# Surface Science Division
# Fachverband Oberflächenphysik (O)

Axel Groß
Universität Ulm
Institut für Theoretische Chemie
Albert-Einstein-Allee 11
89069 Ulm
axel.gross@uni-ulm.de

## Overview of Invited Talks and Sessions

(Lecture Rooms: TRE Phy, TRE Ma, GER 38, PHY C 213, WIL A317, WIL C107, WIL C307; Posters: P1 and P2)

### Invited Talks

| | | | | |
|---|---|---|---|---|
| O 1.1 | Mon | 9:30–10:15 | TRE Phy | **Building blocks for molecular spintronics: From C60 to Spin-Shuttles on Surfaces** — •Thomas Greber |
| O 12.1 | Mon | 15:00–15:45 | TRE Phy | **Uncovering Molecular Orbitals by ARPES** — •Achim Schöll |
| O 24.1 | Tue | 9:30–10:15 | TRE Phy | **Elementary Steps in Surface Reactions: Mechanisms, Kinetics and Thermodynamics** — •Swetlana Schauermann |
| O 33.1 | Tue | 15:00–15:45 | TRE Phy | **Beyond graphene: silicene and germanene, its silicon and germanium cousins** — •Guy Le Lay |
| O 38.1 | Wed | 9:30–10:15 | TRE Phy | **Understanding STM experiments on single-atom junctions from first-principles** — •Stefan Heinze |
| O 53.1 | Wed | 15:00–15:45 | TRE Phy | **The Many-Body Path Towards Quantitative Modeling of Complex Adsorption Systems** — •Alexandre Tkatchenko |
| O 66.1 | Thu | 9:30–10:15 | HSZ 01 | **Fundamental mechanistic studies in formic acid decomposition on transition metal surfaces** — •Manos Mavrikakis |
| O 76.1 | Thu | 15:00–15:45 | TRE Ma | **Quasi free-standing graphene** — •Carsten Busse |
| O 91.1 | Fri | 9:30–10:15 | TRE Phy | **From organic monolayers to free-standing 2D carbon materials: Carbon nanomembranes, graphene and their heterostructures** — •Andrey Turchanin |
| O 104.1 | Fri | 13:15–14:00 | TRE Phy | **Toward a Dynamical Understanding of Surface Chemistry** — •Alec Wodtke |

### Topical Talks of the Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale (jointly with HL and TT)

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| O 7.1 | Mon | 10:30–11:00 | TRE Ma | **Molecular junction transport: some theoretical and computational considerations** — •Mark Ratner, Matthew Reuter |
| O 7.5 | Mon | 12:00–12:30 | TRE Ma | **Insight into Charge Transport in Molecular Junctions from Ab Initio Theories of Level Alignment** — •Jeffrey B. Neaton |
| O 15.1 | Mon | 16:00–16:30 | TRE Ma | **Simulating heat transport: from large scale molecular dynamics to first-principles calculations** — •Davide Donadio |
| O 28.1 | Tue | 10:30–11:00 | TRE Ma | **Ultrafast relaxation dynamics of Hubbard nanoclusters** — •Michael Bonitz, Sebastian Hermanns, Christopher Hinz, Denis Lacroix |
| O 47.1 | Wed | 10:30–11:00 | TRE Ma | **From Rydberg Crystals to Bound Magnons - Probing the Non-Equilibrium Dynamics of Ultracold Atoms in Optical Lattices** — •Immanuel Bloch |
| O 56.1 | Wed | 16:00–16:30 | TRE Ma | **Theory of nonlinear phononics for coherent light-control of solids** — •Antoine Georges, Alaska Subedi, Andrea Cavalleri |
| O 70.1 | Thu | 10:30–11:00 | TRE Ma | **Localization at the edge of 2D topological insulator by Kondo impurities** — •Boris Altshuler, Igor Aleiner, Vladimir Yudson |

## Topical Talks of the Focussed Session: Towards a Quantitative Understanding of Complex Adsorption Structures: Surface Science goes Organic

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|---|---|---|---|---|
| O 55.1 | Wed | 16:00–16:30 | TRE Phy | **Trends in the energies and entropies of adsorbates on single-crystal surfaces** — •Charles Campbell |
| O 55.5 | Wed | 17:15–17:45 | TRE Phy | **Surface crystallography of organic layers** — •Georg Held |
| O 69.1 | Thu | 10:30–11:00 | HSZ 01 | **Injection/extraction barriers in donor-acceptor blends on metals through core-level spectroscopy** — •Enrique Ortega, Afaf El-Sayed, Patrizia Borghetti, Eli Goiri, Celia Rogero, Luca Floreano, Yutaka Wakayama, Jose Luis Cabellos-Quiroz, Duncan Mowbray, Angel Rubio, Dimas Oteyza |
| O 69.4 | Thu | 11:30–12:00 | HSZ 01 | **Core and valence spectroscopy of physisorbed molecules: Role of substrate** — •Claudia Draxl |
| O 77.1 | Thu | 16:00–16:30 | TRE Phy | **Infrared-Spectroscopy applied to ultrathin organic films.** — •Peter Jakob |

## Gaede Prize Talk

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| O 52.1 | Wed | 12:30–13:00 | HSZ 02 | **Spectroscopy and microscopy of graphene on metals** — •Yuriy Dedkov |

## Invited talks of the joint symposium SYMO: Magnetic/organic Interfaces and Molecular Magnetism (MA jointly with CPP, DS, HL, O, TT)

See SYMO for the full program of the symposium.

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|---|---|---|---|---|
| SYMO 1.1 | Mon | 9:30–10:00 | HSZ 02 | **Molecular quantum spintronics with single-molecule magnets** — •Wolfgang Wernsdorfer |
| SYMO 1.2 | Mon | 10:00–10:30 | HSZ 02 | **EPR Studies of Rare-Earth Molecular Nanomagnets** — •Stephen Hill, Sanhita Ghosh, Dorsa Komijani, Salvador Cardona-Serra, Jose-Jaime Baldovi, Yan Duan, Alejandro Gaita-Arino, Eugenio Coronado |
| SYMO 1.3 | Mon | 10:45–11:15 | HSZ 02 | **On-surface magnetochemistry of spin-bearing metalorganic molecules** — •Peter M. Oppeneer, Kartick Tarafder, Ehesan Ali, Nirmalya Ballav, Christian Wäckerlin, Thomas A. Jung |
| SYMO 1.4 | Mon | 11:15–11:45 | HSZ 02 | **Interfacing single-molecule magnets with metals** — •Andrea Cornia, Valeria Lanzilotto, Luigi Malavolti, Matteo Mannini, Mauro Perfetti, Luca Rigamonti, Roberta Sessoli |
| SYMO 1.5 | Mon | 11:45–12:15 | HSZ 02 | **Linking magnetic molecules to themselves, to others and to surfaces** — •Richard Winpenny |

## Invited talks of the joint symposium SYSG: Spin Properties of Graphene (HL jointly with DS, MA, O, TT)

See SYSG for the full program of the symposium.

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|---|---|---|---|---|
| SYSG 1.1 | Tue | 9:30–10:00 | HSZ 02 | **Intrinsic magnetism in graphene** — •Irina Grigorieva |
| SYSG 1.2 | Tue | 10:00–10:30 | HSZ 02 | **Defect Induced Magnetic Moments in Graphene** — •Roland Kawakami |
| SYSG 1.3 | Tue | 10:30–11:00 | HSZ 02 | **Role of MgO barriers for spin and charge transport in Co/MgO/graphene spin-valve devices** — •Bernd Beschoten |
| SYSG 1.4 | Tue | 11:15–11:45 | HSZ 02 | **Defect-Mediated Spin Relaxation and Dephasing in Graphene** — Mark Lundeberg, Silvia Folk, •Joshua Folk |
| SYSG 1.5 | Tue | 11:45–12:15 | HSZ 02 | **Electron spin relaxation in graphene: resonant scattering off local magnetic moments** — •Jaroslav Fabian, Denis Kochan, Martin Gmitra |

## Invited talks of the joint symposium SYMS: Molecular Switches and Motors at Surfaces (O jointly with BP, CPP)

See SYMS for the full program of the symposium.

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|---|---|---|---|---|
| SYMS 1.1 | Wed | 9:30–10:00 | HSZ 02 | **Imaging and manipulation of single functional molecules on surfaces** — •Leonhard Grill |
| SYMS 1.2 | Wed | 10:00–10:30 | HSZ 02 | **Adiabatic quantum motors** — •Felix von Oppen |
| SYMS 1.3 | Wed | 10:30–11:00 | HSZ 02 | **Operation of molecular devices and machines on surfaces** — •Saw Wai Hla |
| SYMS 1.4 | Wed | 11:15–11:45 | HSZ 02 | **Driving and Controlling Molecular Surface Rotors with a Terahertz Electric Field** — •Raymond Dean Astumian |
| SYMS 1.5 | Wed | 11:45–12:15 | HSZ 02 | **Unidirectional motion by inelastic electron tunneling** — •Karl-Heinz Ernst |

## Invited talks of the joint symposium SYOM: One-dimensional metals: Reality of Fiction (DS jointly with HL, O, TT)

See SYOM for the full program of the symposium.

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| SYOM 1.1 | Fri | 9:30–10:10 | HSZ 02 | **Atomic-scale dopant wires for quantum computer architectures** — •Michelle Y Simmons |
| SYOM 1.2 | Fri | 10:10–10:50 | HSZ 02 | $1+\delta$**: Tuning the Dimensionality of Organic Conductors** — •Martin Dressel |
| SYOM 1.3 | Fri | 11:10–11:50 | HSZ 02 | **Spectral and transport properties of one-dimensional correlated electrons** — •Volker Meden |
| SYOM 1.4 | Fri | 11:50–12:30 | HSZ 02 | **Atomic nanowires on surfaces: Spectroscopic reality versus theoretical fiction** — •Ralph Claessen |

## Sessions

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|---|---|---|---|---|
| O 1.1–1.1 | Mon | 9:30–10:15 | TRE Phy | **Invited Talk (Thomas Greber)** |
| O 2.1–2.5 | Mon | 9:30–12:15 | HSZ 02 | **Symposium Magnetic/Organic Interfaces and Molecular Magnetism SYMO (MA jointly with CPP, DS, HL, O, TT)** |
| O 3.1–3.9 | Mon | 9:30–12:15 | ZEU 222 | **Organic Electronics and Photovoltaics I (DS jointly with HL, O)** |
| O 4.1–4.14 | Mon | 9:30–13:15 | BEY 81 | **Transport: Quantum Dots, Quantum Wires, Point Contacts I (TT jointly with O)** |
| O 5.1–5.11 | Mon | 9:30–12:30 | POT 051 | **Topological Insulators: Mostly Structure and Electronic Structure (HL jointly with MA, O, TT)** |
| O 6.1–6.11 | Mon | 10:30–13:15 | TRE Phy | **Organic/bio Molecules on Metal Surfaces I** |
| O 7.1–7.8 | Mon | 10:30–13:15 | TRE Ma | **Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale** |
| O 8.1–8.10 | Mon | 10:30–13:00 | GER 38 | **Electronic Structure and Spin-Orbit Interaction I** |
| O 9.1–9.10 | Mon | 10:30–13:00 | PHY C 213 | **Surface Chemical Reactions and Heterogeneous Catalysis I** |
| O 10.1–10.11 | Mon | 10:30–13:15 | WIL A317 | **Solid-liquid Interfaces I** |
| O 11.1–11.11 | Mon | 10:30–13:15 | WIL C107 | **Nanostructures at Surfaces I** |
| O 12.1–12.1 | Mon | 15:00–15:45 | TRE Phy | **Invited Talk (Achim Schöll)** |
| O 13.1–13.5 | Mon | 15:00–17:30 | HSZ 04 | **Focus Session: New Trends in Molecular Magnetism (MA jointly with O, TT)** |
| O 14.1–14.12 | Mon | 16:00–19:00 | TRE Phy | **Organic/bio Molecules on Metal Surfaces II** |
| O 15.1–15.10 | Mon | 16:00–18:45 | TRE Ma | **Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale II** |
| O 16.1–16.12 | Mon | 16:00–19:00 | GER 38 | **Electronic Structure and Spin-Orbit Interaction II** |
| O 17.1–17.13 | Mon | 16:00–19:15 | PHY C 213 | **Semiconductor Substrates** |
| O 18.1–18.13 | Mon | 16:00–19:15 | WIL A317 | **Solid-liquid Interfaces II** |
| O 19.1–19.12 | Mon | 16:00–19:00 | WIL C107 | **Graphene: Structural properties** |
| O 20.1–20.13 | Mon | 16:00–19:15 | WIL B321 | **Nanostructures at Surfaces II** |
| O 21.1–21.9 | Mon | 16:00–18:30 | HSZ 204 | **Transport: Quantum Dots, Quantum Wires, Point Contacts II (TT jointly with O)** |

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| O 22.1–22.10 | Mon | 15:00–18:00 | ZEU 222 | **Organic Electronics and Photovoltaics II (CPP jointly with DS, HL, O)** |
| O 23.1–23.7 | Mon | 18:00–19:45 | CHE 91 | **Organic Electronics and Photovoltaics III (DS jointly with CPP, HL, O)** |
| O 24.1–24.1 | Tue | 9:30–10:15 | TRE Phy | **Invited Talk (Swetlana Schauermann)** |
| O 25.1–25.5 | Tue | 9:30–12:15 | HSZ 02 | **Symposium Spin Properties of Graphene (HL jointly with DS, MA, O, TT)** |
| O 26.1–26.13 | Tue | 9:30–13:15 | WIL C107 | **Transport: Graphene (TT jointly with O)** |
| O 27.1–27.11 | Tue | 10:30–13:15 | TRE Phy | **Organic/bio Molecules on Metal Surfaces III** |
| O 28.1–28.9 | Tue | 10:30–13:15 | TRE Ma | **Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale III** |
| O 29.1–29.11 | Tue | 10:30–13:15 | GER 38 | **Topological Insulators** |
| O 30.1–30.9 | Tue | 10:30–12:45 | PHY C 213 | **Surface Chemical Reactions and Heterogeneous Catalysis II** |
| O 31.1–31.10 | Tue | 10:30–13:00 | WIL A317 | **Molecular Films: Properties and Preparation** |
| O 32.1–32.9 | Tue | 10:00–12:30 | POT 081 | **Organic Semiconductors: Photovoltaics (HL jointly with CPP, DS, O)** |
| O 33.1–33.1 | Tue | 15:00–15:45 | TRE Phy | **Invited Talk (Guy Le Lay)** |
| O 34.1–34.2 | Tue | 15:00–16:00 | BEY 118 | **Magnetic Adatoms on Surfaces (MA jointly with O)** |
| O 35.1–35.8 | Tue | 14:00–16:00 | HSZ 304 | **Transport: Topological Insulators I (TT jointly with O)** |
| O 36.1–36.105 | Tue | 18:30–22:00 | P1 | **Posters: Bio/organic Molecules on Surfaces, Graphene, Solid/liquid interfaces, Metal Substrates, Electronic Structure Theory** |
| O 37.1–37.110 | Tue | 18:30–22:00 | P2 | **Posters: Plasmonics, Electronic Structure and Spin-Orbit Interaction, Semiconductor and Insulator Surfaces, Nanostructures** |
| O 38.1–38.1 | Wed | 9:30–10:15 | TRE Phy | **Invited Talk (Stefan Heinze)** |
| O 39.1–39.5 | Wed | 9:30–12:15 | HSZ 02 | **Symposium Molecular Switches and Motors at Surfaces (O jointly with BP, CPP)** |
| O 40.1–40.12 | Wed | 9:30–13:00 | HSZ 304 | **Transport: Molecular Electronics I (TT jointly with O)** |
| O 41.1–41.10 | Wed | 9:30–12:15 | POT 051 | **Graphene: Transport (HL jointly with MA, O, TT)** |
| O 42.1–42.7 | Wed | 9:30–11:15 | POT 151 | **Topological Insulators: Theory (HL jointly with MA, O, TT)** |
| O 43.1–43.12 | Wed | 9:30–12:45 | ZEU 260 | **Organic Electronics and Photovoltaics IV (CPP jointly with DS, HL, O)** |
| O 44.1–44.13 | Wed | 9:30–13:00 | BEY 81 | **Low-Dimensional Systems: 2D - Theory (TT jointly with O)** |
| O 45.1–45.7 | Wed | 10:15–12:00 | POT 006 | **Spintronics I (HL jointly with MA, O, TT)** |
| O 46.1–46.10 | Wed | 10:30–13:00 | TRE Phy | **Plasmonics and Nanooptics I** |
| O 47.1–47.10 | Wed | 10:30–13:15 | TRE Ma | **Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale IV** |
| O 48.1–48.11 | Wed | 10:30–13:15 | GER 38 | **Scanning Probe Methods I** |
| O 49.1–49.10 | Wed | 10:30–13:00 | PHY C 213 | **Surface Chemical Reactions and Heterogeneous Catalysis III** |
| O 50.1–50.10 | Wed | 10:30–13:00 | WIL A317 | **Oxide and Insulator Surfaces I** |
| O 51.1–51.10 | Wed | 10:30–13:00 | WIL C107 | **Surface and Interface Magnetism I (O jointly with MA)** |
| O 52.1–52.1 | Wed | 12:30–13:00 | HSZ 02 | **Gaede Prize Talk** |
| O 53.1–53.1 | Wed | 15:00–15:45 | TRE Phy | **Invited Talk (Alexandre Tkatchenko)** |
| O 54.1–54.12 | Wed | 15:00–18:15 | ZEU 260 | **Organic Electronics and Photovoltaics V (CPP jointly with DS, HL, O)** |
| O 55.1–55.10 | Wed | 16:00–19:00 | TRE Phy | **Focussed Session: Towards a Quantitative Understanding of Complex Adsorption Structures: Surface Science goes Organic I** |
| O 56.1–56.11 | Wed | 16:00–19:15 | TRE Ma | **Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale V** |
| O 57.1–57.12 | Wed | 16:00–19:00 | GER 38 | **Plasmonics and Nanooptics II** |
| O 58.1–58.12 | Wed | 16:00–19:00 | PHY C 213 | **Oxide and Insulator Surfaces II** |
| O 59.1–59.13 | Wed | 16:00–19:15 | WIL A317 | **Metal Substrates I** |
| O 60.1–60.13 | Wed | 16:00–19:15 | WIL C107 | **Graphene: Electronic Properties (O jointly with DS, HL, MA, TT)** |
| O 61.1–61.12 | Wed | 16:00–19:00 | WIL B321 | **Nanostructures at Surfaces III** |

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| O 62.1–62.32 | Wed | 17:30–21:00 | P1 | **Posters: Surface Reactions and Dynamics, Nanostructures** |
| O 63.1–63.33 | Wed | 17:30–21:00 | P2 | **Posters: Scanning Probe Methods** |
| O 64.1–64.5 | Wed | 17:00–20:00 | P1 | **Poster: Surfaces, Interfaces and Heterostructures (HL jointly with O)** |
| O 65.1–65.12 | Wed | 17:00–20:00 | P1 | **Poster: Graphene (HL jointly with MA, O)** |
| O 66.1–66.1 | Thu | 9:30–10:15 | HSZ 01 | **Invited Talk (Manos Mavrikakis)** |
| O 67.1–67.9 | Thu | 10:00–12:30 | POT 081 | **Graphene-like Materials: Silicene, MoS2 and Relatives (HL jointly with DY, MA, O, TT)** |
| O 68.1–68.9 | Thu | 10:00–12:15 | POT 151 | **Spintronics II (HL jointly with MA, O, TT)** |
| O 69.1–69.9 | Thu | 10:30–13:15 | HSZ 01 | **Focussed Session: Towards a Quantitative Understanding of Complex Adsorption Structures: Surface Science goes Organic II** |
| O 70.1–70.10 | Thu | 10:30–13:15 | TRE Ma | **Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale VI** |
| O 71.1–71.10 | Thu | 10:30–13:00 | GER 38 | **Plasmonics and Nanooptics III** |
| O 72.1–72.5 | Thu | 10:30–13:00 | PHY C 213 | **Competition for the Gerhard Ertl Young Investigator Award** |
| O 73.1–73.11 | Thu | 10:30–13:15 | WIL A317 | **Scanning Probe Methods II** |
| O 74.1–74.10 | Thu | 10:30–13:00 | WIL C107 | **Surface and Interface Magnetism II (O jointly with MA)** |
| O 75.1–75.1 | Thu | 14:00–14:45 | HSZ 02 | **Plenary Talk (Lukas Novotny)** |
| O 76.1–76.1 | Thu | 15:00–15:45 | TRE Ma | **Invited Talk (Carsten Busse)** |
| O 77.1–77.11 | Thu | 16:00–19:00 | TRE Phy | **Focussed Session: Towards a Quantitative Understanding of Complex Adsorption Structures: Surface Science goes Organic III** |
| O 78.1–78.11 | Thu | 15:00–18:00 | POT 081 | **Graphene: Spintronics, Transistors, and Sensors (HL jointly with DY, MA, O, TT)** |
| O 79.1–79.10 | Thu | 16:00–18:30 | TRE Ma | **Plasmonics and Nanooptics IV** |
| O 80.1–80.12 | Thu | 16:00–19:00 | GER 38 | **Surface Dynamics I** |
| O 81.1–81.12 | Thu | 16:00–19:00 | PHY C 213 | **Oxide and Insulator Surfaces III** |
| O 82.1–82.12 | Thu | 16:00–19:00 | WIL A317 | **Metal Substrates II** |
| O 83.1–83.11 | Thu | 16:00–18:45 | WIL C107 | **Graphene: Adsorption, Intercalation, Doping (O jointly with DS, HL, MA, TT)** |
| O 84.1–84.6 | Thu | 16:00–17:30 | WIL B321 | **Nanotribology** |
| O 85.1–85.5 | Thu | 17:45–19:00 | WIL B321 | **Molecular Simulations** |
| O 86.1–86.8 | Thu | 17:45–19:45 | CHE 91 | **Organic Electronics and Photovoltaics VI (DS jointly with CPP, HL, O)** |
| O 87.1–87.12 | Thu | 17:00–20:00 | P1 | **Poster: Topological Insulators (HL jointly with MA, O)** |
| O 88.1–88.7 | Thu | 17:00–20:00 | P1 | **Poster: Spintronics (HL jointly with MA, O)** |
| O 89 | Thu | 19:30–20:00 | TRE Phy | **Annual General Meeting of the Surface Science Division** |
| O 90 | Thu | 20:00–21:00 | TRE Phy | **Post-Deadline Session** |
| O 91.1–91.1 | Fri | 9:30–10:15 | TRE Phy | **Invited Talk (Andrey Turchanin)** |
| O 92.1–92.4 | Fri | 9:30–12:30 | HSZ 02 | **Symposium One-dimentional Metals: Reality or Fiction (DS jointly with HL, O, TT)** |
| O 93.1–93.9 | Fri | 9:30–12:00 | HSZ 04 | **Topological Insulators (MA jointly with DS, HL, O, TT)** |
| O 94.1–94.6 | Fri | 9:30–11:00 | POT 081 | **Graphene: Bi- and Multi-Layers (HL jointly with MA, O, TT)** |
| O 95.1–95.7 | Fri | 9:30–11:15 | CHE 89 | **Micro- and Nanopatterning (DS jointly with O)** |
| O 96.1–96.10 | Fri | 9:30–12:30 | CHE 91 | **Atomic Layer Deposition (DS jpointly with O)** |
| O 97.1–97.10 | Fri | 10:30–13:00 | TRE Phy | **Organic/bio Molecules on Metal Surfaces IV** |
| O 98.1–98.10 | Fri | 10:30–13:00 | TRE Ma | **Plasmonics and Nanooptics V** |
| O 99.1–99.10 | Fri | 10:30–13:00 | GER 38 | **Scanning Probe Methods III** |
| O 100.1–100.10 | Fri | 10:30–13:00 | PHY C 213 | **Surface Dynamics II** |
| O 101.1–101.8 | Fri | 10:30–12:30 | WIL A317 | **Molecular Films: Electronics, Photovoltaics and Structure** |
| O 102.1–102.7 | Fri | 11:15–13:00 | POT 081 | **Graphene: Interaction with the Substrate (HL jointly with DY, MA, O, TT)** |
| O 103.1–103.7 | Fri | 11:30–13:15 | CHE 89 | **Graphene (DS jointly with TT, MA, HL, DY, O)** |
| O 104.1–104.1 | Fri | 13:15–14:00 | TRE Phy | **Invited Talk (Alec Wodtke)** |

## Annual General Meeting of the Surface Science Division

Thursday 19:30–20:00 TRE Phy

- Report of the chairman
- Election of the new chairmen
- Presentation of the Gerhard Ertl Young Investigator Award
- Miscellaneous

## Post Deadline Session

Thursday 20:00–21:00 TRE Phy

Post Deadline Session followed by the Surface Science Get-Together

# O 1: Invited Talk (Thomas Greber)

Time: Monday 9:30–10:15 Location: TRE Phy

**Invited Talk** O 1.1 Mon 9:30 TRE Phy

**Building blocks for molecular spintronics: From C60 to Spin-Shuttles on Surfaces** — •Thomas Greber — Physik-Institut, Universität Zürich, CH-8057 Zürich, Schweiz

After the discovery of $C_{60}$ it was immediately realized that the hollow carbon shell molecules may host atoms or molecules. If such endofullerenes host unpaired electrons, they act as "spin-shuttles", where the spin is protected from the environment by a diamagnetic carbon cage. Only recently, trimetal nitride cluster fullerenes turned out to have members in the family of single molecule magnets. It was e.g. shown that the three molecules $Dy_nSc_{(3-n)}$ N@$C_{80}$ ($n$=1,2,3), all display magnetic hysteresis, though the interaction between the dysprosium ions in the cage produces distinct ground states, where the $Dy_2$ case is exchange stabilized and has record remanence time in zero field. The magnetic moments do not align parallel to an external magnetic field but remain related to the orientation of the cages and the endohedral clusters. This can be directly seen in the angular dependence of x-ray magnetic circular dichroism of molecules oriented by surfaces. By means of resonant photoelectron diffraction it is possible to access the interplay between conformation, work function and magnetism in detail. The understanding of this interplay might give rise to new opportunities in molecular spintronics.

# O 2: Symposium Magnetic/Organic Interfaces and Molecular Magnetism SYMO (MA jointly with CPP, DS, HL, O, TT)

Time: Monday 9:30–12:15 Location: HSZ 02

**Invited Talk** O 2.1 Mon 9:30 HSZ 02

**Molecular quantum spintronics with single-molecule magnets** — •Wolfgang Wernsdorfer — Institut Néel, CNRS, BP 166, 38042 Grenoble, France

We will address the field called molecular quantum spintronics, combining the concepts of spintronics, molecular electronics and quantum computing. Various research groups are currently developing low-temperature scanning tunnelling microscopes to manipulate spins in single molecules, while others are working on molecular devices (such as molecular spin-transistors, spin valves and filters, and carbon-nanotube-based devices) to read and manipulate the spin state and perform basic quantum operations. For ex., we have built a novel spin-valve device in which a non-magnetic molecular quantum dot, consisting of a Single-Wall Carbon Nanotube, is laterally coupled to a TbPc2 molecular magnet. The localized magnetic moment of the SMM led to a magnetic field-dependent modulation of the conductance in the nanotube with magnetoresistance ratios of up to 300%. Using a molecular spin-transistor, we achieved the electronic read-out of the nuclear spin of an individual metal atom embedded in a single-molecule magnet (SMM). We could show very long spin lifetimes (several tens of seconds). Using the hyperfine Stark effect, which transforms electric fields into local effective magnetic fields, we could not only tune the resonant frequency by several MHz, but we also performed coherent quantum manipulations on a single nuclear qubit by means of electrical fields only.

**Invited Talk** O 2.2 Mon 10:00 HSZ 02

**EPR Studies of Rare-Earth Molecular Nanomagnets** — •Stephen Hill[1], Sanhita Ghosh[1], Dorsa Komijani[1], Salvador Cardona-Serra[2], Jose-Jaime Baldovi[2], Yan Duan[2], Alejandro Gaita-Arino[2], and Eugenio Coronado[2] — [1]Department of Physics and NHMFL, Florida State University, Tallahassee, FL 32310, USA — [2]ICM, Universidad de Valencia, 46980 Paterna, Spain

I will discuss the application of multi-frequency EPR to study the static and dynamic properties of a family of mononuclear Ln(III) (Ln = Ho or Tb) nanomagnets encapsulated in polyoxometallate (POM) cages. The encapsulation offers the potential for spintronics applications on surfaces or in devices, as it preserves the intrinsic properties of the nanomagnet outside of a crystal. A large magnetic anisotropy arises due to a splitting of the Hund's coupled angular momentum ($J = L+S$) ground state in the POM ligand field. High-frequency EPR studies for the Ho(III) compound ($J = 8$) reveal an anisotropic eight line spectrum corresponding to transitions within the lowest $m_J = \pm 4$ doublet, split by a hyperfine interaction with the $I = 7/2$ Ho nucleus. Meanwhile, X-band studies reveal the presence of a large tunneling gap ($\Delta \sim 9$ GHz) within the $m_J = \pm 4$ doublet. Spin-echo measurements allow studies of the coherent spin dynamics, including Rabi oscillations. Remarkably long $T_2$ times are found, even for the most concentrated samples. It is postulated that this is due to the large gap, $\Delta$, which provides an optimal operating point for coherent manipulations at X-band such that the quantum dynamics are relatively insensitive to dipolar fields.

**15 min. break**

**Invited Talk** O 2.3 Mon 10:45 HSZ 02

**On-surface magnetochemistry of spin-bearing metalorganic molecules** — •Peter M. Oppeneer[1], Kartick Tarafder[1], Ehesan Ali[1], Nirmalya Ballav[2], Christian Wäckerlin[3], and Thomas A. Jung[3] — [1]Uppsala University, Uppsala, Sweden — [2]IISER, Pune, India — [3]PSI, Villigen, Switzerland

Planar spin-bearing metalorganic molecules such as metal-porphyrins and -phthalocyanines are paramagnetic in the gas phase, however an interface exchange coupling develops when these molecules are assembled on magnetic surfaces, which induces spontaneous molecular magnetic order at room temperature. To unveil fundamental origins of the exchange interaction leading to the metalorganic molecule/substrate spin-interface we use ab-initio DFT+U calculations with dispersion corrections added. Our calculations provide detailed, orbitally-resolved insight in the molecule-surface exchange interactions as well as the spin-switching induced by additional ligation in the free ligand position of the metal ion by small molecules such as NO and $NH_3$. We find that on-surface coordination chemistry of planar metalorganic complexes gives rise to novel magnetochemical effects, which challenge the notions of classical coordination chemistry. A key to these magnetochemical effects is the weak bonding to the surface, i.e. a "surface" trans effect. Our calculations further reveal that certain systems, as e.g. Cu-phthalocyanine on Co, are liable to formation of novel spin-polarized interface states that are expected to be particularly suited for spin-polarized electron injection in metalorganic layers.

**Invited Talk** O 2.4 Mon 11:15 HSZ 02

**Interfacing single-molecule magnets with metals** — •Andrea Cornia[1], Valeria Lanzilotto[2], Luigi Malavolti[2], Matteo Mannini[2], Mauro Perfetti[2], Luca Rigamonti[1], and Roberta Sessoli[2] — [1]Dip. di Scienze Chimiche e Geologiche, Univ. di Modena e Reggio Emilia & INSTM, Modena, Italy — [2]Dip. di Chimica U. Schiff, Univ. di Firenze & INSTM, Sesto Fiorentino (FI), Italy

Encoding and manipulating information through the spin degrees of freedom of individual molecules are central challenges in molecular scale electronics. With their large magnetic moment and long spin relaxation time, single molecule magnets (SMMs) are of special importance in this field. The electrical addressing of individual SMMs is now well within reach using scanning probe methods, which require organizing molecules on electrically conductive surfaces [1,2]. Herein we present the latest achievements in the deposition of SMMs on metal substrates, like ultraflat surfaces [3] and nanoparticles [4]. Special emphasis is placed on the design of molecular structures that withstand processing by solution [3,4] or vapour-phase [5,6] methods as well as on chemical strategies for controlling molecular orientation. Rewardingly, these efforts have shown that the distinctive property of SMMs, i.e. slow spin relaxation, can persist in metal-wired molecules [3,4].

[1] S. Loth, et al. Science 2012, 335, 196. [2] A. A. Khajetoorians, et al. Science 2013, 339, 55. [3] M. Mannini, et al. Nature 2010, 468, 417. [4] M. Perfetti, et al. Small 2013, DOI: 10.1002/smll.201301617. [5] L. Rigamonti, et al. Inorg. Chem. 2013, 52, 5897. [6] L. Malavolti,

et al. Chem. Commun. 2013, 49, 11506.

**Invited Talk** O 2.5 Mon 11:45 HSZ 02

**Linking magnetic molecules to themselves, to others and to surfaces** — •Richard Winpenny — University of Manchester, United Kingdom

We are learning how to link together polymetallic compounds to give complex structures [1]. During this presentation recent work will be discussed in two distinct approaches. Firstly, we will describe recent work creating new hybrid inorganic-organic rotaxanes [2] and in the second approach we will discuss functionalising polymetallic rings so that they can act as ligands for other metal complexes and surfaces [3,4]. We will also describe the use of pulsed EPR spectroscopy to measure weak interactions between these molecular magnets.

1.G. A. Timco, T. B. Faust, F. Tuna and R. E. P. Winpenny, Chem. Soc. Rev., 2011, 40, 3067-3075. 2.C.- F. Lee, D. A. Leigh, R. G. Pritchard, D. Schultz, S. J. Teat, G. A. Timco and R. E. P. Winpenny, Nature, 2009, 458, 314-318. 3.G. A. Timco, S. Carretta, F. Troiani, F. Tuna, R. G. Pritchard, E. J. L. McInnes, A. Ghirri, A. Candini, P. Santini, G. Amoretti, M. Affronte and R. E. P. Winpenny, Nature Nanotechnology, 2009, 4, 173-178. 4 G. F. S. Whitehead, F. Moro, G. A. Timco, W. Wernsdorfer, S. J. Teat and R. E. P. Winpenny, Angew. Chem. Int. Ed., 2013, 52, 9932-9935.

## O 3: Organic Electronics and Photovoltaics I (DS jointly with HL, O)

small molecules, hybrid materials

Time: Monday 9:30–12:15 Location: ZEU 222

**Invited Talk** O 3.1 Mon 9:30 ZEU 222

**Structure-property relations in perylene bisimids: Charge mobility, exiton diffusion and singlet exciton fission** — •Ferdinand Grozema — Delft University of Technology, Department of Chemical Engineering, Delft, The Netherlands

Perylene diimides (PDIs) represent a class of materials that is promising for application as the active layer in field effect transistors and as an electron accepting material in organic photovoltaic cells. The electronic properties of PDI-based materials strongly depend on the supramolecular order in the material. Therefore, a thorough understanding of the relation between the electronic properties and the organization on the molecular scale can result in design rules for the synthesis of new $\pi$-conjugated organic molecules .

To achieve this we have performed a combined experimental and theoretical study of the electronic properties of a large library of PDI derivatives that differ in the side chains, resulting in subtle differences in the crystal structure. By time-resolved microwave conductivity measurements we show a strong correlation between the supramolecular organization and the charge carrier mobility, with a maximum mobility of 0.41 cm2/Vs. Singlet exciton fission, a process in which a singlet excited state is efficiently converted into two triplets, is also found to be strongly dependent on the supramolecular organization.

This comprehensive study shows that the engineering of the supramolcular organization in PDIs and conjugated molecules in general is viable approach to tailor a variety of electronic properties of such materials over a wide range.

O 3.2 Mon 10:00 ZEU 222

**Influence of morphology on organic solar cell performance comparing crystalline diindenoperylene (DIP) and its amorphous derivative tetraphenyldibenzoperiflanthene (DBP)** — •Stefan Grob, Mark Gruber, Ulrich Hörmann, Theresa Linderl, and Wolfgang Brütting — University of Augsburg, Germany

The DIP molecule, consisting of seven benzene and two cyclopentadiene rings, forms the backbone of the DBP molecule, which has two further benzene rings and four additional, rotatable phenyl groups. Compared to the planar arrangement of DIP, these phenyl groups give DBP a more three-dimensional shape, changing the growth behavior in thin films completely. While we observe crystalline domains of almost upright standing DIP, layers of DBP exhibit an amorphous character and therefore a relatively small exciton diffusion length, being about ten times shorter than that of its crystalline counterpart. However, the drawback of the upright standing arrangement of DIP molecules is the unfavorable orientation of the transition dipole moment resulting in a low absorption coefficient and thus a smaller short-circuit current density. The difference in morphology also leads to different coupling between donor and acceptor molecules at the interface. As a consequence there is an appreciable distinction in the recombination processes occurring within the solar cell. We investigate this phenomenon by temperature-dependent j-V-measurements, electroluminescence and photothermal deflection spectroscopy. Based on these results, we discuss the influence of different film structure and morphology on electrical transport and device performance.

O 3.3 Mon 10:15 ZEU 222

**Spray deposition of zinc oxide nanostructured films for applications in dye-sensitized solar cells** — •Kuhu Sarkar[1], Erik V. Braden[1], Stefan Pogorzalek[1], Shun Yu[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]DESY, Notkestr. 85, 22607 Hamburg

Zinc oxide (ZnO) has emerged as a suitable alternative to titania (TiO2) in the recent years in the field of dye-sensitized solar cells (DSSCs). The inorganic metal oxide films for DSSCs are highly desirable to have an increased surface for enhanced adsorption of a photosensitizer. Hence, nanostructured films of ZnO are synthesized from a solution based approach. Different deposition techniques are investigated to have a significant film thickness for a considerable amount of light absorption. In this respect, spray deposition is shown to be a highly efficient and scalable technique to produce films matching the above-mentioned criteria. Surface as well as bulk morphology of the films have been studied using SEM and GISAXS. These ZnO films are successfully shown to provide good performance in a dye-sensitized solar cell with the highest short circuit current density reported so far.

O 3.4 Mon 10:30 ZEU 222

**Extremely Thin Absorber Solar Cells based on $Sb_2S_3$** — •Eugen Zimmermann, Jonas Weickert, Thomas Pfadler, James Dorman, and Lukas Schmidt-Mende — Universität Konstanz

The introduction of nanostructured metal oxides as electron acceptor resulted in the concept of extremely thin absorber solar cells. Thus, low cost fabricated inorganic semiconductors like $Sb_2S_3$ can be utilized as sensitizer, which typically possess promising properties, such as a tunable band gap and high extinction coefficient. However, optimization of the fabrication process and a detailed characterization of intrinsic properties is unavoidable in order to find the best device architecture and suitable material combinations for highly efficient solar cells. For this purpose, chemical bath deposition conditions and parameters have been examined and resulted in a detailed recipe for fabrication of high quality $Sb_2S_3$ coatings. In combination with optimized layer thicknesses of P3HT, efficiencies of up to 3.2% could be achieved in flat heterojunction architecrue. In order to identify intrinsic limitations, comparative measurements with P3HT:PCBM cells have been, revealing monomolecular recombination processes of excitons, a potential dependency of charge separation, and long charge carrier pathways as main loss mechanisms of fabricated flat heterojunction cells. In addition, investigation of several hole transport materials (HTM) revealed a disadvantageous influence on charge generation due to the parasitic absorption of light by the HTM. Based on these results, the use of nanostructured metal oxides in combination with transparent HTMs is proposed to possibly overcome some of the found limitations.

O 3.5 Mon 10:45 ZEU 222

**Towards low-temperature synthesis of polymer/titania hybrid films for application in photovoltaics** — Martin A. Niedermeier[1], Monika Rawolle[1], Erik V. Braden[1], Kuhu Sarkar[1], Eva M. Herzig[2], Volker Körstgens[1], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]TU München, Munich School of Engineering, James-Franck-Str. 1, 85748 Garching

In a hybrid solar cell an inorganic matrix, such as titania, is combined with a hole-conducting polymer to form a so-called bulk heterojunction. The functionality of such a system depends strongly on the quality of the polymer/semiconductor interface. A very common approach to fabricate that interface is the so-called backfilling of the existing inorganic matrix with the conducting polymer. This approach is generally a two-step process, as the fabrication of the inorganic matrix usually involves high temperatures, which destroy all organic material present in the system. To date the subsequent backfilling of that matrix remains challenging, since a lot of problems have to be overcome. A workaround to these problems is promised by a low-temperature sol-gel process, in which the polymer and the inorganic semiconductor network are fabricated simultaneously. Approaches towards such low-temperature synthesis of polymer/titania hybrid films for application in photovoltaics are presented. These novel routes make use of special tailored block copolymers as structure directing agent. Film morphology and device function are investigated.

**15 min break**

O 3.6 Mon 11:15 ZEU 222

**Photoinduced charge transfer in** $\mathrm{CuInS_2}$ **nanocrystal/polymer composites** — •Rany Miranti[1], Yuliar Firdaus[2], Christopher Krause[1], Mark van der Auweraer[2], Holger Borchert[1], and Jürgen Parisi[1] — [1]Univ. of Oldenburg, Dept. of Physics, Energy and Semiconductor Research Laboratory, 26129 Oldenburg, Germany — [2]Lab. for Photochemistry & Spectroscopy, Div. of Mol. Imaging & Photonics, Chemistry Dept., Katholieke Universiteit Leuven, Celestijnenlaan 200 F B-3001 Heverlee, Belgium.

The photoinduced excited states and the effects properties of charge transfer in $\mathrm{CuInS_2}$ (CIS) nanocrystal/polymer composites were studied by applying quasi steady-state photoinduced absorption (PIA) and steady state photoluminescense as well as time-resolved photoluminescense. The time-resolved properties and excited state dynamics of our systems were studied using the time-correlated single photon counting (TCSPC) technique. We used two different systems of composites with two different kind of polymer, i.e. poly(3-hexylthiophene) (P3HT) and poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)] (PCPDTBT). Optical absorption and emission spectra of thin films of CIS nanocrystal/polymer composites exhibit several interesting features such as luminescence quenching and polaronic photoinduced absorption (PIA) indicating photoinduced charge transfer. The effect of different organic ligands surrounding the CIS nanocrystals on the charge separation process in CIS nanocrystal/ polymer composites will be presented as well.

O 3.7 Mon 11:30 ZEU 222

**Structured growth of ZnO for light trapping enhancement in organic solar cells** — •Nivedita Yumnam and Veit Wagner — Jacobs University, 28759 Bremen, Germany

Organic photovoltaic cells are promising candidates for large-area and low-cost production of solar cells. However, their performance is limited due to the short diffusion length of excitons and low absorption in the active semiconductor layer. The absorption of light can be enhanced by incorporating ZnO nanostructures, which act as scattering centres and hence, they increase the optical path length of light. Our work focuses on the investigation of light trapping mechanism of solar cells based on electrochemically grown ZnO nanorod and active layer of conjugated polymer P3HT and PCBM. The size and the structure of the ZnO nanorods are varied by changing the parameters of electrochemical deposition. Angle resolved scattering measurements are employed to investigate the amount of light scattered by the nanorods. These results are correlated to the performance of the solar cell determined from electrical measurements.

O 3.8 Mon 11:45 ZEU 222

**Temperature-dependent molecular orientation of the organic semiconductor PTCDI-$\mathbf{C_8}$: Optical and structural properties** — •Sebastian Bommel[1,2], Linus Pithan[2], Christopher Weber[2], Anton Zykov[2], Gonzalo Santoro[1], Stephan V. Roth[1], Jörg Megow[2], and Stefan Kowarik[2] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

Optical and structural properties of molecular materials are not only essential for the rational design of opto-electrical devices, but also for the understanding of intermolecular interactions. Here, we report on the structural and optical properties of the organic semiconductor PTCDI-$C_8$ investigated by temperature-dependent Grazing Incidence X-ray Diffraction (GIXD) and photoluminescence (PL) measurements. Our *in situ* studies yield a large impact of temperature on unit cell parameters and optical transitions. The energy of the optical transition $E_{10}$-$E_{01}$ in the PL spectra shifts from 1.80 eV for 273 K to 1.85 eV for 413 K. Furthermore, a rearrangement of the molecular ensemble was found, indicated by a large change of the beta-angle of the PTCDI-C8 unit cell from 107° (273 K) to 102° (413 K). The influence of these structural changes, which are an indication for a change of molecular orientation with temperature, on the optical properties will be discussed in detail. Additionally, the structural and optical properties are supported by temperature-dependent molecular dynamics (MD) simulation based calculations.

O 3.9 Mon 12:00 ZEU 222

**Highly Efficient Silicon/Polythiophene Hybrid Solar Cell Devices** — •Matthias Zellmeier[1], Johannes Frisch[2], Silvia Janietz[3], Norbert Koch[2], Jörg Rappich[1], and Norbert Nickel[1] — [1]Helmholtz-Zentrum Berlin, Institut für Silizium Photovoltaik, Kekulèstr. 5, D-12489 Berlin — [2]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6,D-12489 Berlin — [3]Fraunhofer-Institut für Angewandte Polymerforschung IAP, Abteilung Polymere und Elektronik, Geiselbergstr. 9, D-14476 Potsdam

Highly efficient hybrid solar cell devices based on crystalline silicon with three different solution processed polymer emitter layers are realized. The inorganic part of the device is optimized with a hole-selective back contact (BSF) and a low defect density hot water oxide ($D_{it}=2\times10^{-12}$ eV$^{-1}$cm$^{-2}$), which provides the necessary wetting properties for the solution processed emitter layers. The applied polymer materials, e.g. poly(3-hexylthiophene-2,5-diyl) (P3HT), poly(3-[3,6-dioxaheptyl]-thiophene) (P3DOT), and poly(3-[2,5,8-trioxanonyl]-thiophene) (P3TOT), differ mainly in the oxygen content in the side groups. Substituting the alkyl chains attached to the thiophene rings with ether groups leads to a modified layer formation during spin coating. The results of the optical, electrical and structural characterization of the polymer layers is correlated to the key figures in the final devices. The open circuit voltage $V_{OC}$ increases from 0.3 V to 0.5 V and the short circuit current $j_{SC}$ increases from 15.2 mA cm$^{-2}$ up to 28.3 mA cm$^{-2}$ in the sequence P3HT, P3DOT, P3TOT and results in a power conversion efficiency close to 10 % for a planar Si/P3TOT device.

# O 4: Transport: Quantum Dots, Quantum Wires, Point Contacts I (TT jointly with O)

Time: Monday 9:30–13:15 Location: BEY 81

O 4.1 Mon 9:30 BEY 81

**Transport through nanostructures: Finite time vs. finite size** — •Peter Schmitteckert[1], Sam Carr[2], and Hubert Saleur[3,4] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]School of Physical Sciences, University of Kent, Canterbury CT2 7NH, UK — [3]Institut de Physique Théorique, CEA, IPhT and CNRS, URA2306, 91191 Gif Sur Yvette, France — [4]Department of Physics, University of Southern California, Los Angeles, CA 90089-0484

Numerical simulations and experiments on nanostructures out of equilibrium usually exhibit strong finite size and finite measuring time $t_\mathrm{m}$ effects. We discuss how these affect the determination of the full counting statistics for a general quantum impurity problem [1]. We find that, while there are many methods available to improve upon finite-size effects, any real-time simulation or experiment will still be subject to finite time effects: in short **size matters**, but **time is limiting**. We show that the leading correction to the cumulant generating function (CGF) at zero temperature for single-channel quantum impurity problems goes as $\ln t_\mathrm{m}$ and is universally related to the steady state CGF itself for non-interacting systems. We then give detailed numerical evidence for the case of the self-dual interacting resonant level model that this relation survives the addition of interactions. This allows the extrapolation of finite measuring time in our numerics to the long-time limit, to excellent agreement with Bethe-ansatz results.

[1] P. Schmitteckert, S. C. Carr, H. Saleur, arXiv:1307.7506

O 4.2 Mon 9:45 BEY 81

**Towards steady state currents on finite systems** — •Tim Collet[1] and Peter Schmitteckert[2] — [1]Theoretical Condensed Matter physics, KIT — [2]Institute for Nanotechnology, KIT

The determination of transport properties of strongly correlated quantum systems by quenches in the charge imbalance is a well established technique. However, the achievable time scales are limited by the system size inducing a finite transit time. Here we present a technique in the spirit of absorbing boundary conditions. This allows to obtain steady states on a finite system and to overcome said limitation from finite transit times. We discuss the application of this concept in the context of transport through quantum impurities.

O 4.3 Mon 10:00 BEY 81

**Kwant - a software package for quantum transport** — •Michael Wimmer[1], Christoph Groth[2], Anton Akhmerov[1], and Xavier Waintal[2] — [1]TU Delft, The Netherlands — [2]CEA Grenoble, France

Computing transport properties numerically is a problem that appears in many different areas of physics. I will present a wave-function based approach to computing transport properties in non-interacting tight-binding systems that scales more favourably than standard algorithms such as the recursive Green's function algorithm.

We have implemented this method in an open-source software package Kwant based on the python language. It allows for an easy definition of arbitrary tight-binding problems using intuitive concepts ("like writing the problem on the blackboard"), and allows to compute transport properties such as the conductance, but also local properties such as electron densities. The software package itself together with extensive documentation, tutorials and examples of research where Kwant has already been used can be found at www.kwant-project.org.

[1] C. W. Groth, M. Wimmer, A. R. Akhmerov, X. Waintal. arXiv:1309.2926 (2013)

O 4.4 Mon 10:15 BEY 81

**Non perturbative approach to transport through Anderson quantum dot: the influence of charge fluctuations** — •Davide Mantelli and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Deutschland

Transport through a strongly interacting Anderson quantum dot is analyzed for tunneling couplings $\Gamma$ comparable or larger than the thermal energy $k_\mathrm{B}T$. In this regime the commonly used sequential tunneling approximation, where tunneling rates are calculated to the lowest order in $\Gamma$, breaks down. By accounting for charge fluctuations accompanying the transfer of one electron onto the dot, "dressed" tunneling rates and the associated current across the dot can be calculated [1]. The difference between the standard lowest order theory and the "dressed" one is carefully analyzed in the weak ($\Gamma \ll k_\mathrm{B}T$), intermediate ($\Gamma \simeq k_\mathrm{B}T$) and strong ($\Gamma \gg k_\mathrm{B}T$) coupling regimes. At low temperatures features typical of the Kondo resonance are recovered.

[1] J. Kern and M. Grifoni, Eur. Phys. J. B **86**, (2013) 384

O 4.5 Mon 10:30 BEY 81

**Energy current cotunnelling features for the Anderson quantum dot** — •Niklas M. Gergs[1], Christoph B. M. Hörig[1], Dirk Schuricht[1], and Maarten R. Wegewijs[2,3,4] — [1]Institute for Theoretical Physics, Utrecht University, Netherlands — [2]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany — [3]JARA–Fundamentals of Future Information Technology — [4]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

We discuss the particle and energy current through an Anderson quantum dot with a strong Coulomb interaction $U$ subject to both voltage and temperature bias. A diagrammatic perturbation theory up to second order in the tunnel rates $\Gamma$ is set up in Liouville space. We find that pair tunnelling features show up in the particle and energy current, while pure inelastic cotunnelling spinflip features are absent in the energy current. The latter cotunnelling processes do appear however when assisted by sequential tunnelling (COSET). Therefore, the energy current contains more distinctive features than the particle current. Thus one can use the energy current for enhanced spectroscopy of quantum dot systems.

O 4.6 Mon 10:45 BEY 81

**Non-equilibrium transport through a Josephson quantum dot** — •Jan Frederik Rentrop[1,2], Severin Jakobs[1,2], and Volker Meden[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [2]JARA Fundamentals of Future Information Technology, 52056 Aachen, Germany

We investigate a quantum dot featuring Hubbard interaction coupled to superconducting leads. Applying a bias voltage across the system leads to a time-dependent periodic Hamiltonian. This implies that the observable, namely the current through the system, aquires a periodic time-dependence (AC Josephson effect). The non-equilibrium feature of so called Multiple Andreev Reflections (MAR), known from the non-interacting case, is observed in the static component of the current.

The self-energy on the dot is calculated with the functional renormalization group method. The derived first and second order truncation schemes allow for a "quasi-static" (i.e. allowing for the periodic time-dependence but not more) approximation of the self-energy. Model and method allow for asymmetric choices of the super-conducting gaps, the lead temperatures, the lead-dot couplings, tuning of the Hubbard interaction, shifting of on-site energy and applying a magnetic field. Numerical results are presented for symmetric choices at zero magnetic field and zero temperature, while lead-dot coupling, on-site energy and Hubbard interaction are tuned. Also, first order self-consistent perturbation theory results are presented as a benchmark.

We discuss limitations that the MAR physics impose on any perturbative scheme that expands in small orders of the interaction.

O 4.7 Mon 11:00 BEY 81

**Magneto-electric spectroscopy of Andreev bound states in Josephson quantum dots** — •Nils Wentzell[1], Tobias Meng[2], Volker Meden[3], Sabine Andergassen[1], and Serge Florens[4] — [1]University of Vienna — [2]University of Basel — [3]RWTH Aachen University — [4]CNRS Grenoble

We theoretically investigate the behavior of Andreev levels in a single-orbital interacting quantum dot in contact to superconducting leads, focusing on the effect of electrostatic gating and applied magnetic field, as relevant for recent experimental spectroscopic studies. In order to account reliably for spin-polarization effects in presence of strong correlations, we further extend here two simple and complementary approaches that are tailored to capture effective Andreev levels: the static functional renormalization group and the self-consistent Andreev bound states theory. We provide a systematic analysis of the Andreev level spectroscopy for the full electric and magnetic tuning available in quantum dot devices.

**15 min. break.**

O 4.8 Mon 11:30 BEY 81

**In gap and out of gap features in the cotunneling spectroscopy of a superconductor coupled quantum dot** — •Sascha Ratz and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We present a nonequilibrium real-time diagrammatic theory for the systematic investigation of low temperature quantum transport properties of a superconductor contacted quantum dot in an individual single wall carbon nanotube. In the low temperature regime particle transport is dominated by cotunneling and Andreev reflection processes. As recent experiments show, elastic/inelastic cotunneling features are clearly visible inside the Coulomb blockade regime, sharpened by the superconducting leads. The proximity induced higher order Andreev reflection processes result in subgap features, however. Temperature dependent measurements show in addition rich features inside the superconducting gap which can be attribute to thermally excited quasiparticles. More detailed experimental investigations and theoretical calculations are in progress to understand the experimental findings.

O 4.9 Mon 11:45 BEY 81

**Unconventional superconductivity in quantum dot systems** — Björn Sothmann[1], •Stephan Weiss[2], Michele Governale[3], and Jürgen König[1] — [1]Departement de Physique Theorique, Universite de Geneve, Switzerland — [2]Theoretische Physik, Universität Duisburg-Essen and CENIDE, Germany — [3]School of Chemical and Physical Sciences, Victoria University of Wellington, New Zealand

Conventional superconductivity of electrons is well described in terms of the BCS theory. Fermi statistics dictates the overall symmetry of e.g. the order parameter. The single ingredients could take either symmetric or antisymmetric properties, hence spin as well as spatial degrees of freedom and time might independently change sign and unconventional pairing amplitudes emerge [1]. We show how quantum dot setups may be used to create unconventional pairing between electrons. Brought into proximity to a conventional SC, Cooper pairs tunnel into the double (quadrupel)-quantum dot (DQD/QDD) system [2,3]. Locally, manipulations of the electronic state is possible by tuning electric and/or magnetic fields. An inhomogeneous magnetic field between the dots breaks the SU(2) symmetry of the spin. This results in nonzero unconventional order parameters. We study the emergence and decay of even/odd singlet and triplet order parameters in different geometries. For DQD and QDD setups spectroscopic properties and signatures of unconventional correlations in the Andreev current are studied.

[1] F. S. Bergeret, et al., Rev. Mod. Phys. 77, 1321 (2005).
[2] M. Governale, et al., Phys. Rev. B 77, 134513 (2008).
[3] J. Eldridge, et al., Phys. Rev. B 82, 184507 (2010).

O 4.10 Mon 12:00 BEY 81

**The interplay of the proximity and Kondo effects in spin-resolved transport through quantum dots** — •Krzysztof P. Wójcik and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland

Transport properties of hybrid quantum dots coupled to ferromagnetic (FM) and superconducting (SC) leads are studied by means of the numerical renormalization group method [1,2]. By constructing the full density matrix of the system [3], the linear conductance and respective spectral functions are calculated. Aiming to emphasize the role of Andreev processes in transport, we model the quantum dot coupled to the superconductor by an effective Hamiltonian in the limit of large superconducting gap [4]. First, a three-terminal setup is considered, for which we study the proximity effect on the spin-dependent current flowing between the two FM leads. Then, the transport properties in a two-terminal setup, with one FM and one SC lead, are analyzed. In this case we focus on the interplay of the exchange field induced by FM lead, the Kondo effect and the Andreev processes. We show that the conductance generally depends on the ratio of these three quantities, leading to nontrivial transport behavior.

[1] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[2] We use the open-access Budapest NRG code, O. Legeza, C. P. Moca, A. I. Toth, I. Weymann, G. Zarand, arXiv:0809.3143 (2008).
[3] A. Weichselbaum, J. von Delft, Phys. Rev. Lett. **99**, 076402 (2007).
[4] Y. Tanaka, N. Kawakami, A. Oguri, J. Phys. Soc. Jap. **76**, 074701 (2007).

O 4.11 Mon 12:15 BEY 81

**The electroluminescence of the transmission line driven by a biased quantum point contact** — •Jinshuang Jin[1,2,3], Michael Marthaler[2,4], Andreas Heimes[2,4], and Gerd Schön[2,4] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Karlsruhe, Germany — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology(KIT), Karlsruhe, Germany — [3]Department of Physics, Hangzhou Normal University, Hangzhou, China — [4]DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, Karlsruhe, Germany

A transmission line resonator driven by a biased quantum point contact is investigated. The quantum point contact (QPC) is not only an efficient detector but also a light emission device. We find that the excited photon number in the resonator is monotonically increased with the bias voltage for $eV > \hbar\omega_r$ with $V$ the applied bias voltage and $\hbar\omega_r$ the frequency of the resonator. The linewidth and the height of the emission spectrum are sensitive to the parameters of the QPC, such as the tunneling rate, the applied bias voltage, and the coupling strength between the QPC and resonator. Moreover, we demonstrate that the noise spectrum of the current through QPC has characteristic features showing peak and dip, which is closely related to the excited photon dynamics of the resonator.

O 4.12 Mon 12:30 BEY 81

**Accumulation of spin anisotropy in a nanoparticle in the mesoscopic Stoner regime** — •Philipp Stegmann[1], Björn Sothmann[2], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [2]Départment de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

We theoretically discuss the accumulation of spin-quadrupole moment [1, 2] in an isotropic system giving rise to a large spin anisotropy although the spin-dipole moment remains strongly suppressed. Our system is a nanoparticle weakly tunnel coupled to two ferromagnetic leads. For such system, it has been demonstrated that the spin fluctuations give rise to enhanced shot noise [3]. Here, large positive spin-quadrupole moments are generated by abruptly switching off the bias voltage for parallel leads' polarizations. Moreover, applying an oscillating bias voltage results in large negative spin-quadrupole moments for parallel or antiparallel polarizations.

[1] B. Sothmann, and J. König, Phys. Rev. B **82**, 245319 (2010).
[2] M. M. E. Baumgärtel, M. Hell, S. Das, and M. R. Wegewijs, Phys. Rev. Lett **107**, 087202 (2011).
[3] B. Sothmann, J. König, and Y. Gefen, Phys. Rev. Lett. **108**, 166603 (2012).

O 4.13 Mon 12:45 BEY 81

**Overhauser effect in spin blockaded double quantum dots-the case of dual hysteresis** — •Bhaskaran Muralidharan and Siddharth Buddhiraju — Electrical Engineering Department, Indian Institute of Technology Bombay, Mumbai, India

In the spin blockade transport regime through GaAs double quantum dots (DQD), experiments [1] revealed that the hyperfine interaction with host nuclei can have profound consequences on the electron-spin dynamics. One of which, is the observation of bistablity and flat-topped behavior in the current versus applied DC magnetic-field characteristics. In this talk, we will first explain the essence of this flat-topped hysteretic behavior using a simple six-state model that captures the multiple-feedback mechanisms that are involved. We will then consider a more detailed model that elucidates the role of the physical parameter space of the DQD set up and a feedback mechanism involving the difference Overhauser field caused by the two separate nuclear spin baths of the DQD set up.

[1] K. Ono and S. Tarucha, Phys Rev Lett., 92, 256803 (2004).

O 4.14 Mon 13:00 BEY 81

**Fixing the Energy Scale in Scanning Tunneling Microscopy on Semiconductor Surfaces** — Gerhard Münnich[1], •Andrea Donarini[2], Jascha Repp[1], and Martin Wenderoth[3] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany — [3]IV. Physikalisches Institut der Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In scanning tunneling experiments on semiconductor surfaces, the energy scale within the tunneling junction is usually unknown due to

tip-induced band bending. Here, we experimentally recover the zero point of the energy scale by combining scanning tunneling microscopy with Kelvin probe force spectroscopy. With this technique, we revisit shallow acceptors buried in GaAs [1]. Enhanced acceptor-related conductance is observed in negative, zero, and positive band-bending regimes. An Anderson-Hubbard model is used to rationalize our findings, capturing the crossover between the acceptor state being part of an impurity band for zero band bending and the acceptor state being split off and localized for strong negative or positive band bending, respectively.
[1] G. Münnich, A. Donarini, J. Repp, and M. Wenderoth, Phys. Rev. Lett. 111, 216802 (2013)

## O 5: Topological Insulators: Mostly Structure and Electronic Structure (HL jointly with MA, O, TT)

Time: Monday 9:30–12:30 Location: POT 051

O 5.1 Mon 9:30 POT 051

**InAs/GaSb compound quantum wells for electrically tunable topological insulator devices** — •Georg Knebl[1], Matthias Dallner[1], Robert Weih[1], Sven Höfling[1,2], and Martin Kamp[1] — [1]Universität Würzburg, Deutschland — [2]University of St Andrews, Scotland

InAs/GaSb compound quantum wells (CQW) sandwiched between two AlSb layers and a front/back gate were proposed by Liu et al. [1] to show a topological insulator phase. The advantage of this structure is the possibility to tune the phase transition from a normal to a topological insulator via the front and back gate voltage. In addition, this material combination allows the use of established III/V semiconductor technology for epitaxy and device processing.

We present results on the growth of InAs/GaSb CQWs via molecular beam epitaxy on GaSb and GaAs substrates using different buffers. Furthermore, we will discuss device fabrication on InAs/GaSb layer structures, which requires special care since oxidation or process induced damage can lead to the formation of conducting surface channels. Electrical characterization of Hall bars and the tunability of the transport properties via gates will be reported.

[1] C. Liu, et al., Phys. Rev. Lett. 100, pp. 1-4, (2008)

O 5.2 Mon 9:45 POT 051

**Resolving the linear dispersion relation of topological insulator nanowires** — •Johannes Gooth, Bacel Hamdou, August Dorn, Robert Zierold, and Kornelius Nielsch — Institute of Applied Physics, Universität Hamburg, Hamburg, Germany

Due to the linear dispersion relation, charge carriers in the surface states of a topological insulator (TI) behave like relativistic particles described by the Dirac equation for spin-1/2 particles leading to exotic new physics and applications. In bulk topological insulators the linear dispersion relation at the surface has been resolved by angle-resolved photoemission spectroscopy (ARPES). On nanostructures ARPES measurements have not been successful, due to the limited sample size. Instead magnetoelectrical transport measurements became the most common way to indicate the existance of surface states in nanomaterials. However, the linear dispersion relation has not been directly resolved in nanostructures to date.

Here, we show that the linear dispersion relation on the surface of a $Bi_2Te_3$ nanowire can directly be deduced from gate dependend magnetototransport measurements. Further carrier concentration, mobility and effective mass of the dirac fermions are determined as a function of gate voltage. It can be shown that at 2K the transport in the surface states is dominated by electron-electron interaction.

O 5.3 Mon 10:00 POT 051

**Temperature-dependent surface band gap of Dirac fermions observed at the (111) surface of the crystalline topological insulator Pb-Sn-Se** — •Partha S. Mandal[1], Gunther Springholz[2], Günther Bauer[2], Valentine V. Volobuev[2], Andrei Varykhalov[1], Oliver Rader[1], and Jaime Sánchez-Barriga[1] — [1]Helmholtz-Zentrum Berlin — [2]Johannes-Kepler-Universität Linz

Using angle-resolved photoemission, we studied (111)-oriented epitaxial films of Pb-Sn-Se grown by molecular beam epitaxy. The topological-to-trivial-insulator phase transition [1] is monitored probing the bulk valence band as a function of Sn concentration and temperature between 30 K and room temperature. In the topological phase, the topological surface state opens a band gap indicating a mass aquisition that is not caused by broken time reversal symmetry. We discuss this phenomenon in comparison to conventional topological insulators [2] protected by time-reversal symmetry.

[1] P. Dziawa, B. J. Kowalski, K. Dybko, R. Buczko, A. Szczerbakow, M. Szot, E. Łusakowska, T. Balasubramanian, B. M. Wojek, M. H. Berntsen, O. Tjernberg, T. Story, Nature Mat. 11, 1023 (2012).

[2] T. Sato, K. Segawa, K. Kosaka, S. Souma, K. Nakayama, K. Eto, T. Minami, Y. Ando, and T. Takahashi, Nature Phys. 7, 840 (2011).

O 5.4 Mon 10:15 POT 051

**Surface-Dominated Transport on a Bulk Topological Insulator** — •Lisa Kühnemund[1], Lucas Barreto[2], Frederik Edler[1], Christoph Tegenkamp[1], Jianli Mi[3], Martin Bremholm[3], Bo Brummerstedt Iversen[3], Christian Frydendahl[2], Marco Bianchi[2], and Philip Hofmann[2] — [1]Leibniz Universität Hannover, Inst. f. Festkörperphysik — [2]Aarhus University, Dep. of Physics and Astronomy, iNANO — [3]Aarhus University, Center for Materials Crystallography, iNANO

Topological insulators are guaranteed to support metallic surface states on an insulating bulk, and one should thus expect that the electronic transport in these materials is dominated by the surfaces states. Alas, due to the high remaining bulk conductivity, surface contributions to transport have so-far only been singled out indirectly via quantum oscillations, or for devices based on gated and doped topological insulator thin films, a situation in which the surface carrier mobility could be limited by defect and interface scattering. Here we present a direct measurement of surface-dominated conduction on an atomically clean surface of $Bi_2Te_2Se$. Using nano-scale four point setups with variable contact distance, we show that the transport at 30 K is two-dimensional rather than three-dimensional and by combining these measurements with angle-resolved photoemission results from the same crystals, we find a surface state mobility of 390(30) $cm^2V^{-1}s^{-1}$ at 30 K at a carrier concentration of $8.71(7)\times10^{12}$ $cm^{-2}$.

O 5.5 Mon 10:30 POT 051

**Room temperature high frequency transport of Dirac fermions in MBE grown $Sb_2Te_3$ based topological insulators** — •T. Herrmann[1], P. Olbrich[1], S.N. Danilov[1], Ch. Weyrich[3], J. Kampmeier[3], G. Mussler[3], D. Grützmacher[3], L. Plucinski[3], C.M. Schneider[3], M. Eschbach[3], L.E. Golub[2], V.V. Bel'kov[2], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Peter Grünberg Institute (PGI) & Jülich Aachen Research Alliance (JARA-FIT), Research Center Jülich, Jülich, Germany

We report on the observation of terahertz (THz) laser radiation induced currents in epitaxially grown $Sb_2Te_3$ based topological insulators (TI) [1]. We demonstrate that the excitation of the sample with linearly polarized THz radiation results in a photoresponse solely stemming from the surface states of the 3D TI. Our analysis shows that the photocurrent is caused by the photogalvanic effect [2], which emerges in the surface states but is forbidden in the centrosymmetric bulk material. As an important result our measurements demonstrate that the high frequency transport can be obtained in the Dirac fermion system even at room temperature.

[1] Plucinski et al.; J. Appl. Phys. **113**, 053706 (2013)

[2] Weber et al.; Phys. Rev. B **77**, 245304 (2008)

O 5.6 Mon 10:45 POT 051

**Topological Insulator Nanowires by Chemical Vapour Deposition** — •Piet Schönherr and Thorsten Hesjedal — Department of Physics, Clarendon Laboratory, University of Oxford, Oxford OX1 3PU, United Kingdom

Topological insulators (TIs) are a new state of quantum matter which insulates in the bulk and conducts on the surface. The study of bulk TIs has been hindered by high conductivity in the bulk, arising from crystalline defects. Such problems can be tackled through compositional engineering or the synthesis of TI nanomaterials. We combined both approaches in a systematic study of various growth parameters to achieve uniform, high purity nanowires with high substrate coverage.

The highlight of this study is the development of a new growth route for nanowires, based on a $TiO_2$ catalyst rather than the conventional Au. Comparative studies demonstrate that Au significantly contaminates the nanowires, whereas $TiO_2$ stays well separated. Details of the Au and $TiO_2$-catalysed growth mechanism were investigated. For Au it was found that the growth mechanism is vapour-liquid-solid. For $TiO_2$ nanoparticles, in contrast, the growth mechanism can be described in the vapour-solid scheme.

Nanowires of the doped compound $(Bi_{0.78}Sb_{0.22})_2Se_3$ were studied using synchrotron radiation. It was discovered that the material mainly adopts an orthorhombic phase known from $Sb_2Se_3$. The Raman spectrum is reported and matched with the structural information for the first time. Furthermore, a method to control the length and diameter of $Bi_2Se_3$ nanowires through laser-cutting was developed.

## Coffee break (15 min.)

O 5.7 Mon 11:15 POT 051

**Optoelectronic flow trajectories in topological insulators** — •Paul Seifert[1], Christoph Kastl[1], Tong Guan[2], Kehui Wu[2], X. Y. He[2], Yongqing Li[2], and Alexander W. Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München — [2]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

We report on the optoelectronic properties of thin films of the topological insulator $(Bi_xSb_{1-x})_2Te_3$ grown by molecular beam epitaxy. In spatially resolved experiments, we observe photocurrent patterns with positive and negative amplitude [1]. We interpret the patterns to originate from a local photocurrent generation due to potential fluctuations [1]. Exploiting the local photocurrent generation in combination with a sub 100-nm lithography, we visualize the current flow in nanoscale circuits based on topological insulators [2].

[1] C. Kastl, T. Guan, X. Y. He, K. H. Wu, Y. Q. Li, and A. W. Holleitner, Appl. Phys. Lett. 101, 251110 (2012). [2] C. Kastl et al., (2014).

We gratefully acknowledge financial support from the DFG-project HO3324/8 within the SPP 1666 on topological insulators.

O 5.8 Mon 11:30 POT 051

**Polarization-controlled picosecond spin currents in topological insulators** — •Christoph Kastl[1], Christoph Karnetzky[1], Helmut Karl[2], and Alexander W. Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, 85748 Garching, Germany — [2]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Controlling spin currents in topological insulators may lead to applications in future spintronic devices [1]. Here, we show that surface currents in Bi2Se3 can be controlled by circularly polarized light on a time-scale of a picosecond with a fidelity near unity even at room temperature. We reveal the temporal interplay of such ultrafast spin currents with photo-induced thermoelectric and drift currents in optoelectronic circuits [2].

[1] C. Kastl, T. Guan, X. Y. He, K. H. Wu, Y. Q. Li, and A. W. Holleitner, Appl. Phys. Lett. 101, 251110 (2012).

[2] C. Kastl et al., (2014).

We gratefully acknowledge financial support from the DFG-project HO3324/8 within the SPP 1666 on topological insulators.

O 5.9 Mon 11:45 POT 051

**Scanning Tunneling Microscopy of Ultrathin Topological Insulator $Sb_2Te_3$ Films on Si(111) grown by Molecular Beam Epitaxy** — •Martin Lanius, Jörn Kampmeier, Gregor Mussler, and Detlev Grützmacher — Peter Grünberg Institut, Forschungszentrum Jülich, Germany

Topological insulators (TIs) are a class of materials in the field of condensed matter physics. In addition to the fascinating electronic properties, the Van der Waals growth mode of TIs, i.e. the TI epilayer is only weakly bonded to the substrate, which allows the use of substrates with high lattice mismatch, is of high interest. In this case we have studied the nucleation and growth process of the TI $Sb_2Te_3$ on Si(111) substrates by STM (Scanning Tunneling Microscopy) and AFM (Atomic Force Microscopy). The thin films from several nanometers thickness down to one quintuple layer thickness have been grown by molecular beam epitaxy. To determine the thickness and composition of the films we used x-ray reflectivity and x-ray diffraction. Further investigations of $Ge_2Sb_2Te_3$, which is a phase-changing material and a topological insulator, and the comparison to the growth mode of $Sb_2Te_3$ will be presented.

O 5.10 Mon 12:00 POT 051

**Transport of Dirac fermions in the presence of spin-orbit impurities** — •Pierre Adroguer[1], Dimitri Culcer[2], and Ewelina Hankiewicz[1] — [1]Institute for Theoretical Physics and Astronomy, Würzburg University, Würzburg, Germany — [2]School of Physics, University of New South Wales, Sidney, Australia

The recent exprimental realizations of three dimensional topological insulators (3DTI) have provided a new tool to investigate Dirac physics.

Indeed, these materials exhibit an insulating bulk and a single metallic surface state described by Dirac fermion physics.

In the regime of weak scalar disorder, Dirac fermions do not backscatter because of time-reversal symmetry. Further, this absence of backscattering leads to a weak antilocalization correction (an increase in conductivity in the absence of magnetic field, due to quantum interference of conjugated paths) [1,2].

In this presentation, we will review these phenomena, and show how these features are modified when there are spin-orbit impurities in the Dirac fermion systems.

We acknowledge financial support via grant HA 5893/4-1 within SPP 1666.

[1] G. Tkachov and E. M. Hankiewicz, Phys. Rev. B 84, 035444 (2011)

[2] P. Adroguer, D. Carpentier, J. Cayssol, and E. Orignac, New Journal of Physics 14, 103027 (2012)

O 5.11 Mon 12:15 POT 051

**Oscillatory surface dichroism of the insulating topological insulator** $Bi_2Te_2Se$ — •Susmita Basak[1], Madhab Neupane[2], Hsin Lin[1], N. Alidoust[2], S.-Y. Xu[2], Chang Liu[2], I. Belopolski[2], G. Bian[2], J. Xiong[2], H. Ji[3], S. Jia[3], S.-K. Mo[4], M. Bissen[5], M. Severson[5], N. P. Ong[2], T. Durakiewicz[6], R. J. Cava[3], A. Bansil[1], and M. Z. Hasan[2] — [1]Department of Physics, Northeastern University, Boston, Massachusetts, USA — [2]Joseph Henry Laboratory and Department of Physics, Princeton University, Princeton, New Jersey, USA — [3]Department of Chemistry, Princeton University, Princeton, New Jersey, USA — [4]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, USA — [5]Synchrotron Radiation Center, Stoughton, Wisconsin, USA — [6]Condensed Matter and Magnet Science Group, Los Alamos National Laboratory, Los Alamos, New Mexico, USA

We present a study of the effect of angular momentum transfer between polarized photons and topological surface states of the insulating topological insulator $Bi_2Te_2Se$ using circular dichroism-angle resolved photoemission spectroscopy. The photoelectron dichroism demonstrate a dramatic sign flip with the change of photon frequency and we show that this is a consequence of a strong coupling between the photon field and the spin-orbit nature of the initial Dirac states on the surface. Our studies reveal the intrinsic dichroic behavior of topological surface states and point toward the potential utility of bulk insulating topological insulators in opto-spintronics device applications.

# O 6: Organic/bio Molecules on Metal Surfaces I

Time: Monday 10:30–13:15 Location: TRE Phy

O 6.1 Mon 10:30 TRE Phy

**Deposition and Characterization of Large Magnetic Molecules on Surfaces** — •Judith Niedenführ[1], Bastian Feldscher[2], Jan-Philipp Broschinski[2], Thorsten Glaser[2], Andrei Postnikov[3], and Daniel Wegner[1] — [1]Westfälische Wilhelms-Universität, Münster, Germany — [2]Universität Bielefeld, Bielefeld, Germany — [3]Université de Lorraine, Metz, France

A key to building functional devices on the basis of single molecule magnets (SMMs), be it for potential high-density memory storage or molecular-electronics applications, is the ability to deposit and manipulate these nanomagnets on surfaces in a controllable and reproducible way. The typical evaporation process is not applicable, because it would lead to dissociation of these large organic molecules. We used two different unconventional preparation techniques, namely pulse injection and rapid heating, for in-situ deposition of the Cu$_3$-triplesalen complex onto a Au(111) surface. These complexes are the building blocks for a new generation of promising SMMs, which combine a high-spin ground state with a large magnetic anisotropy. The comparison of both techniques allows us to evaluate their advantages and drawbacks. The Cu$_3$-triplesalen molecules have been studied using a combination of scanning tunneling microscopy (STM) and spectroscopy (STS). We discuss details of the electronic structure and its consequences on the internal spin coupling and compare these with first-principle calculations within the framework of the density-functional theory. The comparison is also done for the slightly modified Cu$_3$-triplesalalen complex which is designed to exhibit an enhanced ferromagnetic coupling.

O 6.2 Mon 10:45 TRE Phy

**Addressing the metal centers in multi-spin-center macromolecule on Au(111)** — •Maciej Bazarnik[1], Bernhard Bugenhagen[2], Annika Frank[2], Jens Brede[1], Marc H. Prosenc[2], and Roland Wiesedanger[1] — [1]Institute of Applied Physics, University of Hamburg, D-20355 Hamburg, Germany — [2]Institute of Inorganic Chemistry, University of Hamburg, D-20146 University of Hamburg, Germany

The use of magnetic molecules opens a gateway to a flexible design of novel spintronic devices to store, manipulate, and read spin information at the nanoscale. Crucial is the precise knowledge of molecular properties at the interface towards an electrode. Progress in this field relies on resolving and understanding the physics at the relevant interfaces. In particular the role of individual molecular constituents and the impact of the atomic environment on molecular properties determine device relevant parameters, such as conductance and spin polarization.

Here, we applied scanning tunneling microscopy to address individual metallic centers of multi-spin-center macromolecules. The analysis focuses on different triplesalophene molecules which have been deposited in vacuo on a Au(111) substrate by either using thermal sublimation or electrospray deposition. The triplesalophene constitutes of three organic salene-like ligands and can be functionalized with various metal ions in order to modify, e.g. the molecular spin state, and/or termination groups to manage the molecule-molecule interactions. We will discuss the influence of terminal groups on the physicochemical properties of the molecules.

O 6.3 Mon 11:00 TRE Phy

**Tuning the electronic structure of metal-organic complexes at the molecule-substrate interface** — •Pascal Raphael Ewen[1], Jan Sanning[1], Nikos Doltsinis[2], Cristian Alejandro Strassert[1], and Daniel Wegner[1] — [1]Physikalisches Institut, Westfälische-Wilhelms Universität Münster, Deutschland — [2]Institut für Festkörpertheorie, Westfälische-Wilhelms Universität Münster, Deutschland

The coupling of molecules at surfaces ranging from the weak (physisorption) to the strong interaction regime (chemisorption) plays a crucial role both in the physical and chemical behavior. Fundamental processes such as conformal changes, dissociation and charge transfer have been observed upon adsorption. A systematic investigation of the adsorption and the electronic structure of slightly differing phosphorescent Pt(II) complexes offers information about the influence of ligands and substituents on their interactions with neighbors and the substrate. We have studied the impact of molecule-surface and intermolecular interactions on the self-assembly and electronic structure of Pt-complex monolayers on Au(111) using scanning tunneling microscopy (STM) and spectroscopy (STS) at low temperature. By determining energies and spatial distributions of several frontier orbitals, we are able to evaluate the impact of coupling and hybridization on the molecular electronic states.

O 6.4 Mon 11:15 TRE Phy

**Electronic structure and relaxation behavior of a thin Fe(II) spin-crossover film** — •Eric B. Ludwig[1], Holger Naggert[2], Matthias Kalläne[1], Sebastian Rohlf[1], Erik Kröger[1], Alexander Bannwarth[2], Arndt Quer[1], Kai Rossnagel[1], Lutz Kipp[1], and Felix Tuczek[2] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel — [2]Institut für anorganische Chemie, Universität Kiel, D-24098 Kiel

Coordinative Fe(II) complexes are model systems for organic molecules, whose optical, electronic and magnetic properties can be manipulated by external stimuli. Moreover, the temperature- and irradiation-dependent spin transitions observed in a number of these materials may provide a suitable testbed toward the development of future spintronic devices.

Here, we present a ultraviolet photoelectron spectroscopy study on a vacuum-deposited thin film of Fe(H$_2$bpz)$_2$(phen) on Au(111). Spectral features sensitive to the spin transition can be identified via comparison of the results of density functional calculations with the results of valence band measurements at different temperatures and varying irradiation conditions.

Our results provide evidence for a VUV-induced spin-state trapping effect at low temperatures. Furthermore, a high optical photon flux seems to stabilize the metastable high-spin state far above the LIESST transition temperature. The overall high- to low-spin relaxation behavior, however, shows similarities to amorphous samples of a related system.

O 6.5 Mon 11:30 TRE Phy

**Fe on metalloporphyrin arrays: Site-selective adsorption, atomic switching and modification of magnetic moments** — Saranyan Vijayaraghavan[1], •Willi Auwärter[1], David Ecija[1], Knud Seufert[1], Uta Schlickum[2,3], Markus Etzkorn[2,3], Stefano Rusponi[3], Pardeep K. Thakur[4], Sebastian Stepanov[2], Torsten Houwaart[5], Philippe Sautet[5], Marie-Laure Bocquet[5], Harald Brune[3], and Johannes V. Barth[1] — [1]Technische Universität München, Department of Physics, E20, Garching, Germany — [2]Max Planck Insitut für Festkörperforschung, Stuttgart, Germany — [3]Ecole Polytechnique Fédérale de Lausanne, Institut de Physique de la Matière Condensée, Lausanne, Switzerland — [4]European Synchrotron Radiation Facility, Grenoble, France — [5]Ecole Normale Supérieure de Lyon, Laboratoire de Chimie, Lyon, France

The confinement and ordering of nanoscale objects as individual atoms or molecules on substrates has gained widespread attention in recent years leading to the realization of individually addressable quantum arrays. Here, we use highly regular metalloporphyrin (Co-TPP) arrays on a Ag(111) support as template for the site-specific adsorption of Fe. Our multi-technique approach combining scanning tunneling microscopy, X-ray magnetic circular dichroism and complementary density functional theory calculations reveals an interaction between the Fe and the Co center of the porphyrin, reviving the magnetic moment of the latter, which was quenched upon adsorption. Furthermore, individual Fe atoms can be switched between four equivalent positions on the porphyrin macrocycle, reflecting the molecular saddle-shape.

O 6.6 Mon 11:45 TRE Phy

**On the role of Entropy in conformational molecular switching of porphyrins on Cu(111)** — Stefanie Ditze[4], Michael Stark[4], Florian Buchner[4], Andre Aichert[1], Norbert Jux[2], Nicola Luckas[3], Andreas Görling[3], Wolfgang Hieringer[3], Joachim Hornegger[1], Hans-Peter Steinrück[4], and •Hubertus Marbach[4] — [1]Lehrstuhl für Mustererkennung — [2]Lehrstuhl für Organische Chemie II — [3]Lehrstuhl für Theoretische Chemie — [4]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

We observe and induce conformational switching of individual molecules via scanning tunneling microscopy (STM) at and close to room temperature. 2H-5,10,15,20-Tetrakis-(3,5-di-tert-butyl)-phenylporphyrin (2HTTBPP) adsorbed on Cu(111) forms a peculiar supramolecular ordered phase: the molecules arrange in alternating rows, with two distinct appearances in STM, which are assigned to concave and convex intramolecular conformations. Around room temperature, frequent bidirectional conformational switching of individual molecules from concave to convex and vice versa is observed. From the temperature dependence, detailed insights into the energy barriers and entropic contributions of the switching processes are deduced. With this contribution, we demonstrate that entropic effects can be a decisive factor for the self-assembly and the conformational switching behaviour of molecules at these temperatures.

O 6.7 Mon 12:00 TRE Phy

**Switching and charging of a ruthenium dye** — •Nadine Hauptmann[1], Christian Hamann[1], Hao Tang[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]CEMES/CNRS 29, rue Jeanne Marvig, B.P. 94347, 31055 Toulouse Cedex, France/ Université de Toulouse, UPS, 31055 Toulouse, France

The ruthenium dye N3 (cis-bis(isothiocyanato)bis-(2,2'-bipyridyl-4,4'-dicarboxylato)-ruthenium(II)), is deposited on metal surfaces by ultrahigh vacuum electrospray ionization and is investigated using low-temperature scanning tunneling microscopy. Scanning tunneling spectroscopy of single molecules reveals vibronic excitations that are related to the lowest unoccupied molecular orbital. Switching of N3 molecules attached to Ag(111) step edges may be induced and modifies the energy of the negative ion resonance as well as the vibrational progression. Moreover, charging of the molecule is induced at reversed bias. This data suggests a surprisingly weak electronic coupling of N3 to the Ag substrate. A double-barrier model reproduces the essential spectral features.

O 6.8 Mon 12:15 TRE Phy

**Charge switching in a self-assembled acceptor-donor complex** — •Paul Stoll[1], Janina N. Ladenthin[1], Tobias R Umbach[1], Christian Lotze[1], Isabel Fernandez Torrente[1], Nacho Pascual[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin — [2]CIC NanoGUNE, San Sebastian

The switching mechanisms between metastable states in molecules is based on fundamental quantum physics and is potentially valuable for future applications in molecular electronics. We investigate the charge-transfer complex tetracyanoethylene (TCNE) and tetrathiafulvalene (TTF) on a Au(111) surface using low temperature scanning tunneling microscopy and spectroscopy. The molecules self-assemble in highly ordered islands with different stoichiometries. The TCNE molecules are found in two different charge states that are identified by the presence or abscence of a Kondo resonance. The rates of the random switching between these states are controlled by the tunneling current and the applied bias.

O 6.9 Mon 12:30 TRE Phy

**Diarylethene molecules on a Ag(111) surface: stability and electric field-induced switching of single molecules** — •Nino Hatter[1], Jonas Wirth[2], Robert Drost[1], Tobias R. Umbach[1], Sara Barja[1], Marc Zastrow[3], Karola Rück-Braun[3], Jose I. Pascual[4], Peter Saalfrank[2], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]Institut für Chemie, Universität Potsdam, Germany — [3]Institut für Chemie, Technische Universität Berlin, Germany — [4]CIC nanoGUNE, Dondostia-San Sebastian, Spain

Diarylethene derivatives are photochromic molecular switches, existing in two different forms, a ring-closed one with a conjugated $\pi$ electron system and a ring-opened, where the conjugation is broken. Light irradiation can induce a reversible ring-opening/closing reaction, as has been shown for molecules in solution and bulk crystals. However, little is known about their switching behaviour when adsorbed on surfaces.

We present a combined approach of scanning tunneling microscopy/spectroscopy (STM/STS) and density functional theory (DFT) calculations of 4,4'-(4,4'-(Perfluorocyclopent-1-ene-1,2-diyl)bis(5-methylthiophene-4,2-diyl)dipyridine (PDTE) adsorbed on a Ag(111) surface. The STM measurements show only one isomer present on the surface after evaporation of PDTE which can be switched by controlled manipulation with the STM tip. Comparison to the DFT calculations suggests that the manipulation with the tip induces the ring-closure reaction.

O 6.10 Mon 12:45 TRE Phy

**STM Induced Light Emission from Organic Molecules on Surfaces** — •Maren C. Cottin, Ebru Özen, Tobias Roos, Doris Steeger, Detlef Utzat, Willy Platz, Rolf Möller, and Christian A. Bobisch — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

Most STM techniques rely on the elastic part of the tunneling current. In contrast, STM induced light emission (STM-LE) experiments analyze the excitation mechanisms in the tip sample junction due to inelastic tunneling processes. Laterally resolved photon maps reveal the specific sites of excitation [1,2], while spectra of the overall light intensity as a function of bias voltage as well as energy resolved spectra of the emitted light can be used to characterize and identify the involved radiative decay channels [3]. Here, we use STM-LE to characterize various organic/metal interfaces. E.g., we present intermolecularly resolved photon maps of the archetype molecule $C_{60}$ on different substrates. From energy resolved spectra of the emitted light we try to identify the involved decay channels.

[1] R. Berndt et al., Science **262**, 1425 (1993).
[2] C. Chen et al., Phys. Rev. Lett. **105**, 217402 (2010).
[3] R. Berndt et al., Ultramicroscopy **42 − 44**, 355 (1992).

O 6.11 Mon 13:00 TRE Phy

**Investigation of novel partial charge-transfer compounds based on triangulene derivatives by ultraviolet photoelectron spectroscopy (UPS) and near-edge X-ray adsorption fine structure (NEXAFS)** — •Alisa Chernenkaya[1,2], K. Medjanik[2], M. Kivala[3], P. Nagel[4], M. Merz[4], S. Schuppler[4], T. Shubina[5], M. Baumgarten[3], K. Müllen[3], and G. Schönhense[2] — [1]Graduate School Materials Science in Mainz, 55128, Mainz, Germany — [2]Inst. für Physik, JGU, 55128, Mainz, Germany — [3]MPIP, 55021 Mainz, Germany — [4]KIT, Inst. für Festkörperphys., 76021 Karlsruhe, Germany — [5]Comp.-Chem.-Cent., 91052 Erlangen, Germany

A new class of donors and acceptors is represented by derivatives of the (4,4,8,8,12,12-hexamethyl-4*H*,8*H*,12*H*-benzo[1,9]quinolizino[3,4,5,6,7-defg]acridine) [1], so-called triangulene. We present UPS and NEXAFS results for molecular beam deposited thin films of triangulene and its trimethoxy derivative donors in complexes with the strong F4-TCNQ acceptor in comparison with density functional theory (DFT) calculations. The whole information about density of states (occupied valence states and unoccupied ones as well) in these charge-transfer systems is provided by these techniques as previously shown for pyrene derivatives [2]. We also compared CT complexes formation and film growth mechanisms in two systems that differ in three methoxy groups only.

Funded by DFG (Transregio TR49).

[1] M. Kivala et. al., Chem. Eur. J., 19, 8117-8128 (2013).
[2] K. Medjanik et. al., JACS 134, 4694-4699 (2012).

# O 7: Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale

Non-equilibrium processes such as charge and heat transport are central to electronic and thermoelectric applications. Understanding these phenomena at the nanoscale challenges both theory and experiment. Basic theoretical issues are related to the role of quantum mechanics, the interplay of ballistic, diffusion and hopping processes, the importance of dissipation, the effect of electronic correlation, and the signatures of unusual quantum states. On the experimental side devising measurements to unravel these phenomena in a controlled way poses severe difficulties. In this regard, optical lattices of cold atoms are emerging as a powerful laboratory to test theoretical models and discover unforeseen phenomena.

This symposium will cover current issues in the field by bringing together scientists working in different specific areas with the aim of fostering interdisciplinary discussion, assessing current theoretical understanding, and indicating future goals with emphasis on electronic structure theory.

Organizers: Roberto Car (Princeton), Kristian S. Thygesen (Lyngby) and Matthias Scheffler (Berlin)

Time: Monday 10:30–13:15 Location: TRE Ma

**Topical Talk** O 7.1 Mon 10:30 TRE Ma

**Molecular junction transport: some theoretical and computational considerations** — •Mark Ratner[1] and Matthew Reuter[2] — [1]Chemistry, Northwestern University, Evanston Illinois 60208 USA — [2]Chemistry, Northwestern University, Evanston Illinois 60208 USA

Following the development of break junction techniques, and very elegant measurements by many labs worldwide, the understanding of the community for single molecule transport junctions on the experimental side has been very nicely unified. While there are still challenges, interpretations of the transport (and indeed of some second-order response properties) is now quite sophisticated.

There have been major advances in the computational approaches also, and in many cases, computations and measurements can be compared quantitatively. But there are some remaining difficulties in the computational and theoretical approaches, and this talk will discuss a few of them.

The topics addressed will be: single molecule aspects, histograms and their usage, time-dependence of the transport, and ghost transmission and computational accuracy.

O 7.2 Mon 11:00 TRE Ma

**On the description of biased nanocontacts from ab initio** — •Steven Achilles[1], Jürgen Henk[1], Michael Czerner[2], Christian Heiliger[2], and Ingrid Mertig[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany — [2]I. Physikalisches Institut, Justus Liebig University, D-35392 Giessen, Germany

A suitable description of arbitrary shaped and biased nanocontacts is very important for investigating and predicting physical effects of materials on the nanometer scale. In particular, the electronic transport properties under finite bias voltages are of great interest.

To account for systems under finite bias we extended our Korringa-Kohn-Rostoker Green's function method [1] to the Keldysh formalism [2]. The method was developed for different types of geometries, i.e. planar junctions [3] and embedded real-space clusters [4]. Both implementations include a self-consistent treatment of the electronic structure under external bias using the nonequilibrium density.

We present ab initio results of voltage drops, the charge relaxation under finite bias voltage and current-voltage characteristics for different types of geometries.

[1] R. Zeller, P.H. Dederichs, B. Ujfalussy, L. Szunyogh, and P. Weinberger, Phys. Rev. B 52, 8807 (1995).; P. Zahn, I. Mertig, R. Zeller, and P.H. Dederichs, Mat. Res. Soc. Symp. Proc. 475, 525 (1997).
[2] L.V. Keldysh, Sov. Phys. JETP 20 (4), 1018-1026 (1965).
[3] S. Achilles et al., Phys. Rev. B 88 (12), 125411 (2013).
[4] S. Achilles et al., to be published

O 7.3 Mon 11:15 TRE Ma

**Elasticity changes in molecular junctions under bias: an ab-initio study** — •Clotilde S. Cucinotta[1], Meilin Bai[1,2], Ivan Rungger[1], Shmin Hou[2], and Stefano Sanvito[1] — [1]School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2, Ireland — [2]2Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China

Non-conservative current induced forces are at the origin of a rich variety of dynamical processes, including vibrations, rotations, phonon energy flow, desorption and reactions. The ability to simulate these phenomena paves the way for crucial advances in interface physics and in molecular electronics. New insights into how the presence of non-conservative forces can affect the vibrational spectrum of prototypic Au-H2-Au nano-junctions are obtained by the Non Equilibrium Green Functions approach combined with Density Functional Theory as implemented in the Smeagol code [1]. The modification of the phonon spectrum of the junction in the presence of an external bias is for the first time analysed, in terms of charge redistribution caused by the electron flow, potential drop and differences in an average distance collective variable. Phonon modes changes are related to a change in bias of some of the elastic constants.The importance of electric field vs. current effects is compared. The elasticity changes of the molecular junction with bias are interpreted in terms of the current flowing through the system. [1] http://www.smeagol.tcd.ie/SmeagolDownloads.htm.

O 7.4 Mon 11:30 TRE Ma

**Carbon nanotubes decorated with magnetic clusters: magnetism, electron transport and gas sensing** — •Zeila Zanolli[1] and Jean-Christophe Charlier[2] — [1]Forschungszentrum Juelich, PGI and IAS, Juelich, Germany — [2]IMCN, Université catholique de Louvain (UCL), Belgium

In this work, first-principles techniques and non-equilibrium Green's function approaches are used to investigate magnetism and spin-polarized quantum transport in carbon nanotubes (CNTs) decorated with transition metal magnetic nanoclusters (NC).

For small cluster sizes ($< 1$ nm), *ab initio* calculations predict a considerable local magnetic moment that induces spin polarization in the host CNT due to a strong mutual interaction with the magnetic NC. Such a huge local magnetic perturbation can be tailored by molecular adsorption on the metallic NC, thus modifying both the magnetization and the spin-dependent conductance of the hybrid CNT-NC system. The adsorption of benzene on Ni- or Pt-decorated metallic CNTs has been investigated as a test case. The ab initio simulations demonstrate that the magnetization change due to the absorption of a single $C_6H_6$ molecule should be large enough to be detected experimentally using either magnetic-AFM or SQUID magnetometer. Consequently, the present research suggests a novel approach for single molecule gas detection, based on local magnetic moment measurements in CNT-NC hybrid systems [1].

[1] Z. Zanolli, J.-C. Charlier, ACSnano **6** (2012) 10786-10791.

**15 min. break**

**Topical Talk** O 7.5 Mon 12:00 TRE Ma

**Insight into Charge Transport in Molecular Junctions from Ab Initio Theories of Level Alignment** — •Jeffrey B. Neaton — Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — Department of Physics, University of California, Berkeley, Berkeley, CA — Kavli Energy Nanosciences Institute, Berkeley, CA

Recent scanning tunneling microscope-based break-junction experiments of molecular junctions – devices formed by trapping organic molecules between macroscopic metallic electrodes – have reported robust conductance, thermopower, switching behavior, quantum interference effects, spin-filtering phenomena, and even nonlinear effects such as rectification, establishing such junctions as unique and revealing windows into the physics of charge transport at the molecular scale. In this talk, I will summarize a predictive approach to compute and understand the transport properties of molecular junctions with good accuracy. Our approach includes important exchange and correlation effects missing in standard DFT Kohn-Sham junction level alignment, building on self-energy corrections within a GW approximation. Advantages and limitations of our approach will be discussed quantitatively in the context of a direct comparison with recent photoemission and transport measurements. I will also describe applications of this approach to select junctions exhibiting novel trends in conductance, thermopower, and nonlinear IV characteristics, where new physical insight is obtained by relating computed transport phenomena to junction structure and chemistry.

O 7.6 Mon 12:30 TRE Ma

**Towards First-Principles Modeling of Solvent Effects in Photo-Catalytic Water Splitting** — •Stefan Ringe, Harald Oberhofer, Sebastian Matera, and Karsten Reuter — Technische Universität München, Germany

In the context of solar energy conversion the search for new materials for photo-catalytic water splitting has received new impetus. While in general powerful, computational screening approaches are struggling with the complexity of the underlying physical processes at the solid-liquid interface. Recent work points in particular at the necessity to include at least an efficient description of solvent screening effects to compute meaningful descriptors even in simple computational hydrogen electrode approaches. To this end, we present an implementation of the modified Poisson-Boltzmann (MPB) implicit solvation model in the highly parallel and numerically efficient all-electron DFT code FHI-aims. Optimally integrating into this code environment, we solve the MPB equation in a novel approach based on an expansion of the electrostatic potential in the localized basis functions of FHI-aims. In contrast to common numerical multi-grid solvers this approach can directly make use of the optimized integration schemes used to reach self-consistency and removes the need for numerical interpolation between different grids. We demonstrate the approach and its efficiency for a range of molecular test systems, and show first results for catalytic water splitting on gold nano-clusters.

O 7.7 Mon 12:45 TRE Ma

**Towards a combined QM/MM and implicit solvent description of photoelectrochemical processes** — •Markus Sinstein[1], Daniel Berger[1], Ran Jia[2], Volker Blum[3], Harald Oberhofer[1], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Jilin University, P.R. China — [3]Duke University, USA

Photoelectrochemical systems are widely explored to drive energy-relevant redox reactions like water splitting or $CO_2$ reduction. The detailed analysis of the involved elementary processes via first-principles calculations is challenged by the necessity to simultaneously account for the extended semiconductor photocatalyst and the liquid electrolyte. Especially for charge (proton and/or electron) transfer steps traditionally employed periodic boundary condition approaches involve charged supercells with difficult to control finite size errors. To this end, we present a solid state QM/MM embedding approach, in which only a finite cluster model of the photocatalyst surface is treated quantum mechanically and the correct Madelung potential of the periodic system is obtained by embedding into a charge field. For the efficient modeling of photoelectrochemical processes we combine this approach with an implicit solvation scheme within the DFT package FHI-aims. Finally, we also show early test results of the combined QM/MM implicit solvent model.

O 7.8 Mon 13:00 TRE Ma

**Ab-initio Simulation of Molecular Networks on the Surface of Water** — •Ralph Koitz, Marcella Iannuzzi, Ari P Seitsonen, and Jürg Hutter — University of Zurich, Zurich, Switzerland

Molecules adsorbed on surfaces play an important role in catalysis, surface science, and nanotechnology. Traditionally, research has focused on various adsorbates atop metals and metal oxides using computational and surface-science techniques. More recently, however, it was demonstrated that ordered monolayer networks can also be formed on the surface of liquid water by using metal ions to bind together multidentate precursor molecules. As these assemblies are difficult to characterize, computational methods can provide valuable insight into their formation and structure.

In this contribution we present large-scale DFT-based molecular dynamics simulations of the formation of a network of *tris*-terpyridine-derived molecules (TTPB) on a water slab. In particular, we focus on the structure of the molecule on the surface, the mechanism of $Zn^{2+}$ ion insertion from the solution and the subsequent linking of molecules into aggregates. We employ the metadynamics method to quantify the free energy surface of the involved processes. Our results provide detailed insight into on-surface and subsurface diffusion in this system and chemical reactions of TTPB on the surface of water.

## O 8: Electronic Structure and Spin-Orbit Interaction I

Time: Monday 10:30–13:00 Location: GER 38

O 8.1 Mon 10:30 GER 38

**Depending on how you look at it - (un)conventional spin topology in the unoccupied band structure of Bi/Ag(111)** — •Sune N. P. Wissing[1], Anke B. Schmidt[1], Christian R. Ast[2], Hossein Mirhosseini[3], Jürgen Henk[4], and Markus Donath[1] — [1]Westfälische Wilhelms-Universität Münster, Germany — [2]Max-Planck-Institut für Festkörperforschung Stuttgart, Germany — [3]Johannes Gutenberg-Universität Mainz, Germany — [4]Martin-Luther-Universität Halle-Wittenberg, Germany

We report on the challenge to determine the spin of the electronic structure out of a spin-polarized (inverse) photoemission experiment. For this purpose, we present a study on the unoccupied electronic structure of Bi/Ag(111) with spin- and angle-resolved inverse photoemission. Above the Fermi level, we identify several states with distinct spin character.

We focus our attention on the two $p_{xy}$-derived surface states. For the downward dispersing $m_j = 1/2$ state, theoretical calculations [1] predict a complex spin topology, where the spin polarization changes sign at the band maximum. Our experimental findings, however, indicate a spin splitting compatible with the conventional Rashba model. To shed more light on this issue, we investigated the spin topology with the help of first-principles electronic-structure and photoemission calculations. We will discuss the dependence of the measured spin topology on the polarization of the emitted light and the symmetry of the involved electronic states.

[1] G. Bihlmayer *et al.*, Phys. Rev. B **75**, 195414 (2007)

O 8.2 Mon 10:45 GER 38

**Spin-flip scattering in the surface bands of $BiAg_2$/Ag(111)** — •Gustav Bihlmayer[1], Lydia El-Kareh[2], Matthias Bode[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute of Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Since its discovery, the surface alloy $BiAg_2$/Ag(111) has attracted considerable attention due to the 'giant Rashba' splitting in the occupied surface bands. Recently, also the unoccupied part of the spectrum was investigated by scanning tunneling microscopy. But, although theory predicted a rather complex spin-texture of these bands [1], the quasiparticle interference patterns seem compatible with a conventional Rashba-type spin-polarization of these bands [2]. Close examination of the spin- and orbital resolved bandstructures obtained by density functional theory show, that the orbital structure allows spin-flip scattering processes that can reconcile experimental evidence with theoretical predictions. Our calculations and experiments show that this behavior is not only characteristic for the Bi-based surface alloy, also in the $PbAg_2$/Ag(111) system these spin-flip scattering events are observed. The same mechanism also blocks quasiparticle interference in forward scattering, while other scattering events are explicitly forbidden by time-reversal symmetry.

[1] G. Bihlmayer et al., Phys. Rev. B **75**, 195414 (2007)

[2] L. El-Kareh et al., Phys. Rev. Lett. **110**, 176803 (2013)

O 8.3 Mon 11:00 GER 38

**Rashba-split surface states of $(\sqrt{3}\times\sqrt{3})$Pb/Ag(111)$R30°$** — •Lydia El-Kareh[1], Gustav Bihlmayer[2], Arne Buchter[3], Hendrik Bentmann[3], Friedrich Reinert[3], Stefan Blügel[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Peter Grünberg Institut and Institute of Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [3]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We report on a combined low-temperature scanning tunneling spectroscopy (STS), angle-resolved photoemission spectroscopy (ARPES), and density functional theory (DFT) investigation of the $(\sqrt{3}\times\sqrt{3})R30°$ Pb/Ag(111) surface alloy which provides a giant Rashba-type spin-splitting [1,2]. By means of STS and quantum interference mapping we determined the band onsets, splitting strengths, and dispersions for two Rashba-split bands. The unambiguous assignment of scattering vectors is achieved by comparison to ARPES measurements. The detailed analysis of the spin and orbital character of both bands as obtained by DFT calculations allows to solve an apparent deviation between experimentally observed scattering events and the theoretically predicted spin polarization [3].

[1] D. Pacilé *et al.*, Phys. Rev. B **73**, 245429 (2006).
[2] G. Bihlmayer *et al.*, Phys. Rev. B **75**, 195414 (2007).
[3] L. El-Kareh *et al.*, Phys. Rev. Lett. **110**, 176803 (2013).

O 8.4 Mon 11:15 GER 38

**The Unoccupied Band Structure of Pb/Ag(111)** — •Katharina T. Ritter, Sune N. P. Wissing, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany

Surface alloys of heavy elements on noble metal fcc(111) surfaces are known to exhibit strongly Rashba-split band structures. Especially the surface alloys with $(\sqrt{3}\times\sqrt{3})R30°$ reconstruction have been in the focus of theoretical and experimental reasearch. So far, most experimental data result from photoemission experiments and hence are limited to the occuppied electronic states.

Here, we perform spin- and angle-resolved inverse photoemission to access the unoccupied band structure of Pb/Ag(111). Above the Fermi level, we identify several states with distinct spin dependence. We determine their nature concerning symmetry, bulk vs. surface character, energy vs. momentum dispersion, and spin character. As we recently also investigated the related surface alloy Bi/Ag(111), we will compare the results of both systems and analyse systematic changes accompanying the reduction of the number of valence electrons of the adsorbate by one.

O 8.5 Mon 11:30 GER 38

**Bulk and surface Rashba states in ferroelectric GeTe: combined experimental and theoretical SX-ARPES study** — H. Volfova[1], J. Krempasky[2], H. Dill[2], V. Strocov[2], J. Braun[1], H. Ebert[1], K. Hricovini[6], R. Calarco[3], R. Bertacco[4], S. Picozzi[5], and •Jan Minar[1] — [1]LMU Munich, Munich, Germany — [2]PSI, Villigen, Switzerland — [3]PDI Berlin, Germany — [4]Politecnico Milano, Italy — [5]CNR-SPIN L'Aquila, Italy — [6]Universite de Cergy-Pontoise, France

The recent theoretical investigations of Picozzi et al. [1] predicted a huge Rashba effect originating from bulk states in ferroelectric GeTe, which spin polarisation can be switched by reversing its ferroelectric polarisation. However, detailed experimental and theoretical studies of the electronic structure by means of the angle resolved photoemission (ARPES) are until now missing. Here we present a combined theoretical and experimental study of the electronic structure of GeTe investigated with the aid of the bulk sensitive soft X-ray (SX)-ARPES [2]. It will be shown that a proper description of the photoemission process is necessary to understand the experimental results. These effects are included in the one-step model of photoemission implemented in the SPR-KKR package [3], which presents clear evidence for the predicted bulk Rashba state. [1] Di Sante et al., Andvanced materials 25, 509 (2013) [2] A. Gray, J. Minar et al., Nat. mat. 10, 759 (2011) [3] H. Ebert et al., Rep. Prog. Phys. 74, 096501 (2011)

O 8.6 Mon 11:45 GER 38

**Chiral magnetism of magnetic adatoms from Rashba electrons** — •Juba Bouaziz[1], Manuel dos Santos Dias[1], Abdelhamid Ziane[2], Mouloud Benakki[2], Stefan Blügel[1], and Samir Lounis[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Laboratoire de Physique et Chimie Quantique, Faculté des Sciences, Université Mouloud Mammeri, 15000 Tizi-Ouzou, Algeria

We investigate chiral magnetic long-range interactions among adatoms mediated by surface states spin-splitted by spin-orbit coupling. Using the Rashba model, the tensor of exchange interactions is extracted wherein a two-ion anisotropy term is found besides the usual isotropic exchange interaction (J) and the Dzyaloshinskii-Moriya interaction (DM). The inter-adatom distance controls the strength of these terms which we exploit to design chiral magnetism in Fe nanotructures on Au(111) surface. In contrast to [1], we include without approximation the contribution of the integrable singularity observed at the extremum of the dispersion curve. When the magnetic moments are out-of-plane, we demonstrate within a simple approach that J and DM are respectively related to superpositions of the out-of-plane and in-plane components of the skyrmionic magnetic waves induced by the adatoms in the surrounding electron gas [2].

This work is supported by the HGF-YIG Programme VH-NG-717 (Functional Nanoscale Structure and Probe Simulation Laboratory).

[1] H. Imamura *et al.* Phys. Rev. B **69**, 121303 (2004)
[2] S. Lounis *et al.* Phys. Rev. Lett. **108**, 207202 (2012)

O 8.7 Mon 12:00 GER 38

**Quasiparticle spin-interference by scattering off magnetic atoms on metal surfaces with spin orbit coupling** — •Philipp Rüssmann, Phivos Mavropoulos, Nguyen H. Long, David S. G. Bauer, and Stefan Blügel — Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We present density-functional calculations of the quasiparticle interference at surfaces due to scattering off magnetic adatoms. Our focus is on 3*d* impurities on Au(111) where the spin-orbit coupling (SOC) causes a Rashba-type splitting of the surface state. The spin polarization of the quasiparticle waves shows a non-collinear texture because of SOC. We investigate the dependence of the polarization on the orientation of the impurity magnetic moment. We compare to previous model-based results [1] and discuss the relation to the scattering properties of the impurity, taking into account the non-zero probability of time-reversed transitions due to the magnetic moment. In our calculations we employ the KKR-Green function method for the electronic structure and scattering properties at defects [2]. We acknowledge financial support from the DFG (SPP-1666) and from the Virtual Institute Topological Insulators of the Helmholtz Association and computational support from the JARA-HPC Supercomputing Center at the RWTH Aachen.

[1] S. Lounis, A. Bringer, and S. Blügel, Phys. Rev. Lett. **108**, 207202 (2012).
[2] S. Heers, PhD Thesis, RWTH Aachen (2011); D.S.G. Bauer, PhD Thesis, RWTH Aachen (2013).

O 8.8 Mon 12:15 GER 38

**Giant splitting of unoccupied surface resonant state on Tl/Si(111)** — •Sebastian D. Stolwijk[1], Kazuyuki Sakamoto[2], Anke B. Schmidt[1], Peter Krüger[3], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster — [2]Department of Nanomaterials Science, Chiba University, Chiba 263-8522, Japan — [3]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster

The Tl/Si(111)-(1 × 1) surface features outstanding properties - a unique spin pattern in momentum space and an unoccupied surface state with giant spin splitting at the $\bar{\mathrm{K}}$ point [1,2]. In this contribution, we focus on the unoccupied surface electronic structure along the $\bar{\Gamma}\bar{\mathrm{M}}$ direction. Spin- and angle-resolved inverse photoemission experiments with sensitivity to the in-plane and out-of-plane components of the spin polarization vector are conducted with the help of our recently developed **RO**tatable **S**pin-polarized **E**lectron source (ROSE). Along $\bar{\Gamma}\bar{\mathrm{M}}$ only in-plane polarization is found. Moreover, we identify a spin-orbit-split surface resonant state, which exhibits a Rashba-type splitting. Remarkably, the size of the Rashba splitting is comparable to the giant splitting found for the Bi/Ag(111) surface [3].

[1] K. Sakamoto et al., Phys. Rev. Lett. **102**, 096805 (2009)
[2] S. D. Stolwijk et al., Phys. Rev. Lett. **111**, 176402 (2013)
[3] C. Ast et al., Phys. Rev. Lett. **98**, 186807, (2007)

O 8.9 Mon 12:30 GER 38

**Spin-split surface states in the unoccupied electronic structure of Tl/Ge(111)-(1x1)** — •Philipp Eickholt[1], Sebastian D. Stolwijk[1], Anke B. Schmidt[1], Peter Krüger[2], and Markus

Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms Universität, Münster, Germany — [2]Institut für Festkörpertheorie, Westfälische Wilhelms Universität, Münster, Germany

The unoccupied electronic structure of Tl/Si(111)-(1x1) exhibits a unique spin-orbit-split surface state with rotating polarization vector and giant energy splitting at the $\overline{\mathrm{K}}$ point [1]. Here, we present spin- and angle-resolved inverse-photoemission results on the unoccupied electronic structure of the isoelectronic Tl/Ge(111)-(1x1) surface, which is expected to show similar properties [2]. In fact, along the $\overline{\Gamma\mathrm{K}}$ direction, a similar spin-orbit-split surface state is found with comparable properties as observed on Tl/Si(111). Differences between the two surfaces can be seen along $\overline{\Gamma\mathrm{M}}$, where a Rashba-type spin-split surface state on the Tl/Ge(111) surface lies well within a band gap, while it is degenerate with the bulk bands on the Si substrate. Remarkably, our measurements feature a spin asymmetry directly at the $\overline{\mathrm{M}}$ point where spin degeneracy should prevail.

[1] Sebastian D. Stolwijk et al., Phys. Rev. Lett. **111**, 176402 (2013)

[2] Y. Ohtsubo et al., J.Phys.: Condens. Matter **24**, 092001 (2012)

O 8.10 Mon 12:45 GER 38

**Hysteretic melting of a soliton lattice in a commensurate charge modulation** — •Tobias Mauerer[1], Pin-Jui Hsu[1], Matthias Vogt[1], J.J. Yang[2], Yoon Seok Oh[3], S-W. Cheong[2,3], Matthias Bode[1], and Weida Wu[3] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Laboratory for Pohang Emergent Materials and Department of Physics,Pohang University of Science and Technology, Pohang 790-784, Republic of Korea — [3]Rutgers Center for Emergent Materials and Department of Physics and Astronomy,Rutgers University, Piscataway, New Jersey 08854, USA

We report on the observation of the irreversible transition of a commensurate charge modulation in $\mathrm{IrTe_2}$ from transport and scanning tunneling microscopy (STM) studies. Below the transition ($T_\mathrm{C} \approx 275\,\mathrm{K}$ on cooling) a $q = 1/5$ charge modulation was observed, which is consistent with previous studies [1,2]. Additional modulations [$q_n = (3n+2)^{-1}$] appear below a second transition at $T_\mathrm{S} \approx 180\,\mathrm{K}$ on cooling. The coexistence of various modulations persist up to $T_\mathrm{C}$ on warming. The atomic structures of charge modulations and the temperature-dependent STM studies suggest that 1/5 modulation is a periodic soliton lattice which partially melts below $T_\mathrm{S}$ on cooling. Our results provide compelling evidence that the ground state of $\mathrm{IrTe_2}$ is a commensurate 1/6 charge modulation, which originates from periodic dimerization of Te atoms visualized by atomically resolved STM images.

[1] J. J. Yang *et al.*, Phys. Rev. Lett. **108**, 116402 (2012).

[2] S. Pyon *et al.*, J. Phys. Soc. Jap. **81**, 053701 (2012).

# O 9: Surface Chemical Reactions and Heterogeneous Catalysis I

Time: Monday 10:30–13:00 Location: PHY C 213

O 9.1 Mon 10:30 PHY C 213

**In-situ investigation of the growth and oxidation of $\mathrm{Mo_2C}$/Mo(100) using high-resolution X-ray photoelectron spectroscopy** — •Udo Bauer, Christoph Gleichwald, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Molybdenum carbide has been proposed as a noble metal free catalyst for a variety of reactions. We used our supersonic molecular beam setup to carburize a Mo(100) single crystal. Ethylene adsorption at 900 K and subsequent oxidation of the carburized system at 1200 K were followed in-situ in the C 1s and Mo 3d core levels by fast X-ray photoelectron spectroscopy (XPS) performed at the synchrotron facility BESSSY II. We observed three different species in the C 1s core level during the $\mathrm{C_2H_4}$ deposition. Starting with the growth of a precursor carbide, surface and bulk carbide species arise and saturate after an exposure of 1200 L. Subsequent annealing to 1300 K removed excess carbon, resulting in the desired $\mathrm{Mo_2C}$ stoichiometry. Oxidation of the molybdenum carbide revealed a very fast diffusion of bulk carbon to the surface, refilling empty sites occurring due to CO desorption.

O 9.2 Mon 10:45 PHY C 213

**Etching of Graphene on Ir(111) with Molecular Oxygen** — •Ulrike A. Schröder[1], Elin Grånäs[2], Timm Gerber[1], Mohammad A. Arman[2], Karina Schulte[3], Jan Knudsen[2,3], Jesper N. Andersen[2,3], and Thomas Michely[1] — [1]Universität zu Köln, II. Physikalisches Institut, Germany — [2]Lund University, Division of Synchrotron Radiation Research, Sweden — [3]Lund University, MAX IV Laboratory, Sweden

Although oxidation of carbon has been studied for decades, it remains unclear how oxygen attacks and oxidizes closed and submonolayer graphene on the atomic scale level. We provide new insights by using the well-defined system graphene on Ir(111) and exposing it to molecular oxygen.

Using scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and thermal desorption spectroscopy (TDS), we find that etching is a thermally activated process and depends on temperature and Gr morphology. For submonolayer Gr films, etching sets in at 550 K. The molecular oxygen dissociates on the free Ir(111) surface. Real time STM measurements reveal that oxygen then attacks Gr via the edges. Free edges are preferentially etched, compared to Gr bound to Ir steps. Perfectly closed Gr films are remarkably stable against oxygen etching, which only starts above 700 K. At this temperature, 5-7 defects stemming from the Gr growth process act as dissociation sites for the $\mathrm{O_2}$ molecules. At higher etching temperatures, large hexagonal etch holes are visible in the STM: Zigzag edges are more stable against etching than armchair edges.

O 9.3 Mon 11:00 PHY C 213

**From qualitative to atomistic: First-principles kinetic modeling of Pd surface oxide reduction by CO** — •Max J Hoffmann and Karsten Reuter — TU München, Germany

Obtaining detailed atomistic insight into oxide formation and reduction at metal surfaces is a key step to understand and ultimately engineer the function of these surfaces in a multitude of applications, not least in oxidation catalysis. On the modeling side, the analysis of kinetic measurements in terms of reaction rate laws is traditionally employed to extract qualitative information. First-principles calculations, on the other hand, describe the microscopic processes underlying the actual phase transition. First-principles microkinetic models offer the prospect to join these two strands and subject atomistic models to scrutiny against measured kinetic data. We illustrate this approach with first-principles kinetic Monte Carlo (1p-kMC) simulations of the reduction of a $(\sqrt{5} \times \sqrt{5})R27^\circ$ surface oxide on Pd(100) in a CO atmosphere, and reference against kinetic data derived from X-ray photoelectron spectroscopy [1]. In full agreement with the experimental rate law analysis our atomistic simulations demonstrate that the reduction process can not occur via a homogeneous decomposition of the oxide phase. We overcome prevalent limitations to lattice-based 1p-kMC through a novel multi-lattice approach and present a mechanistic model that includes the full transformation from oxide to metal. This model fully rationalizes the measured data and proves that under the investigated gas-phase conditions the reduction is a phase-boundary controlled process. [1] V.R. Fernandes *et al.*, Surf. Sci. (in press).

O 9.4 Mon 11:15 PHY C 213

**Cu/ZnO nanocatalysts in response to environmental conditions: Surface morphology, electronic structure, redox state and CO2 activation** — Luis Martínez-Suárez[1], •Johannes Frenzel[1], Bernd Meyer[1,2], and Domink Marx[1] — [1]Theoretische Chemie, Ruhr–Universität Bochum,44780 Bochum, Germany — [2]ICMM and CCC, Uni Erlangen-Nürnberg, 91052 Erlangen, Germany

By performing extensive DFT calculations in combination with a thermodynamic formalism we establish an atomistic understanding of gas phase-induced changes of surface morphology, redox properties and reactivity of ZnO supported Cu nanocatalyst [1] which shows strong metal-support interactions (SMSI) [2-7]. Being subject to electronic charge transfer processes across the metal-support interface [7,8] we explore surface stabilization and site dependent redox state of both catalyst components in response to the redox properties of the surrounding gas phase . Further, *ab initio* molecular dynamics unveils the vital nature of the deposited metal which, besides reduced Zn in the ZnO support, enhances CO2 activation over Cu.

[1] Martínez-Suárez, L., Frenzel, J., Meyer,. B., and Marx, D., PRL **110**, 086108 (2013) [2] Tauster, S. J., Fung, S. C., Baker, R. T. K., and Horsley, J. A., Science **211**, 1121 (1981). [3] Clausen, B. S., et al., Top. Catal. **1**, 367-376 (1994). [4] Wagner, J. B., et al., J. Phys. Chem. B **107**, 7753 (2003). [5] Wilmer, H., and Hinrichsen, O., Catal. Lett. **82**, 117-122 (2002). [6] Behrens, M., *et al.*, Science **336**, 893 (2012). [7] Frost, J. C., Nature (London) **334**, 577 (1998) [8] Liao, F., *et al.* Angew. Chem. Int. Ed. **51**, 5832 (2012).

O 9.5 Mon 11:30 PHY C 213

**Complex surface structure determination through first-principles global geometry optimization: $c(2\times2)$-$RuO_2(100)$** — •Tongyu Wang, Dennis Palagin, Saskia Stegmaier, and Karsten Reuter — Technische Universität München, Germany

"Ruthenium" catalysts exhibit a remarkable change of CO oxidation activity with reactant pressure [1]. Current understanding rationalizes the high activity at near-ambient conditions with a change of oxidation state. The enigmatic deactivation observed under oxidizing conditions is in turn assigned to a microfacetting of (otherwise highly active) $RuO_2(110)$ facets into an inactive $c(2\times2)$-$RuO_2(100)$ phase [2]. A detailed structural model of the latter phase would be an important step towards understanding (and possibly suppressing) the deactivation mechanism. Yet, despite detailed experimental characterization, such a model could not be established to date. To this end, we perform density-functional theory based global geometry optimization using a basin hopping approach. Combined within *ab initio* thermodynamics we assess the relative stabilities of the obtained structural candidates and discuss their properties in light of the existing experimental data. [1] H. Over, Chem. Rev. **112**, 3356 (2012); [2] J. Assmann *et al.*, Angew. Chem. Int. Ed. **44**, 917 (2005).

O 9.6 Mon 11:45 PHY C 213

**From macro to micro: Kinetics of HCl oxidation on $RuO_2(110)$** — •Farnaz Sotoodeh[1], Patrick Gütlein[1], Irene M. N. Groot[2], Joost W. M. Frenken[2], and Karsten Reuter[1] — [1]TU München, Germany — [2]Leiden University, Netherlands

A large portion of $Cl_2$ is used in industries that produce HCl as a waste byproduct [1]. The catalytic conversion of waste HCl back to high purity $Cl_2$ through oxidation (Deacon process) is thus highly desirable. However, the current process is expensive since it requires the precious metal Ruthenium. As this process is important to most industries, even small improvements in its efficiency will have a global economic and environmental impact by extending catalyst life time and stability. Therefore, designing an active and stable catalyst in the sustainable $Cl_2$ production is extremely valuable. Optimizing the catalyst activity under often "harsh" industrial implementations, requires an in-depth understanding of reaction kinetics over a wide range of operating conditions. Here, macrokinetic models including power-law and Langmuir-Hinshelwood are applied to measured activities. On the way towards microkinetics, the Langmuir-Hinshelwood kinetics is scrutinized closely by looking at elementary steps on $RuO_2(110)$ surface, with reaction barriers and binding energies of surface species calculated using DFT. The adaptability of the examined models are compared to available ones [2] where the model parameters were estimated by fitting to a restricted range of operating conditions.

[1] H. Y. Pan *et al.*, Ind. Eng. Chem. Res. **33**, 2996 (1994).

[2] D. Teschner *et al.*, J. Catal. **285**, 273 (2012).

O 9.7 Mon 12:00 PHY C 213

**Simulation of $Ni/CeO_2$ surfaces for $CO_2$ catalysis** — •Konstanze Hahn[1] and Jürg Hutter[2] — [1]University of Cagliari, Monserrato, Italy — [2]University of Zurich, Zurich, Switzerland

Combined metal-metal oxide systems are important materials for numerous technological applications such as microelectronics, photovoltaics, gas sensors and in particular in oxide-supported metal catalysts. Deposition of small metal particles on metal oxides such as $Al_2O_3$, $CeO_2$ and $TiO_2$ has led to enhanced catalytic activity, for example, for the water gas shift reaction or CO oxidation. Metal oxide supported materials are also promising catalysts for hydrocarbon production from $CO_2$, a reaction process interesting for alternative energy production since it provides high energy density fuel from $CO_2$ which is omnipresent in our environment. In fact, $CeO_2$-supported Ni particles have proven to be promising materials for the activation of methanation of $CO_2$. Here, density functional theory within the Gaussian and plane waves formalism has been used for the simulation of Ni cluster formation on $CeO_2(111)$ surfaces. Stabilization of Ni particles has been observed with increasing cluster size up to ten atoms. It has been found that O diffusion from the subsurface layer of $CeO_2(111)$ to the surface layer is facilitated in the presence of Ni particles on the surface. Furthermore, the adsorption and dissociation of $CO_2$ has been investigated on clean $CeO_2(111)$, on non-supported Ni clusters in the gas phase and on the $Ni/CeO_2(111)$ system. This study gives fundamental insight into the metal-metal oxide interactions and its function for $CO_2$ catalysis.

O 9.8 Mon 12:15 PHY C 213

**Combining High-Resolution Scanning Probe Microscopy Studies with Reactivity Experiments** — •Stefanie Stuckenholz, Christin Büchner, Hendrik Ronneburg, Gero Thielsch, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

We use thin metal supported MgO films as a model system to understand the correlation between morphology, electronic structure and reactivity of heterogeneous catalysts on the atomic scale.

For investigation of our samples we operate a scanning tunnelling microscope (STM) and noncontact atomic force microscope (nc-AFM). With the dual mode microscope we study the sample morphology and perform spectroscopic measurements, such as field emission resonance(FER) and Kelvin probe force microscopy (KPFM). The influence of a thin MgO film on the Mo(001) local work function, as well as differences between pristine terrace sites and line defect sites will be discussed.

To connect the findings of the dual mode microscope with reactivity studies we are setting up a new temperature programmed desorption (TPD) experiment. Here, desorption of gaseous species, e.g. CO from MgO surfaces, will be studied. This reaction serves as a model for the interaction of CO with an ionic surface.[1, 2] First results of the low temperature TPD setup will be presented.

[1] R. Wichtendahl, *et al.*, Phys. Status Solidi A **173**, 93 (1999)

[2] M. Sterrer, *et al.*, Surf. Sci. **596**, 222 (2005)

O 9.9 Mon 12:30 PHY C 213

**Near ambient pressure XPS investigation of the interaction of ethanol with $Co/CeO_2(111)$** — •Sandra Krick Calderón[1], Óvári László[2], Lykhach Yaroslava[1], Libuda Jörg[1], Erdohelyi Andras[3], Papp Christian[1], Kiss János[2,3], and Steinrück Hans-Peter[1] — [1]Physikalische Chemie II, University of Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany — [2]MTA-SZTE Reaction Kinetics and Surface Chemistry Research Group, H-6720 Szeged, Rerrich Béla tér 1, Hungary — [3]Department of Physical Chemistry and Materials Science, University of Szeged, H-6720 Szeged, Aradi vértanúk tere 1, Hungary

The adsorption of ethanol on a $CeO_2(111)$ surface and a $Co/CeO_2(111)$ model catalyst was studied with near ambient XPS at pressures up to 1 mbar. The main species adsorbed on the surface was found to be ethoxide, formed by dissociative adsorption. Upon ethanol exposure on pristine ceria at 300 K a gradual reduction with increasing pressure was observed; reduction was even further enhanced by heating to 600 K at 0.1 mbar. This effect was attributed to increased diffusion of the $Ce^{3+}$ centers or lattice oxygen at elevated temperatures. Partial reduction of the ceria layer upon Co deposition was observed. Ethanol strongly reduced the Co particles leaving almost solely metallic Co on the concurrently reduced $CeO_2$ surface at 600 K. While no coke formation occurred during reaction with the pristine $CeO_2$ layer, carbonaceous species were observed at 600 K on the $Co/CeO_2$ model catalyst.

O 9.10 Mon 12:45 PHY C 213

**Imaging mass transfer limitations in in-situ model catalyst studies** — •Sebastian Matera[1], Sara Blomberg[2], Max J. Hoffmann[1], Johan Zetterberg[2], Johan Gustafson[2], Edvin Lundgren[2], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Lund University, Sweden

A central goal in in-situ studies of defined model catalysts is to establish a correlation between surface micro-structure and observed reactivity. In corresponding near-ambient environments this observable reactivity may be intricately influenced by macroscale heat and mass transport limitations in the reactor. We investigate such effects with a first-principles based multi-scale modeling approach integrating kinetic Monte Carlo simulations into a fluid dynamical treatment [1]. Recent methodological advances [2] allow the full consideration of the experimental reactor geometry, which we illustrate with the application to recent Planar Laser Induced Fluorescence measurements [3] of CO oxidation at Pd(100). Experiment and theory consistently reveal strong mass transfer limitations under near-ambient operation conditions. Intriguingly, the detailed comparison of calculated and measured gas-phase concentration profiles offers an unprecedented route to draw conclusions on the prevalent surface phases and reaction pathways. [1] S. Matera and K. Reuter, Catal. Lett. 133, 156 (2009); Phys. Rev. B 82, 085446 (2010); J. Catal. 295,261 (2012). [2] S. Matera, M. Maestri, A. Couci, and K. Reuter, in preparation. [3] J. Zetterberg et al., Rev. Sci. Instrum. 83, 053104 (2012)

## O 10: Solid-liquid Interfaces I

Time: Monday 10:30–13:15 Location: WIL A317

O 10.1 Mon 10:30 WIL A317

**On the stability of strained Cu overlayers on Pt(1 1 1), Au(1 1 1) and Au(1 0 0) electrodes under low potential conditions and in presence of CO and CO$_2$** — •Christian Schlaup and Sebastian Horch — Center for Individual Nanoparticle Functionality (CINF), Department of Physics, Technical University of Denmark (DTU), DK–2800 Kongens Lyngby, Denmark

Copper is known for its outstanding catalytic activity for the electroreduction of carbon dioxide. However, a tremendous overpotential in the order of 1 V needs to be overcome in order to drive this reaction. An approach to tune the reactivity of copper surfaces is to introduce strain into the surface, yielding in different binding situations of the involved reaction species.

A convenient experimental access to such strained copper surfaces is the electrodeposition of pseudomorphic films on electrodes with a bigger lattice constant. Yet, their stability under the desired reaction conditions is of crucial importance. By means of in-situ STM, the influence of CO$_2$ and the important reaction intermediate CO has been studied under low potential conditions. For the Pt(1 1 1) substrate, a CO induced restructuring, driven by attractive Pt-CO bindings was found. In contrast, Au-CO bindings are much less attractive, however, for Au(1 1 1) the stability of Cu films is limited by desorption of coadsorbed anions at low potentials. For Au(1 0 0) neither effect was found, instead an surface alloy forms under the desired reaction conditions.

O 10.2 Mon 10:45 WIL A317

**Structural degradation of PtRu model electrodes during CO electrooxidation and its influence on the reaction characteristics** — •Albert K. Engstfeld, Jens Klein, Sylvain Brimaud, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

The stability of an (electro-)catalyst under reaction conditions is important for the proper understanding of the underlying (electro-) catalytic processes. In this work we present the structural modifications of a PtRu model electrode during the electrooxidation of CO and the resulting changes in the electrocatalytic behavior.

The electrodes are prepared by deposition of Pt ($\leq$ 1 ML) on Ru(0001) under ultra high vacuum (UHV) conditions, leading to Pt monolayer islands with different sizes and densities. Subsequent to the structural characterization by scanning tunneling microscopy (STM), the samples are transferred to a pre-chamber equipped with an electrochemical laminar flow cell. The electrochemical/-catalytic properties of the PtRu electrodes were characterized by base cyclic voltammetry in 0.5 M H$_2$SO$_4$ (potential range of 0 V to 0.9 V or 1.25 V) and by evaluating their activity for CO bulk electrooxidation. Subsequently, the samples were transferred back to the UHV to study modifications of the electrode surface structure by STM. After exposure to higher potentials the surface shows pronounced modifications of the Ru(0001) surface and small Pt islands, which influences the CO oxidation in a distinct way. Correlations between electrode structure / structure modification and reactivity will be discussed.

O 10.3 Mon 11:00 WIL A317

**Photoelectrochemical CO2 reduction on silicon electrodes functionalized with pyridine** — •Qi Li[1], Sebastian Lindner[1], Anton Tosolini[1], Katrin Bickel[1], Simon Filser[1], Konrad Schönleber[1], Ignaz Höhlein[2], Bernhard Rieger[2], Irene Grill[3], Regina Wyrwich[3], Joost Wintterlin[3], and Katharina Krischer[1] — [1]Nonequilibrium Chemical Physics, Physics Department, Technical University Munich, Germany — [2]WACKER-Lehrstuhl für Makromolekulare Chemie, Chemistry Department, Technical University Munich, Germany — [3]Chemistry Department, Ludwig-Maximilians-Universität Munich, Germany

Solar driven CO2 conversion to fuels or basic chemicals could provide an exciting new energy storage pathway. Attempts of creating such a photochemical solar cell have to deal with the large activation barrier of CO2 reduction which leads to low yields and efficiencies. Bocarsly et al. reported that in the presence of dissolved pyridine, CO2 can be electrochemically reduced to methanol at illuminated p-GaP electrodes at a comparably low overpotential [1]. We demonstrate that a functionalized p-Si electrode constitutes a promising interface for CO2 reduction. The interface consists of pyridine molecules which are immobilized via an electrografting process to the Si-surface. Modified electrodes have been characterized using electrochemical methods and XPS. Besides its protective attributes against surface oxidation, the pyridine layer on top of the p-Si electrode shows increased electrochemical reactivity towards CO2 reduction. [1] E. Barton, D. Rampulla, A. B. Bocarsly; J. Am. Chem. Soc., 2008, 130, 6342-6344

O 10.4 Mon 11:15 WIL A317

**Implicit solvation model for the first-principles description of methanol electro-oxidation on Pt electrodes** — •Sung Sakong and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

Within a conventional density functional theory (DFT) framework, the atomistic description of the electrochemical reactions in a direct methanol fuel cell often ignores the presence of the aqueous environment or the dispersion interactions between reaction intermediates and electrode that can be crucial for a realistic modeling. Recently, Arias has introduced a joint scheme to treat solute/solvent simultaneously with combining DFT calculations and an implicit solvent based on the polarizable continuum model [Modelling Simul. Mater. Sci. Eng. **21** (2013) 074005], which allows to assess electrochemical systems including the electrolyte within a first-principles approach.

Using the method, we address the electro-oxidation of methanol on Pt electrodes and compare it to the corresponding reaction steps at Pt in vacuum. Practically, we model the electrode as a Pt(111) surface and investigate the energetics of the reaction intermediates with and without implicit solution. Furthermore, we test the influence of an explicit water bilayer at the interface in addition to the implicit solution on the energetics. The contribution of dispersion interaction to the stability of reaction intermediates and the height of reaction barriers in both vacuum and an aqueous environment will also be addressed using a correction scheme suggested by Tkatchenko and Scheffler [Phys. Rev. Lett. **102** (2009) 073005].

O 10.5 Mon 11:30 WIL A317

**The structure of water at metal interfaces** — •Tanglaw Roman and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

The structure of water and adsorbed ions at the interface between a metal electrode and an electrolyte solution directly impacts the electrode potential, and vice versa [1]. Although water has been the subject of countless experimental and theoretical investigations, the details of its structure at electrochemical interfaces are still the subject of debate [2]. In this talk, we will discuss ab initio molecular dynamics investigations for interfaces involving Cu, Pt, and Ag. Water is introduced using different surface area densities through supercells that are unbiased to the formation of bilayers. Dispersion corrections are added to energies obtained using the RPBE functional which is necessary in order to obtain the correct wetting behavior of water [3].

[1] S. Schnur and A. Groß, New J. Phys. 11, 125003 (2009). [2] T. Roman and A. Groß, Catal. Today. 202, 183 (2013). [3] K. Tonigold and A. Groß, J. Comput. Chem. 33, 695 (2012).

O 10.6 Mon 11:45 WIL A317

**Development of a Neural Network Potential for Protonated Water Clusters** — •Suresh Kondati Natarajan, Tobias Morawietz, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr

Universität Bochum, D-44780 Bochum, Germany

Protonated water clusters are important model systems for the dissociation of water, proton transport and acids in aqueous solution. Many classical force fields are not applicable to the dissociation of water or proton transport due to their inability to describe the making and breaking of bonds. Recently, high-dimensional neural networks (NNs) [1-2] have been introduced as an efficient way to represent interatomic potentials based on electronic structure calculations. Here, we present a NN potential for protonated water clusters with up to eight water molecules. The results are discussed and compared to density functional theory data.

[1] J. Behler and M. Parrinello, Phys. Rev. Lett., vol. 98, p.146401, 2007.

[2] J. Behler, Phys. Chem. Chem. Phys., vol. 13, p.17930, 2011.

O 10.7 Mon 12:00 WIL A317

**The electrostatic double layer of Pt/water interfaces from first principles molecular dynamics.** — •Clotilde S. Cucinotta and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2, Ireland

The formation of the electrostatic double layer is the most basic phenomenon taking place at electrified interfaces. However, even in the relatively simple case of a Pt/water interface, none of the current theoretical approaches provides a realistic microscopic view of this double layer (DL), accounting for electronic, polarization and solvent reorganization effects. Here we provide for the first time a comprehensive description of the DL of a Pt-water interface, based on ab initio computations, including charge polarization effects at both sides of the interface, explicit solvent and its rearrangements upon changing the electrode polarization. This interface has been modeled with up to 1000 atoms. A simple, fully dissociated salt in solution has been explicitly included. Varying the relative number of cations and anions provides a way to control the charge on the electrode, controlling, in turn, the applied potential. The proposed approach allows to provide a detailed description of the structure of the Pt/water DL reproducing the localization of electric field and potential energy drop within a microscopic distance from the metal surface. An a posteriori calibration of the relation between charge and potential is performed, analyzing the potential energy profile vs. the distance from the electrode for any given charge, providing for the first time a realistic ab initio determination of the interface capacitance and the point of zero charge.

O 10.8 Mon 12:15 WIL A317

**Ab initio molecular dynamics approach to adsorption processes of water molecules on Pt surface** — •Maryam Naderian and Axel Gross — Institute of Theoretical Chemistry, University of Ulm, D-89069 Ulm, Germany

The processes involved in the interaction of water with surfaces play a very important role in the fields of electrochemistry and surface science. We perform ab initio molecular dynamics (AIMD) simulations to address the adsorption process of water molecules on Pt(111). The AIMD simulations are based on periodic density functional theory calculations using the RPBE funtional in connection with disperssion correction, as the correct wetting behavior of water on close-packed metal surfaces is reproduced by using the RPBE-D3 aproach [1]. Special attention is paid to the role of the internal degrees of freedom of the water molecules upon impinging on the Pt substrate, as temporary kinetic energy from the center-of-mass motion might be transferred into vibrations and rotations thus leading to a more efficient energy dissipation which is crucial for molecular adsorption [2]. Furthermore, the sticking probability will be presented as a function of initial kinetic energy of water and/or water coverage. Also the initial processes of the water network formation on metal surfaces shall be addressed based on AIMD trajectories.

[1] K. Tonigold and A. Groß, J. Comput. Chem. 33, 695-701 (2012) .
[2] A. Groß *et al*, Surf. Sci. 539, L542-L548 (2003).

O 10.9 Mon 12:30 WIL A317

**Copper (110) surface in thermodynamic equilibrium with water vapor - Entropy effect** — •Amirreza Baghbanpourasl[1], Kurt Hingerl[1], and Wolf Gero Schmidt[2] — [1]Johannes Kepler University Linz — [2]University of Paderborn

In this contribution we study the interaction of Cu(110) surface with water vapor in a wide range of environment conditions. Theoretical and experimental studies for determining the adsorption structures of water on Cu(110) surface, are mostly performed for/in UHV and low temperature condition. For extending the validity of the studies to higher pressure and temperature it is needed to include the thermodynamic properties of water in the environment and the effect of vibrations of adsorbed molecules in the calculation of free energy. We applied Density Functional Theory on a relatively large group of known structures of locally stable water/Hydroxyl on Cu(110) surface, as a starting point, to calculate different contributions to adsorption free energy, coming from electronic interaction, zero point and thermal vibrations. The study shows that vibrational effects are negligible on the phase diagram. The net effect of zero point and thermal vibrations is increasing the temperature of the phase transition (for each pressure) with about 20 K.

O 10.10 Mon 12:45 WIL A317

**First-principles study of the water structure on flat and stepped Pb surfaces** — •Xiaohang Lin and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

The geometric structure and electronic properties of single water layers on flat and stepped Pb surfaces have been addressed by periodic density functional theory (DFT) calculations. Pb is often used as an electrode material in electrochemical applications such as the electrochemical atomic-scale quantum conductance switch [1]. As a first step in the modeling of this switch, we had considered Pb deposition and diffusion processes on stepped Pb surfaces. As the next step, we study the interaction between water and and flat and stepped Pb substrates which is important for an understanding of the switching processes. Because of the large lattice constant, water layers on Pb surfaces exhibit completely different structures than, e.g., on transition metals such as Au, Ag and Pt [2, 3]. In order to understand the structure formation and the Pb-water interaction, the electronic structure of water layers on Pb surfaces, in particular on stepped surfaces, will be discussed.

[1] F.-Q. Xie *et al.*, Phys. Rev. Lett. **93**, 128303 (2004).
[2] X. Lin and A. Groß, Surf. Sci. **606**, 886 (2012).
[3] S. Schnur and A. Groß, New J. Phys. **11**, 125003 (2009).

O 10.11 Mon 13:00 WIL A317

**Insights on the Microscopic Mechanisms of Anisotropic Growth of Gold Nanorods from Molecular dynamics simulations** — •Santosh Meena and Marialore Sulpizi — Condensed Matter Theory, Institute of Physics, Johannes Gutenberg University, Staudingerweg 7, 55128 Mainz, Germany

Gold nanorods are normally prepared using seed-mediated growth technique, which require gold seeds, ascorbic acid and aqueous cetyltrimethylammonium bromide (CTAB) solution of HAuCL4. Crystal twinning of seeds results into formation of pentatetrahedral nanorod structure with different facets[1]. Although possible mechanism have been proposed, the microscopic understanding of the anisotropic growth is still missing. We provide the first atomistic model of adsorption of CTAB on different surfaces, namely (111), (110) and (100) in growing electrolyte solution. We find that on all the investigated surfaces, the CTAB form a layer of distorted cylindrical micelles where channels among micelles would provide direct ions access to the surface. In particular, we show how AuCl2- ions, can freely diffuse from the bulk solution to the gold surface[2]. Furthermore, we investigate the effect of halide ions (X= Cl- , Br- and I-) on adsorption of CTAX on the (111) surface and we provide a rational for the influence of halide ions on anisotropy of gold nanoparticles.

[1] C. J. Murphy, T. K. Sau, A. M. Gole, C. J. Orendorff, J. Gao, L. Gou, S. E. Hunyadi, T. Li, J. Phys. Chem. B 2005, 109, 13857-13870

[2] S. K. Meena, M. Sulpizi, Langmuir 2013, DOI: 10.1021/la403843n

# O 11: Nanostructures at Surfaces I

Time: Monday 10:30–13:15 Location: WIL C107

O 11.1 Mon 10:30 WIL C107

**Two Dimensional Square-like Bismuth Oxyiodine Nanosheets with High Efficient Visible-Light Driven Photocatalytic Activity** — •Yan Mi, Min Zhou, Liaoyong Wen, and Yong Lei — Ilmenau University of Technology, Institute of Physics & IMN MacroNano(ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau (Germany)

Two dimensional (2D) square-like bismuth oxyiodine (BiOI) nanosheets with thickness of about 10 nm and exposed {001} facets are obtained by a facile hydrothermal route without any surfactant and speical solvent. The photocatalytic performance of as-prepared 2D square-like BiOI nanosheets are evaluated by the photodegradation of rhodamine-B (RhB), methyl orange (MO) and phenol under visible-light irradiation. The products show highly efficient photocatalytic performance and good photostability and recyclability under the visible light irradiation. The efficient visible-light driven photocatalytic activity can be ascribed to the thin 2D square shape nanosheet with exposed {001} facet, which provides appropriate diffusion length and self-induced internal static electric fields direction of BiOI, improves the separation efficiency of photoinduced electron-hole pairs in BiOI nanosheets.

O 11.2 Mon 10:45 WIL C107

**Tandem nanostructure for solar water splitting** — •Stefan Bösemann, Liaoyong Wen, Fabian Grote, and Yang Xu — Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK), Prof. Schmidt-Str. 26, 98693 Ilmenau (Germany)

A promising solution to challenge the problems of renewable energies like absence of sufficient storage facilities and energy transportation is offered by water splitting. In order to separate water into hydrogen and oxygen, a theoretical energy of 1.23 eV is needed, which can be up to 1.6 - 2.4 eV considering overpotentials. Besides, the minimum of the conduction band of the active semiconductor has to be lower than the redox potential of H+/H2 and the maximum of the valance band has to be higher than the redox potential of O2/H2O. Furthermore, lights absorption and material stability in electrolytes are very important aspects in regarding to efficient solar water splitting. To fulfill these requirements with only one absorber, a semiconductor with a large bandgap is necessary and thus can only absorb a small fraction of the incident sunlight. Hence, it is essential for an efficient water splitting system to be constructed of more than one absorbing material with different bandgaps to utilize a larger fraction of the incoming light and generate O2 and H2 in a single device. We have developed a tandem structure consisting of two-sided ordered semiconductor nanorods by using anodic aluminum oxide (AAO) templates. The two-sided ordered tandem architecture enables not only the complete water splitting but also a large surface and consequently an increased light absorption and a high surface reaction area.

O 11.3 Mon 11:00 WIL C107

**Ab-initio simulations of copper-modified titania photocatalysts** — •Nicola Seriani — The Abdus Salam ICTP

Titania modified with transition or coinage metals has a great potential as a photocatalyst for the conversion of water and carbon dioxide into hydrocarbons. In particular, copper is interesting for its positive effect on the activity of the system. Still, it is not clear yet what the role of copper is in the overall mechanism, for the photoabsorption, for charge separation and for the chemical reactions taking place on the system. To shed light on these aspects, first-principles simulations based on density functional theory have been performed in three cases: copper doping in bulk titania, small copper clusters on titania surfaces and large particles on titania surfaces. The (101) and (100) surfaces of anatase were considered. Regardless whether copper is present in the bulk or at the surface of titania, its presence has an effect on the local atomic structure of the semiconductor, as well as on the electronic structure of the system. The presence of copper can lead to changes in the edges of valence and conduction bands, but also to the appearance of mid-gap states, depending on the atomic structure of the cluster and the coordination of the copper atoms. Finally, water dissociation has been investigated. These results give an insight over the role of copper in the photoabsorption and in the subsequent steps of the photocatalytic cycle.

O 11.4 Mon 11:15 WIL C107

**Large scale ordered binary nanopatterns via pre-patterned anodic aluminum oxide** — •Liaoyong Wen, Yan Mi, Chengliang Wang, Fabian Grote, Huaping Zhao, Min Zhou, and Yong Lei — Ilmenau University of Technology, Institute of Physics & IMN MacroNano* (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau Ilmenau, Ilmenau, Germany

Multicomponent nanopatterns, such as binary superlattices, consist of two or more kinds of materials or morphologically dissimilar nanocomponents. Unlike single component counterparts, multicomponent nanopatterns offer enormous diversities in the pattern shape, material composition and corresponding functionality. Nevertheless, there are very few simply lithographic techniques capable of constructing such nanopatterns in one single domain area. Nanoporous anodic aluminum oxide (AAO) has been intensively exploited as a template technique for the preparation of many kinds of nanostructures. However, the existing AAO only consist of single-sharp, monodisperse nanopores. Herein, we develop a novel selective etching approach to address this limitation and successfully generate ordered binary nanopores. The size of the binary nanopores is independently tunable without influencing the pattern periodicity and the well-established etching methods are scalable to arbitrary large area processing. More importantly, combing with other growth or deposition techniques, the ordered binary pores can act as a template to realizing different kind of ordered binary nanopatterns, such as binary nanowires, tubes or dots array.

O 11.5 Mon 11:30 WIL C107

**Structure and Self-assembly of Two-dimensional Manganese Gallium Quantum Height Islands and One-dimensional Atomic Chains on Wurtzite GaN (000$\bar{1}$)** — •Jeongihm Pak, Meng Shi, Andrada-Oana Mandru, Abhijit Chinchore, and Arthur Smith — Nanoscale and Quantum Phenomena Institute, Department of Physics and Astronomy, Ohio University, Athens, OH 45701 USA

We describe the spontaneous formation of five and six-monolayer quantum height manganese gallium islands and atomic chains on gallium-rich, nitrogen polar GaN(000$\bar{1}$). From ex-situ MOKE measurements at room temperature, we expect these MnGa islands to be ferromagnetic. The structural evolution is followed from the beginning of growth using reflection high energy electron diffraction, in which a dotted 2x pattern is observed to form. In-situ scanning tunneling microscopy is also used to investigate the islands* structures with atomic resolution. Based on all the observations, we propose possible bulk and surface models for the islands. A possible bonding structure at the substrate/island interface is also discussed in which Mn atoms substitute for Ga atoms within the Ga adlayer thus bonding with nitrogen, making the MnGa islands bonded directly to the last GaN bilayer. The atomic chain model on the six-layer island surface is also discussed. STM observations of atomic-chain interconnection on the six-layer island surface indicate a dynamic system at room temperature. The models presented here should serve as useful starting points for theoretical calculations.

O 11.6 Mon 11:45 WIL C107

**Tunable superradiance in porphyrin chains on insulating surfaces** — •Sebastiaan Vlaming and Alexander Eisfeld — Max Planck Institute for Physics of Complex Systems, Dresden, Germany

Recent experiments have shown that it is possible to synthesize collections of effective one-dimensional chains of non-covalently bound porphyrins on various surfaces.[1,2] We provide a study of the optical absorption properties of these systems, and we show that generally one expects the appearance of multiple superradiant transitions which can be both redshifted or blueshifted with respect to the monomer transitions. In addition, porphyrin chains can simultaneously support both redshifted and blueshifted features in the absorption spectrum. The energies, oscillator strengths and polarizations of the excitonic transitions can be understood in terms of Davydov splitting of chains with one transition per molecule. A distribution over chain lengths is proposed as a mechanism for the broadening of the superradiant transitions.

[1] S. Maier et al., Small 4, 115 (2008); Th. Glatzel et al., Isr. J. Chem. 48, 107 (2008). [2] C. Tröppner et al., Phys. Rev. B 86, 235407 (2012).

O 11.7 Mon 12:00 WIL C107

**Structure formation of lipophilic molecules on surfaces: a computational study** — •Pritam Kumar Jana and Andreas Heuer — Institute of Physical Chemistry, University of Muenster, Corrensstr. 28/30, Muenster, Germany

Understanding of STM images of different adsorbed molecules and the mechanism of structure formation is a very important aspect in the field of surface science due to its technological relevance. Here we are interested in the structure formation of lipophilic molecules, containing a nucleobase as the head group. Recently the group of Prof. Lifeng Chi has observed that N9-substituted adenine derivative in solution form two different types of structures (intercalation vs. stripe patterns) on the surface[1]. Repeating this experiment for vapor deposited molecules, an additional impact of deposition rate and substrate temperature on structure formation can be seen.

We present kinetic lattice Monte Carlo simulations where the molecules are represented in a minimum fashion, keeping the key properties of hydrogen bonding and van der Waals chain-chain interaction. Most model parameters can be taken from quantum-chemical calculations[1]. The quality of structure formation in dependence on flux and temperature as well as the relative fraction of both phases is analysed and compared with the experimental data.

[1] Z. Mu, O. Rubner, M. Bamler, T. Blömker, G. Kehr, G. Erker, A. Heuer, H. Fuchs, and L. Chi, Langmuir 29 (2013) 10737-10743.

O 11.8 Mon 12:15 WIL C107

**Electrostatic interaction between colloids trapped at an electrolyte interface** — •Arghya Majee, Markus Bier, and Siegfried Dietrich — Max Planck Institute IS and University of Stuttgart, Germany

Self-assembly of stably trapped colloidal particles at electrolyte interfaces has attracted much interest in recent years. For large separations between the charged particles, the repulsive part of the interaction can be compared to a dipole-dipole interaction. However for distances close to the particle this simple dipolar picture cannot be applied. In this contribution we will consider the case of colloids situated very close (˜50-100 nm) to each other at an electrolyte interface by going beyond the superposition approximation [1]. Within an appropriate model exact analytic expressions for the electrostatic potential as well as for the surface and line interaction energies are obtained. They demonstrate that the widely used superposition approximation, which is commonly applied to large distances between the colloidal particles, fails qualitatively at small distances and is quantitatively unreliable even at large distances. Our results contribute to an improved description of the interaction between colloidal particles trapped at fluid interfaces.

[1] "Electrostatic interaction between colloidal particles trapped at an electrolyte interface" by A. Majee, M. Bier, and S. Dietrich (submitted).

O 11.9 Mon 12:30 WIL C107

**Nanocomposites with functions of biomedical nanorobots** — •Ievgen Pylypchuk and Petro Gorbyk — Ukraine, Kyiv, Gen. Naumov str. 17

The modern level of nanotechnology permits creating unique means for medicine and biology. Their introduction into practice is the basis of the contemporary progress in diagnostics and therapy, in particular, at the cell and genetic levels. Researchers* interest in magnetosensitive biocompatible nanoparticles arises from the possibilities to control their motion in biological medium by external magnetic *eld, use for targeted drug delivery, form local hyperthermia zones, create new types of adsorbents, means for early diagnostics of diseases, etc.

Recent advances in cross-disciplinary nanoscience and nanotechnology have led to further and rapid developments of new *nanohybrids* as probes for molecular imaging, MRI, neutron capture therapy(NCT), targeted drug delivery, different kinds of therapy which are sensitive to pH, magnetic field, neutron irradiation etc. All of these parametres inherent to biomedical nanorobots.

Developed methods of immobilization of different bio-compounds on to surface of nanosized magnetite. Nanocomposites was characterized by vibrating sample magnetometry, IR-spectroscopy, X-ray diffraction and X-ray photoelectron spectroscopy etc.

O 11.10 Mon 12:45 WIL C107

**Large-scale Replication of Optical Nanostructures Inspired by Blue Morpho Butterflies** — •Claudia Zeiger, Norbert Schneider, Alexander Kolew, Marc Schneider, Radwanul H. Siddique, Hendrik Hölscher, and Matthias Worgull — Institute of Microstructure Technology (IMT), Karlsruhe Institute of Technology (KIT)

Morpho butterflies show an impressive iridescent blue color which does not originate from pigmentation but from sophisticated nanostructures. The "Christmas-tree-like" morphology of these structures has been investigated for a long time since numerous technical applications could benefit from the large-scale replication of Morpho-like structures, ranging from pigment-free colors to thermal imaging sensors and chemical sensors. However, the large-scale replication of sophisticated 3D micro- and nanostructures faces difficulties even today.

We developed a technology to overcome this problem and to fabricate such structures on large scales in a cost-effective way. Our unique combination of hot embossing and microthermoforming allows the easy implementation of other non-optical features like superhydrophobicity and self-cleaning as well. Hot embossing is applied to imprint nanostructures in a polymer foil which is subsequently shaped on the microscale by microthermoforming. This process enables the replication of structure sizes several orders of magnitude smaller than conventional thermoforming. We demonstrate the features of this technique by manufacturing optical structures inspired by Morpho butterflies as well as refractive gratings.

O 11.11 Mon 13:00 WIL C107

**Parallel Fabrication of User Defined Patterns Using Scanning Particle Lens Array** — •Wei Guo — Manufacturing Technology Research Laboratory, B38f Sackville Street Building, School of Mechanical Aerospace and Civil Engineering, The University of Manchester, Manchester, M13 9PL

Direct laser writing of parallel patterns over a large area is achieved by an efficient and low-cost technique using scanning particle lens array. With near-field enhancement created by particle lenses, a single laser beam can be split into millions of nano laser jets. By scanning the laser beam at various angles, user defined patterns such as lines, curves and even letters can be generated simultaneously. Up to 100 million periodic features with nano or sub-micro scale can be produced within tens of seconds over an area of 5 mm * 5 mm. In addition, overwriting same patterns on previous locations can be performed without any relocation or misalignment issues.

# O 12: Invited Talk (Achim Schöll)

Time: Monday 15:00–15:45 Location: TRE Phy

**Invited Talk** O 12.1 Mon 15:00 TRE Phy

**Uncovering Molecular Orbitals by ARPES** — •Achim Schöll — Experimentelle Physik VII, Universität Würzburg, 97074 Würzburg, Germany — Karlsruher Institut für Technologie (KIT), Gemeinschaftslabor für Nanoanalytik, 76021 Karlsruhe, Germany

Electrons are responsible for the structural, chemical and physical properties of materials. As one of the fundamental concepts of quantum mechanics, electrons in molecules are described by molecular orbitals. Consequently, visualizing these wave functions experimentally has been highly desired ever since quantum mechanics was established.

I will demonstrate how Angle Resolved Photoelectron Spectroscopy (ARPES) can provide unprecedented information on molecular orbitals by mapping the angle dependent intensity patterns of photoelectrons with a Photoelectron Emission Microscope (PEEM). The full potential of this tomographic technique becomes obvious by providing three-dimensional images of orbitals in real space. While this has already been proposed theoretically, I will demonstrate how 3D-imaging of molecular orbitals is feasible for the first time by momentum mapping with a PEEM and synchrotron radiation. This allows reconstruction of the molecular orbital in momentum space from the hemispherical k-space tomograms. The phase information, which is usually lost in the experiment but mandatory for the Fourier transformation of the orbital data into real space, can be derived from experiments with circular light polarization. In consequence, the full molecular orbital can be uncovered in 3D in real space, thus providing fascinating insight into the properties of electrons in molecules.

# O 13: Focus Session: New Trends in Molecular Magnetism (MA jointly with O, TT)

Organizers: J. Schnack (U. Bielefeld), O. Waldmann (U. Freiburg)

During the past 25 years molecular magnetism has developed into a broad field. Today's major research directions include applications in quantum computing or as quantum simulators as well as the use as sub-Kelvin magnetic refrigerants. For direct manipulation as part of spintronic systems molecules are deposited and manipulated on surfaces. The progress of this interdisciplinary field is intimately related to the ability of coordination chemists to synthesize unprecedented molecules, to the ability of experimental physicists to characterize them as well as to the ability of theorists to model their properties.

Time: Monday 15:00–17:30 Location: HSZ 04

**Topical Talk** O 13.1 Mon 15:00 HSZ 04

**Spin dynamics in Molecular Nanomagnets** — •Stefano Carretta — Dipartimento di Fisica e Scienze della Terra, Universita' di Parma, I-43124 Parma, Italy

Molecular nanomagnets (MNMs) have been test beds for addressing several quantum phenomena. In particular, one of the major current objectives is to exploit their coherent spin dynamics for quantum information processing (QIP). We show that recently developed instrumentation yields the four-dimensional inelastic-neutron scattering function and enables the direct determination of the spin dynamics [1]. We use the Cr8 antiferromagnetic ring as a benchmark to demonstrate the potential of this approach, which allows us, for instance, to examine how quantum fluctuations propagate along the ring. We show that parameters of the spin Hamiltonian can be reliably calculated ab-initio. In particular, we present a flexible and effective ab-initio scheme to build many-body models for MNMs, and to calculate magnetic exchange couplings and zero-field splittings [2]. We have applied this scheme to three paradigmatic systems, the antiferromagnetic rings Cr8 and Cr7Ni and the single molecule magnet Fe4 and have found excellent agreement with experimental results. At last, we discuss the dynamics of ensembles of spin systems coherently coupled to microwave photons in coplanar waveguide resonators. We introduce a scheme to perform QIP that is based on a hybrid spin-photon qubit encoding [3].

[1] M. Baker et al, Nature Physics 8, 906 (2012); [2] A. Chiesa et al, Phys. Rev. Lett. 110, 157204 (2013); [3] S. Carretta, et al, Phys. Rev. Lett. 111, 110501 (2013).

**Topical Talk** O 13.2 Mon 15:30 HSZ 04

**Exchange interaction in lanthanides** — •Liviu Chibotaru, Liviu Ungur, Naoya Iwahara, and Veaceslav Vieru — Theory of Nanomaterials Group, KU Leuven, Heverlee, Belgium

Using ab initio, DFT and model calculations we analyze the main features of exchange interactions in lanthanide complexes.

Andersons superexchange model is applied for analytical derivation of exchange interaction between total magnetic moments $\mathbf{J}_1$ and $\mathbf{J}_2$ corresponding to ground atomic multiplets of two exchange-coupled lanthanide ions. Despite the common belief that the exchange interaction is of $\sim \mathbf{J}_1 \cdot \mathbf{J}_2$ form, we find it strongly anisotropic. If the crystal field (CF) on Ln sites exceeds significantly the exchange splitting, the exchange interaction between low-lying CF doublet states generally becomes of non-collinear Ising type.

In the case of exchange-coupled lanthanide ion ($\mathbf{J}$) and isotropic magnetic center ($\mathbf{S}$) the exchange interaction is found not to be of the form $\sim \mathbf{J} \cdot \mathbf{S}$, as supposed before, but again very anisotropic. When the CF splitting on Ln exceeds the exchange splitting, the exchange interaction between the low-lying CF doublet on Ln and the isotropic spin generally becomes of collinear Ising type.

Finally, we give arguments why the mixed Ln-TM complexes are more efficient SMMs than pure Ln ones despite less anisotropic magnetic ions involved.

**Topical Talk** O 13.3 Mon 16:00 HSZ 04

**Cool molecules** — •Marco Evangelisti — Instituto de Ciencia de Materiales de Aragón, CSIC - Universidad de Zaragoza, Departamento de Física de la Materia Condensada, 50009 Zaragoza, Spain

The recent progress in molecule-based magnetic materials exhibiting a large magnetocaloric effect at liquid-helium temperatures is reviewed. Advanced applications and future perspectives in cryogenic magnetic refrigeration are also discussed.

**Topical Talk** O 13.4 Mon 16:30 HSZ 04

**Bulk and submonolayer studies of novel single-ion molecular magnets** — •Jan Dreiser — Ecole Polytechnique Federale de Lausanne, Institute of Condensed Matter Physics, 1015 Lausanne, Switzerland — Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Single-ion magnets (SIMs) [1,2] contain a single transition-metal or rare-earth ion embedded in an organic ligand. In contrast to many other mononuclear molecular magnets, SIMs exhibit long magnetization relaxation times at low temperatures ranging from milliseconds to more than hours. In order to exploit their properties in possible applications they should be organized and addressable one-by-one [3]. A promising path to achieve this goal is the deposition of submonolayers of SIMs on to surfaces.

In this talk I will report on our recent studies of the Er(trensal) SIM [2] in which the Er(III) ion is seven-fold coordinated to the very robust tripodal ligand. In addition to the investigations of the bulk phase I will present first results obtained on (sub)monolayer deposits on metallic surfaces using X-ray magnetic circular dichroism and scanning tunneling microscopy.

[1] N. Ishikawa, M. Sugita, T. Ishikawa, S.-y. Koshihara, Y. Kaizu, J. Am. Chem. Soc. 2003, 125, 8694; [2] K. S. Pedersen, L. Ungur, M. Sigrist, A. Sundt, M. Schau-Magnussen, V. Vieru, H. Mutka, S. Rols, H. Weihe, O. Waldmann, L. F. Chibotaru, J. Bendix, J. Dreiser,

submitted; [3] D. Gatteschi, A. Cornia, M. Mannini, R. Sessoli, Inorg. Chem. 2009, 48, 3408.

**Topical Talk** O 13.5 Mon 17:00 HSZ 04

**When Organic Materials Interact with Ferromagnetic Surfaces: A First-Principles Perspective** — •Nicolae Atodiresei — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The adsorption of $\pi$-conjugated organic materials on ferromagnetic surfaces offers the possibility to merge the concepts of molecular electronics with spintronics to build future nanoscale data storage, sensing and computing multifunctional devices. Based on the density functional theory, we performed theoretical studies to understand how to tailor the magnetic properties of organic-ferromagnetic interfaces. For such hybrid systems, the magnetic properties like molecular magnetic moments and their spatial orientation, the spin-polarization and the magnetic exchange coupling can be specifically tuned by an appropriate choice of the organic material and ferromagnetic surface. [1] N. Atodiresei et al., Phys. Rev. Lett. 105, 066601 (2010); [2] N. Atodiresei et al., Phys. Rev. B 84, 172402 (2011); [3] K. V. Raman et al., Nature 493, 509 (2013); [4] M. Callsen et al., Phys. Rev. Lett. 111, 106805 (2013).

## O 14: Organic/bio Molecules on Metal Surfaces II

Time: Monday 16:00–19:00 Location: TRE Phy

O 14.1 Mon 16:00 TRE Phy

**Adsorption behavior of porphycenes on a Cu(111) surface: A scanning tunneling microscopy study** — •Michael Stark, Stefanie Ditze, Michael Lepper, Johannes Träg, Liang Zhang, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The knowledge of the adsorption behavior of large organic molecules, like porphyrin derivatives, on surfaces is a prerequisite to engineer their supramolecular architecture and to finally utilize their functional properties. Herein, we expand the surface science studies of porphyrins to their constitutional isomers, the so-called porphycenes. We investigate 2H-2,7,12,17-tetraphenylporphycene (2HTPPc) and 2H-2,7,12,17-tetrakis-(4-tert-butyl)-phenylporphycene (2HTTBPPc) on Cu(111) with scanning tunneling microscopy (STM) under ultra-high vacuum (UHV) conditions. Thereby, we found a dominant registry of the porphycene core with the substrate, regardless of its peripheral substituents and the actual supramolecular structures formed. Different supramolecular structures were identified depending on the peripheral substituents of the porphycenes. A particular interesting behavior is observed for 2HTPPc which assembles in highly ordered rows separated by rather loosely arranged molecular rows. In the latter we also observe occasional rotation of individual molecules at room temperature. The results will be presented and discussed addressing the role of specific molecule-molecule interactions.

O 14.2 Mon 16:15 TRE Phy

**Interplay of hydrogen bonding and molecule-substrate interaction in self-assembled adlayer structures of tetra($p$-hydroxyphenyl)porphyrin on Ag(110)** — •Lars Smykalla[1], Pavel Shukrynau[1], Michael Hietschold[1], Carola Mende[2], and Heinrich Lang[2] — [1]Technische Universität Chemnitz, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany — [2]Technische Universität Chemnitz, Institute of Chemistry, Inorganic Chemistry, D-09107 Chemnitz, Germany

The construction of desired molecular architectures on surfaces can be achieved by the self-assembly of molecular building blocks. The arrangement of adsorbed molecules is mainly controlled by a complex interplay between intermolecular interactions, such as hydrogen bonds, dispersion and electrostatic interactions, and the molecule-substrate interaction, that is the adsorption on favourable positions on the substrate lattice. We report on the adsorption and self-organisation of 5,10,15,20-tetra($p$-hydroxyphenyl)porphyrin molecules on the highly anisotropic Ag(110) surface. One-dimensional molecular chains as well as three molecular structures with large unit cells, each containing a different number of molecules, were observed using scanning tunnelling microscopy. The molecules in the arrangements form hydrogen bonds and, additionally, show $\pi$-$\pi$ stacking of phenyl-groups. The difference between the unit cells is the number of hydrogen bonds per molecule and correspondingly a different epitaxy. Density Functional Theory calculations are presented to explain the complex adsorption and epitaxial behaviour of these molecules on Ag(110) in detail.

O 14.3 Mon 16:30 TRE Phy

**Fabrication of chemical templates for the selective adsorption of functional molecules by Focused Electron Beam Induced Processing** — •Martin Drost, Fan Tu, Esther Carrasco, Florian Vollnhals, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The fabrication of well-defined nanostructures is usually realized by choosing one of the two main methods: the bottom-up approach, e.g. the self-assembly of supramolecular structures on surfaces, and top-down methods like electron beam lithography. We target at combining both methods such that local surface modifications by focused electron beam induced processing (FEBIP) act as a template for the adsorption of functional molecules, here 2H-Tetraphenylporphyrin (2HTPP). First, the adsorption behavior of 2HTPP on metal surfaces like Cu(111) and Rh(110) with and without adsorbed oxygen was studied. Second, the feasibility of locally altering the surface by FEBIP, e.g. by local electron induced oxygen desorption for the directed adsorption of 2HTPP, was investigated by a combination of Scanning Electron Microscopy (SEM), Auger Electron Spectroscopy (AES) and Scanning Tunneling Microscopy (STM). Latest results will be presented and discussed.

This work was supported by the DFG via grant MA 4246/1-2 and MA 4246/2-1.

O 14.4 Mon 16:45 TRE Phy

**Adsorption geometry and intramolecular conformation of Ni(II)-tetraphenyl-benzoporphyrin on Cu(111)** — •Liang Zhang, Michael Lepper, Michael Stark, Stefanie Ditze, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für PhysikalischeChemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

Self-assembly of molecular building blocks on well-defined surfaces by supramolecular coordination provides a promising approach for the bottom-up fabrication of two-dimensional nanostructures with outstanding properties. In this respect, porphyrins are particularly attractive because of their distinct chemical and physical properties.

In this presentation, we expand our scanning tunneling microscopy studies to the adsorption of Ni(II)-tetraphenyl-benzoporphyrin (NiTPBP) on Cu(111) under ultra-high vacuum (UHV) conditions, mainly at room temperature (RT). NiTPBP shows a peculiar interesting adsorption behavior with coexisting domains of different supramolecular structure and individual molecules exhibiting deviant orientation within a particular supramolecular arrangement. The observed supramolecular assemblies, the corresponding intermolecular interactions and the dynamic behavior of the molecules will be discussed in detail.

O 14.5 Mon 17:00 TRE Phy

**Controlling intramolecular hydrogen transfer** — •Takashi Kumagai[1], Felix Hanke[2], Sylwester Gawinkowski[3], John Sharp[2], Konstantinos Kotsis[2], Jacek Walik[3], Mats Persson[2,4], and Leonhard Grill[1,5] — [1]Fritz-Haber Institute, Berlin, Germany — [2]University of Liverpool, Liverpool, UK — [3]Polish Academy of Science, Warsaw, Poland — [4]Chalmers University of Technology, Göteborg, Sweden — [5]University of Graz, Graz, Austria

Although the local environment of a molecule can play an important role in its chemistry, rarely has it been examined experimentally at the level of individual molecules. We report the precise control of intramolecular hydrogen transfer reactions (i.e. tautomerization) in single porphycene molecules using low-temperature scanning tunneling microscopy (STM) [1]. Single porphycene molecules adsorbed on a Cu(110) surface were imaged by STM at 5 K and found to have only cis configuration in which the inner H-atoms located on the one side in the cavity. The cis-cis tautomerization is induced either by STM via inelastic electron tunneling process at 5 K or thermal activation at elevated temperatures. We found that the tautomerization can be precisely tuned up and down by placing a Cu adatom nearby a molecule. The adatom is controlled using the STM manipulation.

[1] T. Kumagai et al. Nature Chemistry, accepted.

O 14.6 Mon 17:15 TRE Phy

**Copper Phthalocyanine Monolayers and Multilayers on Ag(110) and Ag(111) surfaces** — •Kathrin Schönauer[1,2], Martin Willenbockel[1,2], Benjamin Stadtmüller[1,2], Christian Kumpf[1,2], Sergey Soubatch[1,2], and Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technology, Germany

Organic semiconductors and their potential for applications in electronic devices such as solar cells and organic light emitting diodes make them interesting for fundamental research. Especially interfaces between different organic layers, e.g. PTCDA and CuPc, are subjects of experiments. To create a basis for the understanding of heteroorganic systems, the corresponding homomolecular phases are investigated regarding their geometric and electronic structure upon adsorption on a metal surface. While homomolecular phases of PTCDA on different noble metal surfaces are well-studied, less is known about adsorption and ordering of CuPc. Here we present a combined study employing (SPA)LEED, STM, STS and ARUPS to CuPc monolayers and multilayers adsorbed on the Ag(110) and Ag(111) surfaces.

O 14.7 Mon 17:30 TRE Phy

**Charged adsorbates among each other: Simulating intermolecular interactions of free-base porphine on coinage metal surfaces** — •Moritz Müller, Reinhard J. Maurer, Katharina Diller, and Karsten Reuter — Technische Universität München

Designed through the process of evolution, porphine naturally serves as a basic unit in hemeproteins and chlorophyll. Functionality and robustness of these compounds suggest potential applications tackling photovoltaics, nano-catalysis, data storage, and drug design. Many technical realizations require controllable surface engineered coating of ordered molecular films on two-dimensional boundaries. Adsorbed to coinage metal surfaces, porphine overlayers exhibit a variety of different superstructures [1], depending on the coverage. We report modeling of free-base porphine on clean Ag(111) and Cu(111) surfaces in the framework of dispersion-corrected semi-local Density Functional Theory. The lateral interactions determining the overlayer structure can be expressed as two competing forces: attractive van-der-Waals interactions and repulsive electrostatic interactions between the charge-transfer-induced adsorbate dipoles. Our investigations of the adsorption geometries and the electronic structure display, in agreement with experiment, a substantial amount of charge-transfer to the molecule upon adsorption. Based on our *ab-initio* calculations a simple interaction model is introduced and corresponding conclusions are drawn towards the coverage-dependent supermolecular arrangement and the effects of adsorbate functionalization.

[1] F. Bischoff *et al.*, ACS Nano, **7**, 3139 (2013)

O 14.8 Mon 17:45 TRE Phy

**Chiral Conflict among Different Helicenes Suppresses Formation of One Enantiomorph in 2D Crystallization** — •Johannes Seibel[1], Oliver Allemann[2], Jay S. Siegel[2], and Karl-Heinz Ernst[1,2] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland — [2]Department of Chemistry, University of Zürich, 8057 Zürich, Switzerland

Intermolecular chiral recognition plays a key role in the spontaneous resolution of enantiomers in crystallization or diastereomeric salt crystallization, a common technique for enantiomer separation in industry. Diastereomeric interactions in 2D crystals formed at solid surfaces serve as excellent models to study the underlying molecular recognition processes, where scanning tunneling microscopy provides submolecular resolution. The adsorption of a [5,6,9,10]-dibenzopentahelicene (db[5]H) racemate on Au(111) leads to 2D conglomerate formation, i. e. homochiral mirror domains containing only one enantiomer are observed, which is in contrast to previous results obtained for [7]H on Cu(111). Upon mixing M-[7]H into the monolayer, the balance between the mirror domains shifts gradually, until only the P-db[5]H enantiomorph is left in a monolayer containing 26% M-[7]H. This is explained by a preferred diastereomeric interaction between different helicene species of opposite handedness, suppressing the formation of the pure P-db[5]H enantiomorph by capturing P-db[5]H in non-ordered areas. These results show that dispersive forces can act in a manner comparable to polar forces in chiral discrimination at surfaces.

O 14.9 Mon 18:00 TRE Phy

**Effect of crystal packing on the electronic properties of free base porphyrins** — •Margherita Marsili[1], Paolo Umari[1], Andrea Goldoni[2], and Maddalena Pedio[3] — [1]Dipartimento di Fisica - Università di Padova- 35131 Padova Italy — [2]Sincrotrone Trieste, Area Science Park, 34149 Basovizza, Trieste Italy — [3]IOM-CNR, TASC Area Science Park Buil., 34149 Basovizza, Trieste, Italy

Porphyrins, a group of organic aromatic molecules, are involved in important biological processes such as oxygen transfer in red blood cells, or light harvesting in plants. Similar functions can be exploited in artificial devices, therefore the understanding and control of their electronic properties is of great interest.

In this work we present the combined theoretical and experimental study of metal free H2OEP and H2TPP, addressing the electronic properties from single molecule to molecular solids. Thin films have been investigated combining valence band photoemission, inverse photoemission spectroscopy and XAS, and the results compared with isolated molecule gas phase spectra and state-of-the-art GW calculations.

O 14.10 Mon 18:15 TRE Phy

**From Benzenetrithiolate Self-Assembly to Copper-Sulfide Adlayers on Cu(111): Temperature-Induced Irreversible and Reversible Phase Transitions** — Thomas Sirtl[1,2], •Matthias Lischka[1,2], Atena Rastgoo-Lahrood[1,2], Johanna Eichhorn[1,2], Thomas Strunskus[3], Wolfgang M. Heckl[1,2,4], and Markus Lackinger[1,2,4] — [1]Department of Physics, Technische Universität München, James-Franck-Str. 1, 85748 Garching — [2]Center for NanoScience (CeNS), Schellingstr. 4, 80799 Munich — [3]Institute for Materials Science - Multicomponent Materials, Christian-Albrechts-Universität zu Kiel, Kaiserstr. 2, 24143 Kiel — [4]Deutsches Museum, Museumsinsel 1, 80538 Munich (all Germany)

Self-assembly and thermally activated surface chemistry of 1,3,5-benzenetrithiol on Cu(111) are studied under ultrahigh vacuum conditions. Low energy electron diffraction patterns acquired at room temperature and during subsequent heating reveal irreversible and reversible phase transitions between in total four different long-range ordered phases. X-ray photoelectron spectroscopy of the different phases facilitates to identify major chemical changes for the phase transitions. The structural characterization of each phase is carried out by high resolution scanning tunneling microscopy and adsorption geometries of the phenyl rings are derived from C 1s near edge x-ray absorption fine structure. Combination of the results from this array of experimental techniques leads to a consistent picture from benzene thiolate monolayer to copper sulfide superstructures and underlying processes.

O 14.11 Mon 18:30 TRE Phy

**Structural phase dynamics and intermolecular coupling studied by energy-dispersive NEXAFS** — •Markus Scholz[1,2,3], Christoph Sauer[1,2], Michael Wiessner[1,2], Than-Nam Nguyen[1,2], Achim Schöll[1,2], and Friedrich Reinert[1,2] — [1]Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg — [2]Karlsruher Institut für Technologie (KIT), Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe — [3]Present address: Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg

We study the formation of a 3D geometric structure in molecular films, which emerges from an initially amorphous layer by the means of energy-dispersive near edge x-ray absorption fine-structure spectroscopy. This novel technique allows NEXAFS experiments with full spectroscopic information on the time scale of seconds. On the example of NTCDA multilayer films, we identify several sub-processes involved in the structure formation and quantify thermodynamic parameters [1]. In a particular transient phase, which exists only for several minutes during the structure formation, we observe peculiar changes of the line shape and energy position of the C K-NEXAFS signal with respect to the bulk and gas phase spectra. By a comparison to a theoretical model based on a coupling of transition dipoles, which is established for optical absorption, we demonstrate that the observed spectroscopic differences can be explained by an intermolecular delocalized core hole-electron pair [2]. [1] M. Scholz et al, New J. Phys. 15, 083052 (2013). [2] M. Scholz et al, Phys. Rev. Lett. 111, 048102 (2013).

O 14.12 Mon 18:45 TRE Phy

**Self-assembly of de-novo synthesized functionalized pyrenes on coinage metal surfaces** — •Tobias Kaposi[1], Sushobhan Joshi[1], Tobias Hoh[1], Alissa Wiengarten[1], Tomas Marangoni[2], Davide Bonifazi[2,3], Knud Seufert[1], David Écija Fernández[1], Willi Auwärter[1], and Johannes V. Barth[1] — [1]Physik Department E20, Technische Universität München, Garching, Germany — [2]Dipartimento di Scienze Chimiche e Farmaceutiche and UdR INSTM, Università di Trieste, Trieste, Italy — [3]Department of Chemistry and Namur Research College, University of Namur, Namur, Belgium

Supramolecular architectures on metallic surfaces provide multiple prospects for the engineering of novel nanostructured materials. Of particular interest are building blocks with inherent functional properties, such as single molecule magnets or photoactive groups.

Here we report a scanning tunneling microscopy study on the self-assembly of a family of pyridil- and phenyl-functionalized pyrenes, including an optically active backbone molecule already used in commercial dyes, on Ag(111) and Cu(111). By systematically changing the molecular functionalization and symmetry, different supramolecular synthons are expressed. Phenyl-substituents result in a uniform pyrene distribution on the surface, whereas pyridil-terminations drive the formation of different regular 2D networks, that may surprisingly include metal-organic binding motifs engaging Ag adatoms. The electronic features of these systems were probed by scanning tunneling spectroscopy.

## O 15: Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale II

Time: Monday 16:00–18:45 Location: TRE Ma

**Topical Talk** O 15.1 Mon 16:00 TRE Ma

**Simulating heat transport: from large scale molecular dynamics to first-principles calculations** — •Davide Donadio — Max Planck Institute for Polymer Research, Mainz, Germany

The necessity to design materials and devices able to harness thermal energy, and possibly convert it into more amenable energy forms, has stimulated a major effort in the scientific community to understand heat transport at the mesoscale and the nanoscale. In this talk I will discuss different atomistic approaches to simulate nanoscale heat transport, ranging from large scale molecular dynamics simulations with classical empirical potentials at equilibrium and non-equilibrium conditions, to lattice dynamics calculations with force-constants computed by first principles. Applications will include silicon and carbon nanostructures, phase-change materials and molecular junctions.

O 15.2 Mon 16:30 TRE Ma

**First principles study of thermal conductivity cross-over in nano-structured Zinc-Chalcogenides** — •Ankita Katre[1], Atsushi Togo[2], Ralf Drautz[1], and Georg K. H. Madsen[1] — [1]ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]ESISM, Kyoto University, Sakyo, Kyoto 606-8501, Japan

Nano-structured Zinc-Chalcogenides are interesting for thermoelectric applications due to their low thermal conductivity.[1] A simple model study has reported how the thermal conductivity of ZnS, ZnSe and ZnTe can potentially show a cross-over as a function of the maximal mean free path of the phonons.[2] We have applied the Boltzmann transport equation in the relaxation time approximation to verify this. We find that thermal conductivity of ZnS crosses ZnSe and ZnTe and explain this in terms of the different contributions of phonon modes in these materials. Furthermore, the cross-over is found to be strongly influenced by isotope scattering. The calculated thermal conductivity is found to be strongly dependent on the volume and we explain the observed differences between LDA and GGA calculations. We compare further calculated thermal properties, such as the thermal expansion coefficient, to experiment to validate our approach.

[1] L.Zhen, S.Qiao, D.Y.Xiang, H.Z.Zhong, and Q.L.Gao, J. Mater. Chem. 22, 22821 (2012). [2] N.Mingo and D.Broido, Phys. Rev. Lett. 93, 246106 (2004).

O 15.3 Mon 16:45 TRE Ma

**Density-functional perturbation theory for lattice dynamics with numeric atom-centered orbitals** — •Honghui Shang, Christian Carbogno, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin

The response of the electronic structure to atomic displacements gives rise to a variety of interesting physical phenomena, which can be probed by experimental techniques such as infrared or Raman spectroscopy or neutron diffraction. The response can be conveniently computed from first principles by means of density-functional perturbation theory (DFPT). Here we present our implementation in the all-electron atom-centered numeric orbital code FHI-aims [1]. Our approach combines the accuracy of an all-electron full-potential treatment with the computationally efficiency of localised atom-centered basis sets that is necessary to study large and complex systems. We verified the accuracy of our DFPT implementation by comparing the vibrational frequencies to finite-difference reference calculations and literature values. Due to the atom-centered nature of the integration grids in FHI-aims, the portion of the grid that belongs to a certain atom also moves when this atom is displaced. Here we demonstrate that, unlike for first derivatives (i.e. forces) [2], this moving-grid-effect plays an important role for second derivatives (i.e. vibrational frequencies). Further analysis reveals that predominantly diagonal force constant terms are affected, which can be bypassed efficiently by invoking translational symmetry.

[1] V. Blum et al. Comp. Phys. Comm. 180, 2175 (2009)

[2] B. Delley, J. Chem. Phys. 94, 7245 (1991).

O 15.4 Mon 17:00 TRE Ma

**Breakdown of Fourier law in layered materials** — •Andrea Cepellotti[1], Giorgia Fugallo[2], Francesco Mauri[3], and Nicola Marzari[1] — [1]THEOS, École Polytechnique Fédérale, Lausanne — [2]IMPMC, Universite Pierre et Marie Curie, Paris — [3]LSI, École Polytechnique, Paris

We compute the thermal conductivity in crystalline layered materials by solving the Boltzmann Transport Equation (BTE) for phonons [1], with the phonon-phonon collision rates obtained from density-functional perturbation theory. We find that in 2D materials, such as graphene and related compounds, and even in 3D layered materials, like bulk graphite, the single-mode relaxation time approximation (SMRTA) cannot describe heat transport correctly, underestimating by one order of magnitude or more thermal conductivities and phonons' mean free paths. Instead, we show that the exact self-consistent solution of the BTE provides results in excellent agreement with experimental measurements [2]. The shortcomings of the SMRTA lie in the assumption that heat flow is transferred only by individual phonon excitations, whereas in layered materials the transport can only be explained in terms of collective phonon excitations. The characteristic length of these collective excitations is often comparable with that of the experimental sample - as a result, Fourier's law become questionable, since its statistical nature makes it applicable only to systems larger than a few mean free paths.

[1] G. Fugallo et al., Phys. Rev. B, **88**, 045430 (2013).

[2] A. A. Balandin, Nat. Mater. **10**, 569 (2011).

O 15.5 Mon 17:15 TRE Ma

**High Temperature Thermal Conductivity from First Principles** — •Christian Carbogno[1], Rampi Ramprasad[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Chemical, Materials & Biomolecular Engineering, University of Connecticut, Storrs, USA

In spite of significant research efforts, a first principles determination of the thermal conductivity at high temperatures has remained elusive. Under such conditions, Boltzmann transport techniques [1] that include anharmonic effects only perturbatively become inaccurate or even inapplicable. In this work, we overcome this limitation by performing first-principles Green-Kubo simulations [2], in which all orders

of anharmonicity are incorporated by the means of *ab initio* molecular dynamics. The thermal conductivity is then assessed from the autocorrelation function of the heat flux in thermodynamic equilibrium. We discuss the details of our implementation and the definition of our heat flux that is based on the virial theorem. We validate our approach by presenting calculations for $ZrO_2$ that also showcase the importance of higher order anharmonic effects in materials with low thermal conductivities. Eventually, we discuss how our technique can be coupled to multi-scale models to achieve a computationally efficient and accurate description of the thermal conductivity at the nanoscale.
[1] D. A. Broido *et al.*, *Appl. Phys. Lett.* **91**, 231922 (2007).
[2] R. Kubo, M. Yokota, S. Nakajima, *J. Phys. Soc. Jpn.* **12**, 1203 (1957).

O 15.6 Mon 17:30 TRE Ma

**Accurate Modelling of the Polymorphism and Elastic Response of Molecular Materials from First Principles** — •Anthony Reilly and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Molecular materials are of great fundamental and applied importance in science and industry, with numerous applications in pharmaceuticals, electronics, sensing, and catalysis. A key challenge for theory has been the prediction of their stability, polymorphism and response to perturbations. While pairwise models of van der Waals (vdW) interactions have improved the ability of density functional theory (DFT) to model these systems, quantitative and even qualitative failures often remain. Here, we show how a many-body description of vdW interactions can dramatically improve the accuracy of DFT for molecular materials, yielding quantitative description of stabilities and polymorphism for these challenging systems. Moreover, the role of many-body vdW interactions goes beyond stabilities to response properties. In particular, we have studied the elastic properties of a series of molecular crystals, finding that many-body vdW interactions can account for up to 30% of the elastic response, leading to quantitative and qualitative changes in elastic behavior. We will illustrate these crucial effects with the challenging case of the polymorphs of aspirin, leading to a better understanding of the conflicting experimental and theoretical studies of this system.

O 15.7 Mon 17:45 TRE Ma

**Surface chemistry on nanostructured oxides: do we have to go beyond hybrid DFT?** — •Daniel Berger, Harald Oberhofer, and Karsten Reuter — Technische Universität München, Germany

Nanostructured oxide surfaces are promising candidates for a wide range of energy and catalysis applications. For first-principles modeling of corresponding surface chemical reactions the current state-of-the-art is generally defined by hybrid-level density-functional theory (DFT). Systematic work assessing the achieved accuracy at this level is nevertheless scarce, also owing to the fact that higher-level reference methods are often not available for standard periodic boundary condition supercell calculations. To this end, we present a study benchmarking semi-local and hybrid DFT against (renormalized) second-order perturbation theory (MP2,rPT2) as recently implemented in the FHI-aims package [1]. We make the efficient usage of the latter theories for oxide surfaces possible through a solid-state embedding framework, in which a central cluster region is described quantum mechanically, the long-range electrostatic interactions in the oxide are accounted for through a polarizable monopole field, and a shell of norm-conserving pseudopotentials correctly connects the two regions. We illustrate the performance of the various levels of theories using the water-splitting reaction at ideal and defected $TiO_2(110)$ surfaces as showcase. [1] X. Ren *et al.*, Phys. Rev. B **88**, 035120 (2013)

O 15.8 Mon 18:00 TRE Ma

**Atoms-in-solids perspective on polarizabilities and van der Waals coefficients in semiconductors** — •Guo-Xu Zhang, Anthony M. Reilly, Alexandre Tkatchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

The calculation of response properties of solids including their polarizabilities and van der Waals (vdW) coefficients usually requires the knowledge of the full electronic bandstructure. For non-covalently bound solids, such as noble-gas and ionic crystals, atoms-in-solids model can be successfully utilized to define their polarizabilities. Here we critically assess the atoms-in-solids model for covalently-bound solids, ranging from wide-gap (10 eV) to narrow-gap (below 1 eV) semiconductors. We model their response by assigning a single quantum harmonic oscillator to every atom, where the parameters of the oscillators are defined as functionals of the electron density, following the Tkatchenko-Scheffler method [1]. The response function is then calculated by solving self-consistent screening equations of classical electrodynamics, without any explicit information about the electronic bandstructure [2]. The calculated polarizabilities and vdW coefficients for 23 semiconductors are compared with TDDFT and experimental benchmark data, revealing an overall agreement within 10%. The efficiency of our method and the accuracy of the calculated vdW parameters allows us to demonstrate the crucial role of vdW interactions in the cohesive properties of the 23 semiconductors. [1] Tkatchenko and Scheffler, PRL (2009); [2] Tkatchenko, DiStasio, Car, Scheffler, PRL (2012).

O 15.9 Mon 18:15 TRE Ma

**Adsorption at semiconductor surfaces - an energy analysis method** — •Ralf Tonner and Marc Raupach — Fachbereich Chemie & Materials Sciences Centre, Philipps-Universität Marburg, Germany

The chemical bond is one of the most fundamental concepts in chemistry. Classifications such as covalent, ionic or metallic bonding are central in discussing trends in different compounds and predicting new reactivity. Several very helpful concepts and methods were developed to understand the chemical bond at surfaces.[1] The question about energetic contributions to surface chemical bonds on the other hand did not receive great attention although energy changes are the ultimate driving force in bond formation.

Starting from preliminary work by Philippsen and Baerends,[2] we implemented all terms of an Energy Decomposition Analysis (EDA) to obtain quantitative data about energetic contributions to chemical bonding in periodic systems. This periodic EDA method was applied to questions of chemisorption of organic molecules at semiconductor surfaces where it can shed light on the nature of the surface-adsorbate bonds.

[1] a) A. Nilsson, L. G. M. Pettersson, J. Nørskov, Chemical Bonding at Surfaces and Interfaces, Elsevier, Amsterdam, 2007; b) A. Groß, Theoretical Surface Science, Springer, Berlin, Heidelberg, 2009. [2] P. H. T. Philipsen, E. J. Baerends J. Phys. Chem. B 2006, 110, 12470.

O 15.10 Mon 18:30 TRE Ma

**Non-local density functionals meet many-body dispersion: A hybrid approach for van der Waals interactions** — •Jan Hermann, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Different approaches to treating van der Waals (vdW) interactions in density-functional theory can be loosely divided into the atom-based and the ones based on non-local functionals. The first type comprises a range of methods from atom-pairwise additive schemes by Grimme to many-body dispersion (MBD) approach of Tkatchenko et al. Usually, these methods require precalculated atomic parameters and thus rely on information not explicitly contained in the electron density. The other category consists of nonlocal functionals either of the Langreth and Lundquist or the Vydrov and van Voorhis (VV) type. In these approaches, the vdW interaction is obtained as a functional of the electron density and at most a few tuning parameters are needed.

Here, we show that these two contrasting approaches can be synergistically combined. We use the polarizability from the nonlocal functional of VV within the MBD method of Tkatchenko et al. Such a combination is worthy for several reasons. First, it is an atom-centered approach with no atomic parameters. Second, it puts aside the problem of partitioning electron density between atoms, which can be problematic in some cases. Third, it enables more direct comparison of so far unrelated methods. Fourth, it highlights the idea of combining working elements from different approaches.

# O 16: Electronic Structure and Spin-Orbit Interaction II

Time: Monday 16:00–19:00 Location: GER 38

O 16.1 Mon 16:00 GER 38

**Anisotropic two-dimensional electron gas at $SrTiO_3(110)$ protected by its native overlayer** — •Zhiming Wang[1], Zhicheng Zhong[2], Xianfeng Hao[1], Stefan Gerhold[1], Bernhard Stöger[1], Michael Schmid[1], Jaime Sánchez-Barriga[3], Andrei Varykhalov[3], Cesare Franchini[4], Karsten Held[2], and Ulrike Diebold[1] — [1]Institute of Applied Physics, Vienna University of Technology, Vienna, Austria — [2]Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria — [3]BESSY, Albert-Einstein-Str. 15, D-12489 Berlin, Germany — [4]Faculty of Physics and Center for Computational Material Science, University of Vienna, Vienna, Austria

Two dimensional electron gases (2DEGs) at oxide heterostructures are attracting considerable attention, as these might substitute conventional semiconductors for novel electronic devices. Here we present a minimal set-up for such a 2DEG – the $SrTiO_3(110)$-(4×1) surface, natively terminated with one monolayer of chemically-inert titania. Oxygen vacancies induced by synchrotron radiation migrate underneath this overlayer; this leads to a confining potential and electron doping such that a 2DEG develops. Our angular resolved photoemission spectroscopy (ARPES) and theoretical results show that confinement along (110) is strikingly different from a (001) crystal orientation. In particular the quantized subbands show a surprising “semi-heavy” band, in contrast to the analogue in the bulk, and a high electronic anisotropy. This anisotropy and even the effective mass of the (110) 2DEG is tunable by doping, offering a high flexibility to engineer properties of this system. This work is supported by ERC Advanced Grant and FWF.

O 16.2 Mon 16:15 GER 38

**Electronic structure of $\alpha$- and $\epsilon$-$Fe_2O_3$ nanoparticles: spin state and satellite structures** — Jörg Haeberle[1], •Matthias Richter[1], Petr Brazda[2], Massimo Tallarida[1], and Dieter Schmeisser[1] — [1]Brandenburg University of Technology Cottbus-Senftenberg, Applied Physics and Sensors, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Department of Inorganic Chemistry, Faculty of Science, Charles University in Prague, Czech Republic

We report on spectroscopic investigation of $\alpha$- and $\epsilon$-$Fe_2O_3$ nanoparticles. $\alpha$-$Fe_2O_3$ is commonly used as photocathode for water splitting for the hydrogen production. On the other hand $\epsilon$-$Fe_2O_3$ is of interest because of its magnetic properties. For both well-defined nanoparticles we analyze the electronic structure and determine the partial density of states for the valence and conduction bands. From these data we can derive a band scheme and compare it with recent (band structure) calculations. The resPES data at the Fe2p absorption edge spectra are analyzed to give evidence about the involved spin states in both phases. We find that for the $\epsilon$-$Fe_2O_3$ the majority is due to $Fe3d^5$ HS state. Contributions of the corresponding LS state are small and are found to be higher for the $\alpha$-$Fe_2O_3$ phase. In $\alpha$-$Fe_2O_3$ prepared by ALD we identify in addition a LS $3d^6$L state. In addition, a loss process can be identified upon resonant excitation at the Fe2p edge. It appears predominantly in the $\epsilon$-$Fe_2O_3$ phase. We give a model to describe that loss process. It is used to also explain the appearance of the Fe2p core level satellites that are different for $\alpha$- and $\epsilon$-$Fe_2O_3$ phases.

O 16.3 Mon 16:30 GER 38

**Electronic structure of the Co oxide catalyst for OER** — •Matthias Richter and Dieter Schmeisser — Brandenburg University of Technology Cottbus-Senftenberg, Applied Physics and Sensors, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

The electronic structure of the cobalt oxide based catalysts is analyzed using synchrotron radiation photoelectron spectroscopy. Cobalt oxide is used in photoelectrochemical cells for photocatalytic water splitting in order to produce solar fuels. We discuss our resonant data in terms of the partial density of states of the valence and conduction band. For the individual Co3d states, we determine their configuration, their spin, and their energy level relative to the Fermi energy. At resonant excitation we find the Co2p partial DOS to exhibit sharp features next to the VBM for increased cobalt oxidation state instead for a broad emission at around 6eV below $E_F$ for a low oxidation state. The former are found in $LiCoO_2$ and other Co-oxide systems with a $Co^{3+}$ ground state. We attribute such sharp features to the low spin (LS) configuration of $Co^{3+}$ and deduce that in the Co oxide catalyst layers with increased thickness there is evidence for the corresponding LS contributions. In contrast, our data prove the $Co^{2+}$ ground state for thin pristine cobalt oxide films and demonstrate that it is exclusively in the $Co3d^7$ high spin state. In addition, both cobalt oxide configurations $Co^{2+}$ in a HS state and $Co^{3+}$ in a LS state have characteristic oxygen to Co charge transfer states in the band gap. We attribute the trivalent charge transfer state to be the active state for the oxygen evolution reaction.

O 16.4 Mon 16:45 GER 38

**The role of spin-orbit coupling in the electronic structure of bulk and thin film $CaIrO_3$** — •Kerstin Dörr, Yuriy Mokrousov, Stefan Blügel, and Marjana Lezaic — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Transition-metal oxides (TMO) feature a multitude of interesting properties, such as metal-insulator transitions or high-temperature superconductivity. Furthermore, Mott physics plays a major role, with an enhanced onsite Coulomb repulsion $U$ driving the system into an insulating state. While this is true for well-studied $3d$ TMOs, in $5d$ TMOs the situation is different owing to larger extent of $d$-orbitals and reduced values of $U$. On the other hand the large atomic number of $5d$ elements promotes strong spin-orbit coupling (SOC). The interplay between strong SOC and small Coulomb repulsion can drive the $5d$ TMOs into a novel spin-orbital Mott state. Here, we investigate these effects in Iridium-based TMOs from first principles calculations using the full-potential linearized augmented plane-wave method [1]. In particular, we focus on the perovskite and postperovskite phases of $CaIrO_3$ and investigate the modifications of their bulk bandstructures in thin films.

[1] www.flapw.de

O 16.5 Mon 17:00 GER 38

**A combined LEEM/PEEM study on ferroelectric domains in perovskite crystals** — •Hatice Doğanay[1], Ingo Krug[1], Daniel Gottlob[1,2], Stefan Cramm[1], and Claus M. Schneider[1,2] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich — [2]Fakultät für Physik, Universität Duisburg Essen

We investigated the local electronic structure in domains of BaTiO3(001), which is considered a model perovskite-type ferroelectric oxide with potential for technological applications [1] due to its large dielectric permittivity, spontaneous polarization, piezoelectricity, and nonlinear optical responses. Polarized x-rays and variable photon energy enables photoelectron microscopy (PEEM)with element selective contrast and nanospectroscopy of the electronic structure differences between the ferroelectric domains. AES and LEED show that the surface is BaO terminated with a (2x2) reconstruction. For a clean surface the MEM-LEEM transition shift between different ferroelectric domains was 300 mV. Such a significant value is related to opposite polarizations perpendicular to the surface, pointing either outwards (P+) or inwards (P-). Equally important, in order to study the charge anisotropy with spatial resolution, XAS measurements have been performed. Accordingly, we were able to image the ferroelectric domains with the help of performed and calculated XLD Spectra, recorded at our UE56/1-SGM beamline (BESSY-II, Berlin) with an aberration-corrected LEEM/PEEM. [1] Shimizu et al. J. Phys.: Condens. Matter 25 (2013) 132001

O 16.6 Mon 17:15 GER 38

**The origin of $TiO_2$ shallow gap states evidenced from resonant photoelectron spectroscopy (RPES) and AFM on anatase single crystal (101) surface, nanocrystalline anatase films and ALD titania ante and post annealing** — •Philip Reckers[1], Mariel Dimamay[1], Sara Trost[2], Thomas Riedl[2], Thomas Mayer[1], and Wolfram Jaegermann[1] — [1]Technical University of Darmstadt, Surface Science, Germany — [2]Wuppertal University, Electronic Devices, Germany

Transparent, conductive and catalytic active $TiO_2$ with all its polymorphs is of high interest as it is used e.g. for water splitting, in DSSC and OSC. Gap states in $TiO_2$ play a crucial role as they influence e.g. charge transport and act as recombination centers. We investigated $TiO_2$ samples with respect to gap states by the use of resonant photoelectron spectroscopy. We detected two different band gap states. Deep gap states (DGS), that are attributed to oxygen defects are found around 1.3 eV and shallow gap states (SGS) are occupied from the Fermi level to about 0.35 eV binding energy. On a single crystal (SC) anatase (101) surface only SGS were detected. DGS and SGS states are observed on sintered nanocrystals (NC). Together with images from AFM we were able to ascribe the SGS to under coordinated Ti sites. The measured DOS fits well to the calculated DOS tailing into the energy gap inherent to NC as 1D line defects of under coordinated Ti sites form at (101) intersections[1]. Similar defects are located at edges of terraces on SC surfaces that form along the (101) direction. [1]F.Nunzi, F.De Angelis, E.Environ. Sci.,2013,6,4,1221-1229

### O 16.7 Mon 17:30 GER 38

**SPLEED at metallic and adsorbate-covered surfaces** — •Stephan Borek[1], Dmytro Kutnyakhov[2], Christian Langenkämper[3], Christian Thiede[3], Jan Minár[1], Jürgen Braun[1], Gerd Schönhense[2], Hans Joachim Elmers[2], Markus Donath[3], and Hubert Ebert[1] — [1]Ludwig-Maximilians-Universiät München — [2]Johannes-Gutenberg-Universiät Mainz — [3]Westfälische-Wilhelms-Universität Münster

The development of SPLEED (Spin-Polarized Low-Energy Electron Diffraction) as a surface-sensitive method has been pushed dramatically in theory as well as in experiment during the last decades. In particular, it is a very important tool for the study of the geometry of crystal surfaces as well as the surface potential barrier. Within the development of a multichannel-vector-spin polarimeter at BESSY various sensor materials have been investigated. Starting from this we perform fully relativistic SPLEED calculations using the SPRKKR package to investigate the resulting spin-dependent reflectivity in dependence on the energy and the scattering angles (polar and azimuthal). We present SPLEED calculations for various materials (W(001), Fe(001), Fe(001) p(1x1) O) and show their characteristics in view of reflectivity, asymmetry and the figure of merit. A comparison between experiment and theory will be made. Funded by BMBF (05K13UM1, 05K13WMA).

### O 16.8 Mon 17:45 GER 38

**Efficient photoemission spectroscopy via a MHz high-harmonic light source** — •Andreas Trützschler[1,2], Michael Huth[1], Cheng-Tien Chiang[1,2], Jürgen Kirschner[1,2], and Wolf Widdra[2,1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120, Halle(Saale), Germany — [2]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120, Halle(Saale), Germany

We demonstrate an efficient photoemission setup by combining time-of-flight (ToF) spectroscopy with a laboratory MHz pulsed light source with photon energies from 16 to 40 eV. The light is provided by high-order harmonic generation driven by a compact fiber laser system. The high flux of $10^9$ photons per second (at 25 eV) at the sample position together with the efficient collection of photoelectrons using ToF spectroscopy allows rapid band mapping of the electronic band structure. As an example we demonstrate photoemission experiments on Ag(100), which reveal the valence band electronic structure within 10 seconds measurement time without remarkable space-charge effects.

### O 16.9 Mon 18:00 GER 38

**Electron pair emission detected by time-of-flight spectrometers: new perspectives** — •Michael Huth[1], Cheng-Tien Chiang[1,2], Andreas Trützschler[1,2], Wolf Widdra[2,1], Frank O. Schumann[1], and Jürgen Kirschner[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120, Halle(Saale), Germany — [2]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120, Halle(Saale), Germany

We present results for electron coincidence spectroscopy obtained by using two time-of-flight (ToF) spectrometers. Electron-pair emission from a Cu(111) surface detected in coincidence and excited by electron impact allows to resolve the dispersion of the Shockley surface state in the momentum distribution. By combining the two ToF spectrometers with a high-order harmonic generation light source opens up new perspectives to enable ($\gamma$,2e) spectroscopy in the laboratory that required synchrotron radiation in the past. Utilizing this setup we report results for ($\gamma$,2e) on NiO(001) on Ag(001) excited with light at 30 eV photon energy.

### O 16.10 Mon 18:15 GER 38

**Energy relations in positron-electron pair emission** — •Frank O. Schumann[1], Iuri S. Brandt[1], Zheng Wei[1], and Jürgen Kirschner[1,2] — [1]Max-Planck Institut für Mikrostrukturphysik, Halle, Germany — [2]Martin-Luther Universität, Halle, Germany

The impact of a primary positron onto a surface leads to the emission of a correlated positron-electron pair. By means of a lab-based positron beam we studied this pair emission from a Ag(100) surface. We analyzed the energy spectra in a symmetric emission geometry. We found that the available energy is shared in an unequal manner among the partners. On average the positron carries a larger fraction of the available energy. The unequal energy sharing is a consequence of positron and electron being distinguishable particles. We provide a model which explains the experimental findings.

### O 16.11 Mon 18:30 GER 38

**Spin-orbit-induced spin polarization on W(110)** — •Henry Wortelen[1], Jürgen Henk[2], Anke B. Schmidt[1], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

Despite W(110) being nonmagnetic, its electronic structure exhibits spin-polarized states due to spin-orbit interaction, e.g., a spin-polarized Dirac-cone-like surface state below the Fermi level [1,2]. We report on the unoccupied electronic structure of W(110) investigated with spin-resolved inverse photoemission experiments and calculations. We compare results for $\bar{\Gamma}$-$\bar{N}$ and $\bar{\Gamma}$-$\bar{H}$, which are inequivalent due to the two-fold symmetry. A complex spin structure is observed for the surface states, which even depends on the photon detection angle. This shows that the measured spin polarization does not necessarily resemble the spin structure of the respective electronic state.

[1] K. Miyamoto et al., Phys. Rev. Lett. **108**, 066808 (2012)

[2] H. Mirhosseini et al., New J. Phys. **15**, 033019 (2013)

### O 16.12 Mon 18:45 GER 38

**Spin-split surface state above the Fermi level on Ta(110)** — •Bernd Engelkamp[1], Henry Wortelen[1], Jürgen Henk[2], Anke B. Schmidt[1], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

Recent experimental and theoretical photoemission studies on W(110) have been focused on a spin-polarized Dirac-cone-like surface state within a spin-orbit-induced symmetry gap [1, 2]. Browsing the periodic table for another heavy element with bcc structure yields only tantalum. On Ta(110), with one valence electron less compared to W(110), the spin-orbit-induced symmetry gap is expected above the Fermi level.

Using spin- and angle-resolved inverse photoemission we identified a spin-split surface state along the $\bar{\Gamma}$-$\bar{H}$ direction. We present our experimental results in combination with spectral density calculations in both high-symmetry directions $\bar{\Gamma}$-$\bar{H}$ and $\bar{\Gamma}$-$\bar{N}$.

[1] K Miyamoto *et al.* Phys. Rev. Lett. **108**, 066808 (2012)

[2] H Mirhosseini *et al.* New J. Phys. **15**, 033019 (2013)

# O 17: Semiconductor Substrates

Time: Monday 16:00–19:15 Location: PHY C 213

O 17.1 Mon 16:00 PHY C 213

**Structural sensitivity of the electromechanical coupling at Si surfaces** — •Sandra Hoppe[1], Anja Michl[1,2], Jörg Weissmüller[2,3], and Stefan Müller[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology, Germany — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Germany — [3]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany

Electromechanical coupling describes a relation between a material's mechanical and electronic properties. It has been found for various metal surfaces that an applied strain leads to a change in the work function. While this phenomenon has been studied for silicon nanowires and silicene, surprisingly, no results are available for clean silicon surfaces. We investigated the electromechanical coupling at the silicon (100) and (111) surfaces via density functional theory by calculating the response of the ionization potential and the electron affinity to different types of strain. The highest occupied and the lowest unoccupied molecular orbital (HOMO and LUMO) were obtained from the surface states within the surface band gap. We find large negative response parameters and a high sensitivity of the strain response to surface relaxations. This can be attributed to the directional bonds in covalent semiconductors and discussed in terms of volume and surface contributions to the response of the surface dipole potential and the electronic structure to strain. While we find a considerable volume influence on the dipole potential, the response of HOMO and LUMO seems to be dominated by the local reconstruction geometry.

O 17.2 Mon 16:15 PHY C 213

**Simultaneous nc-AFM/STM characterization of subsurface defects on B:Si(111)-$\sqrt{3}$x$\sqrt{3}$ surface** — •Evan Spadafora[1], Jan Berger[1], Pingo Mutombo[1], Mykola Telychko[1], Martin Ondracek[1], Martin Svec[1], Zsolt Majzik[1], Alastair Mc Lean[2], and Pavel Jelinek[1] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [2]Department of Physics, Queen's University, Kingston, Ontario, Canada

B:Si(111)-$\sqrt{3}$x$\sqrt{3}$ surface has gained a lot of interest in surface science, due to its prominent electronic and structural properties. Compared to bare silicon surface, this system has reduced chemical reactivity, which makes it a suitable candidate for deposition of molecular complexes without a risk of their decomposition. Here we will report combined nc-AFM/STM measurements using qPlus sensor with atomic resolution of the B:Si(111)-$\sqrt{3}$x$\sqrt{3}$ surface supported by total energy DFT calculations. STM reveals slight modulation of the tunneling current over surface area, which we attributed to presence of subsurface boron defects. We combine KPFM and lock-in STS measurements with large-scale DFT calculations to characterize position of boron subsurface defects and their influence on surface electronic structure.

O 17.3 Mon 16:30 PHY C 213

**In situ Scanning Tunneling Microscopy investigation of layered superlattices [(VSe2)n]1.06[(TaSe2)n]** — •Pavel Shukrynau[1], Ryan Atkins[2], Dave C. Johnson[2], and Michael Hietschold[1] — [1]Institute of Physics, Technische Universität Chemnitz, Reichenhainer Straße 70, D-09107 Chemnitz, Germany. — [2]Materials Science Institute and Chemistry Department, University of Oregon, Eugene, Oregon 97403, USA

Variable Temperature Scanning Tunneling Microscopy (VT STM) was used to investigate local structural and electronic properties of the cleaved surface of [(VSe2)n]1.06[(TaSe2)n] layered compound. The original uppermost layer dissipates into small domains of 50x50 nm in size or more. In a region where three domains are in contact, a small triangular area with a side up to 5 nm is usually found, exhibiting a dark depression. The detailed inspection of the interior of the domain reveals a local ordering in a hexagonal-like pattern with rare inclination of surface defects. The observed structure is somehow similar to those obtained previously on other transition metal-chalcogenide surfaces. We were not able to identify unambiguously the chemical identity of the surface layer in STM scans. However, tunneling spectroscopy measurements distinctly show the dominance of the metal atoms in the topmost layer rather than the chalcogen ones.

O 17.4 Mon 16:45 PHY C 213

**Adsorption of Tetrahydrofuran and Diethylether on the Si(001) surface studied by means of STM, XPS and UPS** — •Marcel Reutzel[1], Gerson Mette[1], Michael Dürr[1,2], Ulrich Koert[3], and Ulrich Höfer[1] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — [2]Institut für Angewandte Physik, Justus-Liebig-Universität Giessen, D-35392 Giessen, Germany — [3]Fachbereich Chemie, Philipps-Universität,D-35032 Marburg

A promising possibility to compete with the challenges of miniaturization in semiconductor device physics is the functionalization of inorganic semiconductor surfaces with organic molecules. It is thus important to understand the basic adsorption mechanisms of different classes of organic molecules. In this contribution, we investigate the adsorption properties of tetrahydrofuran and diethylether on the Si(001) surface as representatives for the functional group of ethers. We find a complex adsorption scheme which is similar for the two molecules.

At 50 K, a dative bond is formed via the donation of electron density of an oxygen lone pair into the $D_{\mathrm{down}}$ orbital of the c(4x2) reconstructed Si(001) surface. Heating the sample to 300 K leads to a surface mediated ether cleavage which results in covalently bonded adsorbates on two neighboring dimer rows. While the ring opening reaction of tetrahydrofuran leads to a bridging Si-O-$(CH_2)_4$-Si configuration, the linear diethylether is cleaved and leads to Si-O-$C_2H_5$ and Si-$C_2H_5$ adsorbates. The scission of diethylether further enables a tip induced intrarow hopping of the (-$C_2H_5$) fragment.

O 17.5 Mon 17:00 PHY C 213

**Switching single molecules by STM voltage pulses on the Si(100) surface** — •Anja Nickel[1], Jörg Meyer[1], Robin Ohmann[1], Christian Joachim[2], Gianaurelio Cuniberti[1], and Francesca Moresco[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]CNRS, CEMES, 29 rue J. Marvig, 31055 Toulouse, France

For the development of electronics down to atomic scale, it is of fundamental importance to build atomic-size interconnections in a planar geometry and to be able to controllably switch between different connection paths. Dangling bond wires build on the H:Si(100) are presently intensively investigated as promising candidates to build such interconnections. In this frame, we have investigated by scanning tunneling microscopy (STM) at low temperature Acetylbiphenyl molecules on the Si(100) surface. STM images show that the molecules adsorb along the dangling bond rows of the silicon. By applying voltage pulses with the STM tip, we demonstrate that single Acetylbiphenyl molecules can be reversibly switched between two different configurations. The experiment shows that Acetylbiphenyl is a suitable molecule to be used as molecular latch on a dangling bond based atomic scale circuit.

O 17.6 Mon 17:15 PHY C 213

**Initial-stage oxidation products on Si(111)-(7x7) in AFM and STM** — Jo Onoda[1], •Martin Ondracek[2], Ayhan Yurtsever[3], Pavel Jelinek[1,2], and Yoshiaki Sugimoto[1] — [1]Graduate School of Engineering, Osaka University, Suita, Osaka, Japan — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [3]The Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Osaka, Japan

Studying the defects that form on a silicon surface in the initial stages of oxidation is important from the technological point of view and resolving the existing controversies regarding the structure of these defects can also contribute to better understanding the experimental techniques that were used in the studies. We investigated structures that appear in the initial oxidation stage of the Si(111)-(7×7) surface using the combined techniques of non-contact atomic force microscopy (AFM) and scanning tunneling microscopy (STM). We identified the defects resulting from initial oxidation as the *ins×1* and *ins×2* structures (1 or 2 oxygen atoms in backbonds of Si adatom) and the secondary oxidation product as the *ad-ins×3* structure (3 oxygen atoms in the backbonds and 1 on top). We excluded the presence of adsorbed $O_2$ molecules on the surface. We used *ab initio* simulations with a diverse range of tip models to interpret the experimental data and to clarify the mechanisms that lead to the observed forces and tunneling currents.

O 17.7 Mon 17:30 PHY C 213

***In situ* study of water adsorption on InP(100) surfaces** — •Matthias M. May[1,2], Hans-Joachim Lewerenz[1,3], and Thomas Hannappel[1,4] — [1]Helmholtz-Zentrum Berlin, Institute of Solar Fuels — [2]Humboldt-Universität zu Berlin, Institut für Physik — [3]California Institute of Technology, Pasadena, USA — [4]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik

Photoelectrochemical water splitting with semiconductors promises to harvest solar energy directly and efficiently in the form of chemical energy. The most critical part of potential devices is the solid-electrolyte interface, which has to enable efficient charge-transfer and simultaneously block corrosion.

III-V semiconductors such as GaP or InP are an interesting light absorber material class, but their surface has to be designed appropriately for solar water splitting applications.[1] We perform water (oxygen) adsorption experiments on atomically well-defined InP(100) surfaces prepared by metal-organic vapour phase epitaxy. Monitoring the adsorbate-induced surface modifications of different surface reconstructions with reflection anisotropy spectroscopy and photoelectron spectroscopy, we aim to develop criteria for the design of III-V electrode surfaces.[2] We find that In-rich, $(2 \times 4)$ reconstructed and $p(2\times2)/c(4\times2)$ reconstructed, P-rich surfaces exhibit a distinctly different initial interaction with the adsorbates, which could explain why In-rich InP(100) photocathodes perform so well.

[1] Hannappel et al., in *Photoelectrochemical Water Splitting*, RSC Publishing (2013). [2] May et al., *New J. Phys.* **15**:103003 (2013).

O 17.8 Mon 17:45 PHY C 213

**Frustrated self-assembly of shape-persistent star molecules on HOPG** — •Stefan-S. Jester, Eva Sigmund, Lisa M. Röck, and Sigurd Höger — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Star-shaped organic molecules with a rigid backbone and flexible side chains adsorb at the solution/solid interface to form self-assembled 2D nanopatterns. Scanning tunneling microscopy yields a submolecularly resolved insight into the adsorbate structures and thus an insight on the driving forces of their formation. We investigate the role of alkoxy side chain length on the adsorption patterns: Different dense and porous adsorbate patterns are observed, and for chain length $n = 12$, frustrated self-assembly leads to hierarchically organized superstructures. Up to 10 molecules form triangular aggregates which pack densely into hexagonal patterns with very large (15.5 nm) lattice constants. [1] S.-S. Jester, E. Sigmund, L. M. Röck, S. Höger *Angew. Chem. Int. Ed.* **2012**, *51*, 8555.

O 17.9 Mon 18:00 PHY C 213

**Ultra-thin ZnO on Metal Substrates as ZnO Surface Model** — •Bjoern Bieniek, Oliver T. Hofmann, Patrick Rinke, and Matthias Scheffler — Fritz Haber Institut der MPG, 14195 Berlin

In the context of catalysis and hybrid inorganic/organic systems, metal supported ultra-thin ZnO can be used as model systems. However, it is not clear to what degree the ZnO films resemble the surfaces of ZnO or whether they exibit significantly different properties. We investigate the structure of ultra-thin ZnO films (1 to 4 layers) on the (111) surfaces of Ag, Cu, Pd, and Pt by means of density-functional theory. The free-standing ZnO monolayer adopts an $\alpha$-BN structure. This structure prevails on the metal substrates, and we obtain coincidence structures in good agreement with experiment [1, 2, 3]. Thicker ZnO layers adopt a wurtzite structure. The films exhibit a large random corrugation, which can be regularized by hydrogen adsorption. A hydrogen overlayer with 50% coverage is formed at chemical potentials that range from low vacuum to ultra-high vacuum $H_2$ pressures. For the Ag substrate both $\alpha$-BN and wurtzite ZnO films are accessible in this pressure range, while for Cu wurtzite films are favoured. The surface structure and the density of states of these hydrogen passivated ZnO thin films agree well with those of the bulk ZnO(000$\bar{1}$)-2x1-H surface. [1] C. Tusche *et al.* PRL **99**, 026102 (2007) [2] Y. Martynova *et al.*, J. Cat., **301**, 227-223 (2013) [3] G. Weirum *et al.* J. Phys. Chem. C, 114 (2010)

O 17.10 Mon 18:15 PHY C 213

**A photoelectron diffraction study of the Fe/GaAs(4x2)-interface** — •Dominique Handschak, Frank Schönbohm, Tobias Lühr, Christoph Keutner, Ulf Berges, and Carsten Westphal — Exp. Physik 1/DELTA, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund

In this study we investigate a system of a (4x2)-reconstructed GaAs(001) substrate with an Fe adsorbate. This system is applied in the field of spintronics, which use the GMR (giant magneto resistance) effect. Especially the interface between this two layers has a strong influence on the efficiency of the effect. The method of x-ray photoelectron diffraction (XPD) is an excellent tool for investigating this system, because it is chemical and interface sensitive. The angle-resolved measurement yield structural information due to scattering and diffraction effects of the photoelectron. The GaAs substrate is found in the well ordered (4x2)-reconstructed structure. XPD pattern of Ga 3d and As 3d reveal that the reconstruction is not lifted due to the Fe deposition. The Fe/GaAs interface is formed by a pyramid-like structure of the iron layers. The strongest lateral shift is found in the first Fe-monolayer with regard to the GaAs substrate and decreases evenly to zero with every additional monolayer towards the surface. Thereby the topmost layers are well bcc-ordered with the Fe-lattice constant of a(Fe) = 2.866Å.

O 17.11 Mon 18:30 PHY C 213

**Epitaxial growth of the topological insulator $Bi_2Se_3$ on Si(111): Growth mode, lattice parameter, and strain state** — •M. Vyshnepolsky[1,2], C. Klein[1], A. Hanisch-Blicharski[1], and M. Horn-von Hoegen[1] — [1]Department of Physics, Universität Duisburg-Essen, Lotharstr. 1, D-47057 Duisburg, Germany — [2]Present address: Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, D-44780 Bochum, Germany

The epitaxial growth of $Bi_2Se_3$ films on Si(111), prepared by co- deposition of selenium (Se) and bismuth (Bi) at 200-250°C, was studied by in-situ high resolution spot profile analysis low energy electron diffraction (SPA-LEED), ex-situ atomic force microscopy (AFM) and x-ray diffraction (XRD). The first $Bi_2Se_3$ layer grows as complete quintuple layer and covers the Si substrate before the next layer nucleates. Its lateral lattice parameter is increased by 1% compared with the value of $a_{||} = 4.136$ Å for a 6-nm-thick film. With increasing film thickness, a continuous change of the lattice parameter is observed to an asymptotic value of $a_{||,\infty} = 4.134$ Å, which is explained by a van der Waals-like bonding between the $Bi_2Se_3$ film and the Si substrate [1]. The films are atomically smooth without small angle mosaics or small angle rotational domains. The precise determination of thus determined lateral and the vertical lattice parameter of c = 28.65 Å reveal that films grown at higher temperature exhibit smaller lattice parameters which is attributed to an increased density of Se vacancies. Bulk defects in the film cause a parabolic increase of the width of the diffraction peaks in XRD. [1] M. Vyshnepolsky et al., Appl. Phys. Lett. **103**, 111909 (2013)

O 17.12 Mon 18:45 PHY C 213

**STM study of thin terbium-silicide layers on Si(111)** — •Martin Franz, Robert Kohlhaas, and Mario Dähne — Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany

The growth of rare earth silicides on silicon surfaces leads to the formation of very interesting structures such as self-organized metallic nanowires on the Si(001) and the Si(557) surface [1]. On Si(111), the formation of nanoclusters is observed at very low coverages [2], while at higher coverages two- and three-dimensional layers form [3].

In this work the growth and the atomic structure of Tb silicide films on Si(111) in the coverage regime from submonolayers to several monolayers were studied using scanning tunneling microscopy. In this regime various superstructures were identified. At submonolayer coverages first nanoclusters form before a $2\sqrt{3} \times 2\sqrt{3}$ superstructure is observed. For Tb coverages exceeding 0.5 ML the $1 \times 1$ superstructure of the $TbSi_2$ monolayer appears additionally, and at coverages exceeding one monolayer the three-dimensional $Tb_3Si_5$-multilayer is observed. Furthermore, elongated islands showing a $2 \times 1$ reconstruction on top are found.

This work was supported by the DFG through FOR 1282 project D.

[1] M. Dähne and M. Wanke, J. Phys.: Condens. Matter **25**, 014012 (2013).

[2] M. Franz et al., Surf. Sci. **609**, 215 (2013).

[3] I. Engelhardt et al., Surf. Sci. **600**, 755 (2006).

O 17.13 Mon 19:00 PHY C 213

**Surface characterization of arsenic terminated Si(111) substrates pre-pared in MOVPE for III-V nanowire solar cells** — •Weihong Zhao[1], Agnieszka Paszuk[1], Matthias Steidl[1], Sebastian Brückner[1], Oliver Supplie[1], Anja Dobrich[2], Peter Kleinschmidt[1,3], and Thomas Hannappel[1,2,3] — [1]Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98684 Ilmenau — [2]Helmholtz-Zentru Berlin, Institut für Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

III-V nanowires grown on Si(111) substrates by metal-organic vapor phase epitaxy (MOVPE) enable a promising new solar cell concept meeting the demands of high-quality-low-cost photovoltaics. GaP buffer layers grown on Si(111) substrates represent suitable quasi-substrates since GaP is almost lattice-matched to Si. Apparently, preparation of atomically flat Si (111) surfaces is an essential step for adjacent GaP het-ero-epitaxy. However, little is known about preparation and surface prop-er-ties of Si(111) surfaces in MOVPE with H2 ambient. A contamination-free transfer system enabled us to study the MOVPE prepared surfaces with numerous UHV based surface science tools. A dedicated wet-chemical pretreatment is crucial to obtain atomically flat Si(111) surfaces. Varying the Si(111) surface preparation could control the polarity of the adjacent GaP layer. With the confirmation of FTIR, STM and LEED, we successfully established a controlled arsenic termination procedure during the epitaxy.

## O 18: Solid-liquid Interfaces II

Time: Monday 16:00–19:15 Location: WIL A317

O 18.1 Mon 16:00 WIL A317

**Changes in Potential During Pulsed Galvanostatic Deposition of Zinc Oxide on Gold** — •Martina Stumpp and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Zinc oxide ($ZnO$) is a promising electrode material for the application in various devices in the fields of chemistry, optics and electronics. Electrochemical deposition is an environmentally-friendly and energy-efficient technique for the deposition of crystalline $ZnO$. As a solution-based technique, it allows to prepare films on temperature-sensitive substrates and independent on substrate shape leading to a variety of optional device geometries. Electrodeposition of $ZnO$ was carried out under pulsed galvanostatic conditions from aqueous zinc nitrate solutions on $Au$ wires, sheets, microstructured bands or $Au$-coated polyamide threads. The voltage-time curves attained during these experiments were analyzed and three significant stages were observed for all depositions regardless of the geometry of the substrate despite limitation of the reaction by diffusion processes. The three stages were discussed under variation of the pulsating current density, the deposition time, but also by polarization of only one of two sets of microstuctured band electrodes. A correlation between an abrupt drop in the potential and the completed coverage of the $Au$ electrode surface was seen. The detailed characterization of each stage in the potential-time curves allows to prepare thin compact $ZnO$ films without pinholes on a given substrate.

O 18.2 Mon 16:15 WIL A317

**Current-time characteristics of the electrochemical deposition of zinc-oxide on microelectrodes and a finite element simulation of the diffusion control** — •Christian Lupo and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Zinc oxide ($ZnO$) films were prepared by electrochemical deposition on interdigitated microstructures of gold band electrodes. Electrodeposition was realized at constant electrode potential from an oxygen-saturated aqueous zinc chloride solution in the presence of the xanthene dye $EosinY$. The composition of the solution, the deposition time, the interdigital electrode size, gap width and the number of electrode bands were varied. The current during reduction of $O_2$ and the subsequent growth of $ZnO$ was measured and correlated with results of scanning electron microscopy and of simulations by the finite element method (FEM). The close match of the observed chronoamperometric curves confirms the diffusion-controlled behavior of the oxygen reduction and of the subsequent deposition of $ZnO$. Furthermore the FEM simulation can be used to discuss an influence of an increasing surface area during film growth on the diffusion-limited precipitation reaction. Such application of the FEM to electrochemical deposition reactions can provide useful contributions to the further development towards a controlled electrochemical growth on electrodes with different geometric features on the microscale.

O 18.3 Mon 16:30 WIL A317

**Understanding the crystal growth inhibition: role of acetate at the calcium oxalate/water interfaces** — •Leila Salimi Parvaneh[1,2], Davide Donadio[1], and Marialore Sulpizi[2] — [1]MPI for Polymer Research, Mainz — [2]Physics Department, Johannes Gutenberg University, Mainz

Calcium oxalate occurs widely in kidney stones and among a variety of living organisms[1]. The presence of bio-polymers such as polyglutamate during the formation of calcium oxalate crystal has a great impact on the crystalline phase, morphology and growth rate[2].We have performed DFT-based Born-Oppenheimer Molecular Dynamics (BOMD) simulations to understand the structural and dynamical properties of the interfaces between calcium oxalate dihydrate (COD) (100) and (101) and water. Our study reveals differences in the coordination of calcium ions at the surface with water. We also characterize the interaction between biomolecules and different surfaces of COD. As a first step we consider acetate as a minimal model for glutamate side chain. We estimate the binding free energy on different surfaces and compare it to the binding free energy of calcium and acetate in solution[3]. We also discuss binding structure at different coverage. Preferential binding of carboxylate to the (100) surface is found, providing a rational for recent experimental results on anisotropic growth of COD crystals in the presence of biopolymers[2]. [1] E. L. Prein and C. Frondel, J. Urol. 57, 949, 1947. [2] V. Fischer, K. Landfester and R. Munoz-Espi, Cryst. Growth Des. 11, 1880, 2011. [3] J. Kahlen, L. Salimi, M. Sulpizi, C. Peter, D. Donadio, 2013 (submitted).

O 18.4 Mon 16:45 WIL A317

**Microscopic characterization of the CaF2 / water interfaces.** — •Rémi Khatib[1], Maria J. Perrez-Haro[2], Mischa Bonn[2], Ellen H.G. Backus[2], and Marialore Sulpizi[1] — [1]Johannes-Gutenberg University, Mainz, Germany — [2]Max Planck Institute for polymer research, Mainz, Germany

From biological membranes to heterogeneous catalysis through atmospheric chemistry, interfaces involving liquid water are common on Earth. Vibrational Sum Frequency Generation (SFG) is a spectroscopic technique which allow a selective characterization of interfacial water. In order to rationalize the experimental results obtained for CaF2 / water interfaces, a theoretical approach has been used, based on first principles molecular dynamics simulations.

In particular Born-Oppenheimer Molecular Dynamics (BOMD) have been used on different model systems to describe a wide range of pH of the aqueous solution. Different tools, like the Velocity Density of States (VDOS), Radial Distribution Function (RDF), were employed to analyze the data. The preliminary results are promising: a *free OH* peak measured by SFG under basic conditions can certainly be explained by a substitution of F- by HO- at the interface. Moreover a microscopic characterization of the water species and dynamics at low pH is also provided.

O 18.5 Mon 17:00 WIL A317

**Nanoconfinement Effects on Hydrated Excess Protons in Layered Materials** — •Daniel Muñoz-Santiburcio, Carsten Wittekindt, and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44801 Bochum, Germany

Nanoconfined water has been widely studied in both wire-like and two-dimensional environments. A feature of particular interest in such systems is the behavior of excess protons. While proton transfer in bulk water has been widely studied, almost all efforts in studying excess protons in confined water systems are devoted to water wires due to their importance in biological systems and in view of technological applications such as fuel cells, whereas investigations of hydrated protons at liquid/solid interfaces are scarce. Following our previous work [1] on nanoconfined water between sheets of mackinawite minerals, FeS, which form layer-like superstructures, we address the behavior of hydrated excess protons in this layered material [2]. Even extreme nanoconfinement is shown to not affect the fluxional nature of the topological defect, thus not localizing the excess protons but conserving the efficient structural (Grotthuss) diffusion process known in bulk water. Yet, depending on the width of the slit pore, the defect can bridge the bilayer water structure, thus forcing the excess proton into the water depleted region between the bilayers.

[1] C. Wittekindt and D. Marx, *J. Chem. Phys.* 137, 054710 (2012).
[2] D. Muñoz-Santiburcio, C. Wittekindt and D. Marx, *Nat. Commun.* 4:2349 (2013).

O 18.6 Mon 17:15 WIL A317

**Wetting Transition in a solid/water/oil system mediated by ion and surfactant -adsorption induced interface interactions** — •Bijoyendra Bera, Igor Sîretanu, Michèl H.G. Duits, Martien A. Cohen-Stuart, Dirk van den Ende, and Frieder Mugele — Physics of Complex Fluids (PCF) Group, TNW, University of Twente, Enschede, The Netherlands

Enhanced oil recovery (EOR) processes rely upon wettability alteration in sandstone rock (silica and clay materials). In this study, by changing the salt (NaCl or $CaCl_2$), concentration (1 mM to 1000 mM) and pH, we observe wetting transition on mica in an oil (n-Decane) phase. At all pH and concentration of NaCl, contact angles below macroscopic detection limit (around $1.5^0$) are observed, implying complete wetting. For $CaCl_2$, we observe finite contact angles (up to $10^0$) above a critical concentration of 50 mM. When we add polar amphiphilic molecules (stearic acid) in n-Decane, this wetting transition is more pronounced since for $CaCl_2$ solution, contact angles are as high as $70^0$. In presence of stearic acid, dynamic effects such as autophobing and self-propelling of drops on mica are also observed.

We explain such wetting transition with an ion-adsorption model, causing surface charge reversal at mica/water interface for divalent cations. This proposition is supported with experimental calculations of zeta potential. Based on these values, we calculate surface charge and subsequently, the interaction potential between mica/water and oil/water interfaces. The minimum of this potential corresponds to the film thickness of aqueous phase, which we confirm with ellipsometry.

O 18.7 Mon 17:30 WIL A317

**Activation of surfaces with ultrasound (US): from physical effects to chemistry** — •Matthieu Virot[1], Serguei I. Nikitenko[1], Thomas Zemb[1], and Helmuth Möhwald[2] — [1]ICSM Marcoule, Bagnols sur Cèze (France) — [2]MPI-KG, Potsdam (Germany)

US propagation in liquid media may lead to acoustic cavitation which is the nucleation, growth, and rapid implosive collapse of vapor filled micro-bubbles. At collapse, these bubbles create extreme transient conditions of several thousand of degrees and hundreds of atm., and possibly light emission (sonoluminescence). At the vicinity of an extended solid surface, these conditions go with the generation of shock waves and micro-jets striking the surface with a high velocity. Non-equilibrium conditions therefore generated at surfaces may offer new alternatives to activate surfaces. Recent investigations carried out at surfaces from the macro- to the nanoscale brought to light new physicochemical properties and possibilities never reported before: (i) Sonicated (20 kHz, 10-20°C, Ar) silica glass and crystalline Si surfaces were characterized by their unusual physical and chemical transformations. (ii) Spectroscopic investigations performed at the vicinity of a sonicated (Ce0.9Tb0.1)PO4 pellet surface revealed for the first time that acoustic cavitation can be used as an in-situ source of excitation for photoactive species contained in an extended solid phase via sonoluminescence, while solubilized Ar was found to be excited during the sonication of crystalline Si via mechanoluminescence. (iii) The reductive dissolution of refractory CeO2 was found to be catalyzed by the sonochemical deposition (20-40°C) of Pt NPs at the surface of ceria.

O 18.8 Mon 17:45 WIL A317

**Self-Assembly of Alkyl Phosphonic Acids at $\alpha$-$Al_2O_3$(0001)-Solvent Interfaces** — Christian Meltzer, Wolfgang Peukert, and •Björn Braunschweig — University of Erlangen-Nuremberg; Institute of Particle Technology (LFG), Cauerstrasse 4, 91058 Erlangen

Molecular self-assembly of octadecylphosphonic acids (ODPA) on $\alpha$-$Al_2O_3$ is studied with vibrational sum-frequency generation (SFG) in-situ and in real time. A detailed analysis of SFG spectra shows that both intensity and relative contributions of methylene and methyl bands are excellent indicators for coverage dependent changes in the molecular structure of ODPA self-assembled monolayers (SAMs). Concentrations between 0.1 and 5 mM ODPA in propanol lead to slow adsorption where a SAM is formed over several hours. For concentrations $< 1$ mM, SAMs with low coverage and possibly flat lying molecules are formed even after prolonged adsorption times. For concentrations $>1$mM an equilibrium can be reached, but vibrational spectra still show substantial contributions from gauche defects. Dewetting of these SAMs in $N_2$ gas leads to an increase in SFG intensity that is accompanied by a substantial decrease in SFG contributions from gauche defects. After re-immersing of dried samples in 2-propanol with 5 mM ODPA, SFG spectra remain unchanged and are representative of well-ordered ODPA SAMs. From these observations we hypothesize that before de-wetting coverage and molecular order are already very high, but final improvements in molecular order are accomplished only at the solid-liquid-gas three phase line.

O 18.9 Mon 18:00 WIL A317

**EFFECT OF SONICATION TIME ON THE SELF-ASSEMBLY OF SOLVENT MOLECULE ADSORBED ON HOPG (0001) SUBSTRATE STUDIED BY SCANNING TUNNELING MICROSCOPY AT THE LIQUID-_SOLID INTERFACE** — •Nguyen Thi Ngoc Ha[1], Thiruvancheril G. Gopakumar[2], and Michael Hietschold[1] — [1]Institute of Physics, Solid Surfaces Analysis Group,Technische Universität Chemnitz, Germany — [2]Indian Institute of Technology, Kanpur, India

Self-assembly at the liquid-solid interface depends on several experimental parameters such as temperature, chemical nature of the solvent, functional groups of the solute molecule, concentration of dissolved molecules, etc. which can influence on the interactions between adsorbate, substrate and solvent. The molecular concentration in a solvent has been shown to be a useful control parameter for self-asssembled molecular pattern formation out of solutions on a crystalline substrate. Sonication treatment of the solutions has been demonstrated to be an efficient method to change these concentrations. The adsorption of TMA (trimesic acid)-undecanol mixture on a HOPG substrate has been investigated. It reveals an adsorption pattern consisting of alternating stripes made of TMA and undecanol solvent molecules which changes in dependence on sonication time. There has been found self -assembled deposition also from pure solvents leading to different patterns which can be controlled by sonication also. These types of studies will give better insight into the adsorption process and may also offer exciting opportunities for nano-patterning.

O 18.10 Mon 18:15 WIL A317

**Temperature-controlled 3d self-assembling of benzene-1,3,5-triphosphonic acid observed by scanning tunneling microscopy (STM) at the liquid-solid interface** — •Chau Yen Nguyen Doan[1], Ngoc Ha Nguyen Thi[1], Michael Mehring[2], and Michael Hietschold[1] — [1]Solid Surfaces Analysis Group, Institute of Physics, TU-Chemnitz, Chemnitz, Germany — [2]Institute of Chemistry, TU-Chemnitz, Chemnitz, Germany

Benzene-1,3,5-triphosphonic acid (BTP), which is the phosphonic acid analogue of trimesic acid (TMA), forms a columnar packing in the crystalline solid state that is characterized by strong hydrogen bonds and $\pi$-stacking involving the aromatic rings. Therefore, BTP is an interesting intermediate to design both 3D supramolecular hydrogen-bonded architectures and organic-inorganic hybrid frameworks. The 2D or 3D crystal engineering of molecular architectures on surfaces requires controlling various parameters related respectively to the substrate, the chemical structure of the molecules, and the environmental conditions. We investigate here the influence of temperature on the self-assembly of BTP at the undecanol-HOPG interface using ambient STM. The geometry adsorption of the 3D self-assembled BTP can be precisely tuned by adjusting the substrate temperature from 20°C to 60°C. STM images at different substrate temperature reveal the different co-adsorption structures as well as different packing density of BTP and undecanol solvent molecules. Based on these results, temperature-control has been proven to be a versatile tool to adjust the polymorphism of molecular patterns deposited out of solutions.

O 18.11 Mon 18:30 WIL A317

**Molecular Dynamics Simulations of the Dissolution of Lactose Crystals** — •Berna Dogan, Julian Schneider, and Karsten Reuter — Technische Universität München, Germany

Apart from its widespread use in food industry, Lactose is commonly applied in the pharmaceutical industry as an excipient for drug formulations. This application demands an efficient dissolution of its crystalline alpha lactose monohydrate (alpha-LM) phase to enable a fast uptake of the active pharmaceutical ingredient. Seeking for an understanding of the underlying molecular porcesses, we aim at complementing the available dissolution experiments with force-field molecular dynamics (MD) simulations of the alpha-LM/water interface at the atomistic level.

At near-equilibrium conditions, dissolution is expected to primarily take place at kink sites within step edges. The dissolution velocity of a step edge can then be derived from the kink free energy, as well as the rate constant of the molecular detachment process [1]. Instead of approximating the defect free energies by potential energy differences of rigid crystal arrangements [1], we aim at a precise calculation, including entropic contributions and explicit solvation. We, therefore, present a modification of binding free energy methods of molecular ligand/receptor complexes towards an application to surface defects. Moreover, we show how the molecular rate constants can be calculated at the same level of precision from accelerated molecular dynamics simulations.

[1] R. C. Snyder and M. F. Doherty: Proc. R. Soc. A, **465**, 1145, (2009)

O 18.12 Mon 18:45 WIL A317

**Exploring the formation, lifetime and dissociation statistics of acid-amine bonds** — •Sangeetha Raman and Markus Valtiner — Department of Interface Chemistry and Surface Engineering, Max-Planck-Institut für Eisenforschung GmbH, D-40237, Düsseldorf, Germany

Understanding the scaling of single molecular interaction forces towards an integral interaction between extended surfaces interacting simultaneously through a large number of molecular bonds is a key objective in order to model or predict interactions in realistic situations. Here we study the scaling of interaction forces arising from acid-base bond at both, the single molecular level using force spectroscopy with atomic force microscopy (AFM) and the macroscopic level using surface forces apparatus experiments (SFA). The single molecule experiments reveal two distinct regimes of interaction forces as a function of the bond-loading rate - the equilibrium desorption regime and the force-dependent bond dissociation regime. SFA measurements revealed, that the forces measured in the equilibrium regime using AFM, scale linear with the number density of acid base bonds at the interface. We show that a combined approach of AFM and SFA allows for a detailed understanding of both kinetic aspects of the bond forming and breaking as well as equilibrium scaling of the interaction forces. AFM allows to directly measuring lifetimes of bonds, while SFA allows to directly studying the equilibrium interactions between specific bonds. Our results provide complementary information to predict and model realistic situations of bond forming and breaking.

O 18.13 Mon 19:00 WIL A317

**The Theoretical and Experimental Study on the Dynamic Ice-making system Using Supercooling Water Based on the Nano-fluorocarbon Coating Material** — •Hong Wang — School of civil engineering, Henan Institute of Engineering, Zhengzhou city, China

Supercooling water is used as a superior method to generate ice slurry for its high efficiency and energy conservation. However, the ice blockage occurred in the supercooling heat exchanger is a prominent problem that reduces the efficiency of the ice generation system. In order to avoid or retard ice blockage, a fluorocarbon coating with superhydrophobicity was applied onto the surface of the supercooling heat exchanger to continuously make ice slurry without any additive. The characteristics of the coated surface with fluorocarbon coating was determined and analyzed relatively. The results showed that the nano-fluorocarbon film in the average thickness was only 9.7nm. It was the very thin film made the solid surface superhydrophobicity with the contact angle of 163.01°. This film not only has a good property in anti-icing but also anti-scale. Compared with the uncoated surface, the process of water freezing on the coated surface with nano-fluorocarbon was slower which demonstrated that the icing on the coated surface was restrained in the experiment. It was also found that the supercooling degree in the coated supercooling heat exchanger was higher, the supercooling state was longer, and the time of ice blockage was delayed. Thus, more ice production can be obtained accordingly and the efficiency of the whole ice-making system was enhanced.

## O 19: Graphene: Structural properties

Time: Monday 16:00–19:00 Location: WIL C107

O 19.1 Mon 16:00 WIL C107

**Vertical height of quasi-free standing monolayer graphene on SiC(0001): an XSW study** — •J. Sforzini[1], T. Denig[2], T. L. Lee[3], C. Kumpf[1], S. Subach[1], U. Starke[2], F. C. Bocquet[1], and F.S. Tautz[1] — [1]Peter Grünberg institute (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany — [3]Diamond light source ltd, Harwell oxford, Didcot, Oxfordshire, United Kingdom

We investigated a quasi-free standing monolayer graphene sample[1] on SiC(0001) obtained by decoupling the buffer-layer from Si-terminated surface by hydrogen intercalation. We used X-ray Standing Wave technique (XSW), combining dynamical diffraction and X-ray photoelectron spectroscopy, to detect the coherent distribution of the chemically different species (Si and C) at the interface. Our analysis shows two different carbon species (C in the graphene layer and C in the SiC bulk); we find that the adsorption height of the graphene layer is slightly higher than theoretically predicted. The discrepancy, attributed to the very weak graphene-substrate intercation, is still challenging for theory[2].

[1]Riedl, et. al., PRL, 103, 246804 (2009)

[2]Deretzis , et. al., Nanoscale, 5, 671-680 (2012)

O 19.2 Mon 16:15 WIL C107

**Epitaxial graphene nanostructures on SiC** — •Alexander Stöhr[1], Stiven Forti[1], Ulrike Waizmann[1], Thomas Reindl[1], Jens Baringhaus[2], Alexei Zakharov[3], Christoph Tegenkamp[2], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Institut für Festkörperphysik, Leibniz-Universität Hannover, Hannover, Germany — [3]MAX IV Laboratory, Lund University, Lund, Sweden

In recent years a lot of effort was put into the realization of graphene devices, in view of their unique electronic properties and the potential application in logical circuits. However, for the use in logical electronics a band gap would be required. This can be achieved by confining the electrons into quasi-onedimensional graphene stripes, called graphene nanoribbons. When patterning graphene, the altering of the electronic properties by the mechanical attack on the ribbon edges as well as residual resist is always an issue. For that matter we chose to structure the SiC-samples before growing graphene, using electron beam lithography and reactive ion etching. Subsequently, the graphene was grown at elevated temperatures, which also removed the residual resist. As a result onedimensional stripes could be obtained and were decoupled from the substrate by intercalation of hydrogen. Characterization by low-energy electron microscopy and angle-resolved photoemission spectroscopy proves the development of quasi-free standing monolayer graphene ribbons.

O 19.3 Mon 16:30 WIL C107

**Moiré-induced Brillouin zone backfolding of graphene phonons on Ir(111)** — •Michael Endlich[1], Alejandro Molina-Sánchez[2], Henrique Miranda[2], Ludger Wirtz[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau — [2]Physics and Material Sciences Research Unit, University of Luxembourg, L-1511 Luxembourg

The moiré superstructure of graphene on Ir(111) leaves its characteristic footsteps in the phonon dispersion. Replica of the phonon dispersion branches of singly oriented graphene on Ir(111) have been determined throughout the entire surface Brillouin zone with angle-resolved inelastic electron scattering. These replica are rationalized in terms of phonon backfolding induced by the graphene moiré superlattice.

O 19.4 Mon 16:45 WIL C107

**Back Focal Plane Imaging of Raman Scattering from Graphene** — •Harald Budde, Xian Shi, Nicolai Hartmann, and Achim Hartschuh — Department Chemie und CeNS, LMU München, Germany

Raman Scattering Spectroscopy is a powerful technique for studying graphene and other sp2 carbon materials [1]. We combined Raman Spectroscopy with back focal plane (BFP) imaging , a method used to visualize the angular distribution of emitted or scattered light. As an example BFP imaging allows to determine the orientation of single dipolar emitters [2, 3]. For graphene on glass Raman BFP images mainly reflect the polarization characteristics of the different phonon modes. On thin gold films emission from graphene leads to the excitation of propagating surface plasmon polaritons.

[1] A. Ferrari, D. Basko, Nat. Nanotech 8, 235-246, 2013.

[2] M. Lieb, J. Zavislan, L. Novotny, J. Opt. Soc. Am. B 21, 1210-1215, 2004.

[3] N. Hartmann, G. Piredda, J. Berthelot, G. Colas des Francs, A. Bouhelier, A. Hartschuh, Nano Lett. 12, 177-181, 2012.

O 19.5 Mon 17:00 WIL C107

**Ion Irradiation of Metal-Supported Graphene: Exploring the Role of the Substrate** — •Charlotte Herbig[1], Harriet Åhlgren[2], Sabina Simon[1], Carsten Busse[1], Jani Kotakoski[2,3], Arkady V. Krasheninnikov[2,4], and Thomas Michely[1] — [1]II. Phys. Inst., Universität zu Köln, Germany — [2]Dept. of Phys., University of Helsinki, Finland — [3]Faculty of Phys., University of Vienna, Austria — [4]Dept. of Appl. Phys., Aalto University, Finland

Ion irradiation effects on 2D materials are an emerging subject, triggered by graphene's (Gr) potentials in applications. For supported Gr the effect of the substrate on ion beam damage and annealing is important. We investigate the behavior of high quality Gr, weakly coupled to Ir(111), to low energy noble gas ion irradiation by scanning tunneling microscopy (STM), molecular dynamics simulations, and density functional theory (DFT). For a freestanding layer, sputtered atoms leave the layer either in forward or backward direction. For metal-supported Gr, only C atoms carrying backward momentum are sputtered while atoms carrying forward momentum are trapped. As evident from STM and DFT, trapped C atoms form nm-sized Gr platelets at the interface upon annealing at 1000K, assisted by substrate defects. The incorporation into the Gr layer is suppressed due to high migration barriers, while diffusion into the Ir is energetically unfavorable. By measuring the area fraction of the platelets, we obtain the trapping yield, i.e., the number of trapped C atoms per incident ion. Interestingly, compared to the sputtering yield, the trapping yield for Gr on Ir(111) displays a distinctly different dependence on the ion beam angle of incidence.

O 19.6 Mon 17:15 WIL C107

***Ab initio* study of graphene on O-intercalated Ir(111) surface and its functionalization via molecular adsorption** — •Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

To integrate graphene in molecular electronics and spintronics devices it is crucial to understand how the strength of the graphene–metal electrode interaction can be specifically tuned. One possibility to loose or strengthen this interaction is to intercalate adatoms with different chemical reactivity between graphene and the metal surface in question. We will analyse this approach from first principles by considering the case of the O-intercalated graphene on Ir(111) [1]. Another path is to analyse how the adsorption of $\pi-$conjugated organic molecules can affect the electronic structure of a quasi-freestanding graphene layer. We investigated this issue by performing spin-polarized density functional theory (DFT) for a trioxotriangulene-derivate molecule [2] on graphene. Importantly, as already demonstrated in [3], for such systems it is mandatory to include the dispersion interaction and in our *ab initio* study these long-range van der Waals interactions were considered at a semi-empirical [4] or first-principle [5] level.

[1] E. Grånäs *et al.*, ACS Nano. **6**, 9951 (2012).

[2] Y. Morita *et al.*, Nat. Mater. **10**, 946 (2011).

[3] C. Busse *et al.*, Phys. Rev. Lett. **107**, 036101 (2011).

[4] S. Grimme, J. Comput. Chem. **27**, 1787 (2006).

[5] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004).

O 19.7 Mon 17:30 WIL C107

**From two to three dimensions: The effect on the Coulomb interaction by increasing the dimensionality in layered materials** — •M. Rösner[1], E. Sasioglu[2], C. Friedrich[2], S. Blügel[2], A.I. Lichtenstein[3], M.I. Katsnelson[4], and T.O. Wehling[1] — [1]Institut für Theoretische Physik and Bremen Center for Computational Materials Science, Universität Bremen, Bremen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [3]I. Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany — [4]Radboud University Nijmegen, Institute for Molecules and Materials, AJ Nijmegen, The Netherlands

We study the Coulomb repulsion and the dielectric screening in mono-, bi- and tetralayer graphene as well as in graphite. We discuss the transition from 2D systems to the bulk structure in layered materials with regard to the (non) local Coulomb interactions. Therefore, we use *ab initio* constrained random phase (cRPA) calculations to get reliable data in a first step. By tailoring the resulting Coulomb interaction in classical electrostatic models afterwards, we find the following: In addition to the effective height of each layer especially the direction dependence and the non-locality of the dielectric function are the keys to understand the screening effects in these structures. Thereby, we discuss models to estimate the Coulomb interaction of the 2D systems by using exclusively the bulk data as input. We apply these rules to calculate the Coulomb interaction in graphene on iridium and find a very good agreement with *ab initio* data.

O 19.8 Mon 17:45 WIL C107

**Graphene nanolithography with 2.5 nm precision: combining bottom-up and top-down techniques** — •Antonio J. Martínez-Galera[1,2], Iván Brihuega[1,3], Ángel Gutiérrez-Rubio[1], Tobias Stauber[1,3], and José M. Gómez-Rodríguez[1,3] — [1]Departamento Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Present address: II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany. — [3]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain.

The selective modification of pristine graphene represents an essential step to fully exploit its potential. The work presented here overcomes one of the remaining challenges key for the comprehensive integration of graphene in real devices: the realization of lithography below 10 nm sizes. Specifically, we have developed a perfectly reproducible nanolithographic technique for graphene that allows, by means of an STM tip, to modify with 2.5 nm accuracy the electronic properties of graphene monolayers epitaxially grown on Ir(111) surfaces. This method can be carried out also on micrometer sized regions and the structures so created are stable even at room temperature. As a result, we can strategically combine graphene regions presenting large differences in their electronic structure to design graphene nanostructures with tailored properties. Therefore, this novel nanolithography method could open the way to the design of nanometric graphene-based devices with specific functionalities. In particular, we explore here the possibility of developing a new platform for plasmonics.

O 19.9 Mon 18:00 WIL C107

**Relaxation of compressive stresses in graphene through mobile nanoripples** — •Peter Klaver, Shouen Zhu, Marcel Sluiter, and Guido Janssen — Delft University of Technology, Delft, Netherlands

Graphene monolayers have a far smaller thermal expansion coefficient than the Cu substrates on which they are often grown through CVD at high temperature. Once the Cu substrate and graphene monolayer are cooled down to room temperature, the Cu contracts 1.5-2.0% more than the graphene. Yet various experiments do not show graphene layers on Cu to be under significant compressive stress. We present molecular dynamics simulations that show that under compressive stress, small ripples of just a few nm wide appear that absorb the excess graphene area. These ripples are quite mobile, even at room temperature. Their movement offers a mechanism to remove the compressive stress in graphene while keeping it flat, by absorbing the ripples into larger ripples (like those that have formed around bunches of step edges) or by eliminating the ripples at the edges of graphene islands. The relaxation of stresses through the movement of nanoripples is somewhat analogous to flattening out a red carpet by gradually moving a wrinkle away to the carpet edge instead of pulling the entire carpet all at once. The ease with which stresses in graphene relax, is not directly determined by the corrugation energy.

O 19.10 Mon 18:15 WIL C107

**Epitaxial graphene nanoflakes on Au(111) and Ag(111)** — •Julia Tesch[1], Philipp Leicht[1], Lukas Zielke[1], Riko Moroni[1], Bernd Illing[1], Luca Gragnaniello[1], Felix Blumenschein[1], Elena Voloshina[2], Lukas Hammerschmidt[3], Lukas Marsoner Steinkasserer[3], Beate Paulus[3], Yuriy Dedkov[4], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Institut für

Chemie, HU Berlin — [3]Institut für Chemie und Biochemie, FU Berlin — [4]Fritz-Haber-Institut der MPG, Berlin

In zig-zag edge terminated graphene nanoribbons or nanoflakes (GNFs), confinement of electrons is predicted to give rise to edge states with magnetic moments. However, the experimental observation of edge effects is impeded by the inevitable presence of substrates that interact with the flake edges, hence masking the GNFs' intrinsic properties. In the attempt of reducing the graphene substrate interaction, we use an entirely UHV based approach for the preparation of GNFs on Au(111) and Ag(111) surfaces allowing for flake sizes down to 10 nm. GNFs on Ir(111) are prepared by temperature programmed growth [1] and subsequently covered by deposition of several nm of Au or Ag. After post-annealing, the flakes diffuse through the Au or Ag film and form embedded or floating graphene flakes. In scanning tunnelling microscopy (STM), the edges of floating GNFs are found to be singly hydrogen terminated and entire flakes can be laterally displaced with the STM tip on both Au and Ag surfaces, suggesting a considerable reduction of graphene-substrate interactions compared to other metals. [1] Coraux et al., New J. Phys. 11, 023006 (2009)

O 19.11 Mon 18:30 WIL C107

**Scatttering and electronic structure in graphene nanoflakes on Au(111)** — •Philipp Leicht[1], Lukas Zielke[1], Samuel Bouvron[1], Julia Tesch[1], Felix Blumenschein[1], Luca Gragnaniello[1], Lukas Marsoner Steinkasserer[2], Beate Paulus[2], Elena Voloshina[3], Yuriy Dedkov[4], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Institut für Chemie und Biochemie, FU Berlin — [3]Institut für Chemie, HU Berlin — [4]Fritz-Haber-Institut der MPG, Berlin

Confinement of electrons in graphene quantum dots and nano ribbons with atomically well defined edges represents an exciting field of research, owing to predicted peculiar electronic and magnetic properties.

Here, we present scanning tunneling microscopy (STM) investigations of graphene nano flakes (GNFs) prepared by temperature programmed growth on Ir(111) [1] and subsequent intercalation of Au for electronic decoupling. The electronic properties of the graphene flakes are addressed by scanning tunneling spectroscopy. Within our atomically resolved constant-energy maps we can probe the electronic states of the graphene electrons exploiting the intervalley scattering. The hereby obtained dispersion relation shows a linear behavior and can be unambiguously discriminated from the parabolic dispersion relation of the Au(111) surface state electrons. The intervalley scattering of graphene electrons forms discs in the Fourier transforms of constant-energy maps, which include additional scattering features compared to monolayer graphene.

[1] Coraux, J. et al., New J. Phys. 11, 023006 (2009)

O 19.12 Mon 18:45 WIL C107

**Improved effective theories for edge magnetism** — •Cornelie Koop and Manuel Schmidt — Institut für Theoretische Festkörperphysik, RWTH Aachen University, Deutschland

We consider the effective interaction between edge states in graphene nanoribbons. Low-energy edge states come along with a strongly enhanced density of states near the graphene edges, which makes electron-electron correlation important and gives rise to the so-called edge magnetism. In a pristine nanoribbon in first order, there is a direct ferromagnetic intra-edge coupling and an antiferromagnetic interaction between opposite edges. We study the coupling by means of an effective model yielding a separation between edge and bulk states. In particular we investigate the influence of the bulk states on the effective edge state theory via a second order Schrieffer-Wolff transformation. Using both numeric and analytic methods, we calculate various correlation functions. We discuss the results for the effective correlations between smooth edges as well as between the strongly localized states at rough edge structures.

## O 20: Nanostructures at Surfaces II

Time: Monday 16:00–19:15 Location: WIL B321

O 20.1 Mon 16:00 WIL B321

**3d nanoparticle deposition on a W(110) surface** — •Hendrik Bettermann, Matthias Werner, and Mathias Getzlaff — Institute of Applied Physics, University of Duesseldorf

Nanoparticles and clusters are interesting objects both from a fundamental perspective and for technological applications due to their unique electronic and magnetic behavior. These properties are significantly influenced by size and structure of the particles. Our contribution is focused on FeNi alloy nanoparticles deposited on a W(110) surface, additionally in comparison with other magnetic 3d nanoparticles. The particles are generated by a UHV compatible continously working Arc Cluster Ion Source (ACIS) and subsequently mass selected in a static electric field. Scanning Tunneling Microscopy (STM) is our main method to study these objects. We will report on size and structural properties of FeNi nanoparticles with diameters between 4 and 15 nm which satisfy softlanding conditions at kinetic energies well below 0.1 eV per atom.

O 20.2 Mon 16:15 WIL B321

**FeRh on Cu(100): Cluster substrate interaction in terms of band structure** — •Ivan Baev[1], Torben Beeck[1], Kari Jänkälä[2], Michael Martins[1], and Wilfried Wurth[1] — [1]Institut für Experimentalphysik, Universität Hamburg — [2]University of Oulu

Very small clusters are an important subject for a detailed understanding of emerging physical properties such as catalytic behavior or magnetic moments. Theoretical models are often limited to small scales because of their complexity. But band structure calculations of metallic crystals have already been performed since the 1960's and are by now well understood. This forms an ideal reference for experimental measurements.

We will present measurements of the Cu(100) band structure along the $\Gamma X$ direction measured by photoelectron spectroscopy and the influence of small FeRh clusters deposited via soft landing on the copper surface. Changes to the band structure are very strong and depend on the size and the type of clusters atoms involved.

The hybridization of the clusters with the substrate is distinct and affects the copper band in a symmetry adapted way. We will show how it is able to change the substrate band structure atom by atom. Ideally this will enable the tailoring of perfect systems for each given application by tailoring atomic orbitals: e.g. for magnetism a high density of states at the Fermi edge with high spin polarization is desirable while for catalytic materials a matching of molecular orbitals with the surface electronic states is more favorable.

This work is supported by the collaborative research center SFB 668.

O 20.3 Mon 16:30 WIL B321

**Fabrication of nanoscaled Fe deposits by focused electron beam processes as catalyst for C-nanostructures growth** — •Esther Carrasco, Fan Tu, Martin Drost, Florian Vollnhals, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen, Germany

The fabrication of clean iron nanostructures under UHV conditions is feasible via the technique of electron beam induced deposition (EBID) [1]. Fe is also successfully employed as a catalyst for the growth of carbon nanotubes (CNTs) by chemical vapor deposition (CVD) [2]. Control of the structure and location of individual CNTs with lithographic precision over large substrates is desired for their applications in electronic devices. By using EBID, we are able to design an arbitrary distribution of metal nanostructures, which can be used as a template for the fabrication of secondary C-nanostructures by CVD. The objective is twofold: i) a controlled fabrication of novel carbon nanostructures via catalytic growth from the structured EBID deposits. ii) the fabrication of single wall carbon nanotubes (SWCNTs) with specific characteristics from localized iron dots with diameters below 8 nm. Latest results will be presented and discussed. This work was supported by the DFG via grant MA 4246/1-2, MA 4246/2-1, Funcos FOR 1878 and the Cluster of Excellence Engineering of Advanced Materials of the FAU Erlangen-Nürnberg.

[1] T. Lukasczyk et al., Small 4 (2008) 841

[2] C. Mattevi et al., J Phys. Chem. C 112 (2008) 12207

O 20.4 Mon 16:45 WIL B321

**STXM and NEXAFS study of the autocatalytic growth of EBID precursors** — •Florian Vollnhals, Fan Tu, Martin Drost, Esther Carrasco, Andreas Späth, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen, Germany

Electron beam induced deposition (EBID) is a technique for the direct fabrication of nanostructures on surfaces with full lithographic control.[1] In EBID, a metal-organic precursor is adsorbed on a surface and locally decomposed by a highly focused electron beam. Nonvolatile fragments form a deposit while volatile ones are pumped off.

The generally low purity of the deposits is a major challenge. In the case of Fe(CO)$_5$, the high attainable purity of 95+ %at. is linked to autocatalytic decomposition and subsequent growth of the Fe seeds at RT.[2] To study this behavior, which is also expected for other precursors, we prepared EBI deposits from Fe(CO)$_5$ and Co(CO)$_3$NO on Si$_3$N$_4$ membranes in UHV and used STXM and NEXAFS to find that Fe(CO)$_5$ gives rise to linear growth of nearly pure Fe, while the behavior of Co(CO)$_3$NO is complex and yields oxygen rich CoC$_x$N$_y$O$_z$.

Supported by the DFG via grant MA 4246/1-2, MA 4246/2-1, the excellence cluster Engineering of Advanced Materials of the FAU Erlangen-Nürnberg and two granted beamtimes at the PolLux STXM at the Swiss Light Source.

[1] W. van Dorp et al., J. Appl. Phys. 104 (2008), 0801301.

[2] M.-M. Walz et al., Angew. Chem. Int. Ed. 49 (2010), 4669.

O 20.5 Mon 17:00 WIL B321

**Electron Quantization Effects in Pristine and Isophorone-Modified Gold Nano-Islands on MgO Thin Films** — •Christian Stiehler, Wolf-Dieter Schneider, Niklas Nilius, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Electron quantization is a fundamental phenomenon that accompanies the transition from bulk metals to nanoclusters. The associated opening of a gap at the Fermi level crucially affects various properties of the nanostructures, e.g. its electrical and optical behavior and its performance in catalytic reactions [1]. By using low-temperature STM and related spectroscopy, we have investigated the electronic structure of 2D Au islands on MgO/Ag(001) thin films, containing between 50-200 atoms [2]. The bare islands exhibit characteristic quantum well states (QWS), arising from the spatial confinement of the Au-6p-orbitals. To explore the impact of molecular adsorption on this quantized structure, we have attached small quantities of isophorone (C9H14O) onto the Au islands. For ultra-small aggregates, we find a formation of Au-isophorone hybrid structures with clear fingerprints for the formation of covalent bonds between the two species. For larger islands, preferential adsorption of the molecules along the cluster perimeter is observed as well as a rigid downshift of the Au QWS that can be understood in terms of electron donation to the isophorone.

[1] M. Valden, X. Lai, D. W. Goodman, Science 281, 1647 (1998)

[2] C. Stiehler, Y. Pan, W.-D. Schneider, P. Koskinen, H. Häkkinen, N. Nilius, H.-J. Freund, PRB 88, 115415

O 20.6 Mon 17:15 WIL B321

**From insulator to conductor: infrared reflectivity of inverted fishnet designs** — •Stefano De Zuani[1], Marcus Rommel[2], Helga Kumric[1], Audrey Berrier[1], Jürgen Weis[2], Bruno Gompf[1], and Martin Dressel[1] — [1]1. Physikalisches Institut and Research Center SCoPE, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]Max Planck Institute for solid state research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

Metallo-dielectric nanocomposites at the insulator-to-metal transition show a discontinuity in their static conductivity and real permittivity in the infrared region that can in principle be described by percolation theories, assuming a random distribution of the metallic inclusions inside the insulating matrix. But what happens in ordered structures when random percolation is suppressed? We perform a systematic study on nearly closed, 20 nm thick gold films made of periodically arranged gold squares of size a separated by 10 nm gaps on a dielectric substrate. We perform reflectivity and spectroscopic ellipsometry investigations from the visible to the infrared range, increasing the gold filling factor f by changing the size of the squares a from 100 to 3600 nm. Our measurements reveal that square arrays with f around 0.9 exhibit a strongly decreasing reflectivity in the near-infrared range when a is decreasing. Solving Maxwell's equations under the full 3D boundary conditions leads to a reasonable agreement between theory and experiment. Regions of very large near-field enhancement in the gaps can be seen over a large frequency range and are responsible for the trapping of the incident light in the patterned structure.

O 20.7 Mon 17:30 WIL B321

**Field effect and charging in layered 2D materials** — •Thomas Brumme, Matteo Calandra, and Francesco Mauri — Institut de minéralogie et de physique des milieux condensés, Université Pierre & Marie Curie, Paris, France

In recent years, materials with reduced dimensionality such as graphene, dichalcogenides or chloronitrides have attracted a lot of attention because of their interesting physical properties. Particularly challenging is the possibility of doping these systems by using a field-effect transistor (FET). In an ion-liquid based FET configuration the charging of the nanolayers is substantial and thus allows for the investigation of the transition from a band insulator, to a metal and, eventually, to a superconductor [1]. Despite the extensive use of such FETs, many questions remain open. It is, *e.g.*, unclear what changes are induced in the nanolayer by the large electric field. Furthermore the distribution of the induced charge is usually obtained from simple Thomas-Fermi models, that can be inappropriate. In this work [2], we develop a first-principles framework to describe nanolayers in FET configuration. We include the external electric field and the charging in the calculations of the geometric and electronic structure of different nanolayer systems. In the case of ZrNCl we show that the charge doping profile in the nanolayer is very different from what has been proposed in previous analysis based on simple screening models.

[1] Nat Mater **9**, 125 (2010). Science **338**, 1193 (2012).

[2] T. Brumme, M. Calandra, and F. Mauri, in preparation.

O 20.8 Mon 17:45 WIL B321

**STM-induced Doping on Si(553)-Au** — •Ingo Barke[1], Stefan Polei[1], Paul C. Snijders[2], Steven C. Erwin[3], Franz J. Himpsel[4], and Karl-Heinz Meiwes-Broer[1] — [1]University of Rostock, Institute of Physics, 18051 Rostock, Germany — [2]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA and Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996, USA — [3]Center for Computational Materials Science, Naval Research Laboratory, Washington, DC 20375, USA — [4]Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

One-dimensional systems are notoriously difficult to dope because the dopant atoms interrupt the continuity of the quantum wires. Here we propose an alternative route based on transient doping, where charge injection from the tip of a scanning tunneling microscope drives the quasi one-dimensional system Si(553)-Au into an excited structural phase [1]. Time-dependent measurements enable access to the system's dynamics revealing rapid fluctuations due to a competition between excitation and decay. The current-dependent lifetimes hint at a barrierless decay of the excited (i.e. doped) state, letting the system behave like an optically excited molecule in close analogy to an excimer.

[1] Polei et al., PRL 111, 156801 (2013).

O 20.9 Mon 18:00 WIL B321

**Do you believe in thermodynamics? Towards a predictive modeling of adsorbed clusters.** — •Chiara Panosetti, Dennis Palagin, and Karsten Reuter — Technische Universität München, Germany

Materials applications generally require the stabilization of engineered atomic clusters at solid surfaces. For metal-doped $M$@Si$_\mathrm{n}$ cages this can be achieved either via controlled deposition of preformed clusters or direct silicide formation at Si surfaces. Particularly for the latter, technologically appealing approach quantitative theory could effectively aid experimental design by predicting deposition conditions at which desired cluster structures form spontaneously at the surface. We propose to approach this problem by suitably combining configurational sampling within an *ab initio* thermodynamics framework. Hereby, the stability of globally optimized geometries of different stoichiometry can be compared through evaluation of thermodynamic functions. Our results demonstrate the possibility of a qualitative prediction of experimental mass-spectra abundances of isolated $M$@Si$_\mathrm{n}$ clusters, suggesting thermodynamics to primarily rule cluster formation in the cluster source. The possibility of extending this equilibrium picture towards cluster formation at extended surfaces will be critically evaluated.

O 20.10 Mon 18:15 WIL B321

**Cluster Nucleation and Growth from a Highly Supersatu-**

**rated 2D Phase: Ag/Fe$_3$O$_4$(001)** — •Roland Bliem[1], Lukas Perneczky[1], Zbynek Novotny[1], David Fobes[2], Zhiqiang Mao[2], Michael Schmid[1], Ulrike Diebold[1], and Gareth Parkinson[1] — [1]Vienna University of Technology, Vienna, Austria — [2]Tulane University, New Orleans, Louisiana, USA

The nucleation and growth of Ag clusters at the $(\sqrt{2}\times\sqrt{2})$R45°-Fe$_3$O$_4$(001) surface was studied using scanning tunneling microscopy (STM). This surface functions as a robust adsorption template, stabilizing a complete array of Ag adatoms with a nearest-neighbor distance of 0.84 nm to temperatures as high as 670 K. As the coverage exceeds 1 ML, the number of Ag adatoms exceeds the number of available adsorption sites and the system enters a supersaturated state. Cluster nucleation occurs spontaneously at room temperature and, with mild annealing, the nuclei grow at the expense of the surrounding material. This behavior cannot be reconciled with any of the established growth modes. From an analysis of the denuded zones, or “vacancy trails”, associated with each cluster, three distinct growth processes are discerned. Cluster nuclei are mobile and diffuse to step edges, capturing otherwise stable Ag adatoms encountered along their path. With the clusters immobilized, adatom diffusion and capture takes over as the dominant process. Above 720 K, the $(\sqrt{2}\times\sqrt{2})$R45° reconstruction is lifted, and the system evolves rapidly to large (>10 nm) nanoparticles, consistent with the thermodynamic preference for 3D crystallites.

O 20.11 Mon 18:30 WIL B321

**Unraveling structural and catalytic properties of Au-Pt nanoalloys** — •Linn Leppert[1], Rodrigo Q. Albuquerque[2], Adam S. Foster[3], and Stephan Kümmel[1] — [1]Theoretical Physics IV, University of Bayreuth, Germany — [2]Institute of Chemistry of Sao Carlos, University of Sao Paulo, Sao Carlos, Brazil — [3]COMP/Department of Applied Physics, Aalto University School of Science, Aalto, Finland

The high catalytic activity of Au nanoparticles (NPs) is a prime example for the special properties of metal clusters. By alloying, e.g. with Pt, the properties of Au NPs can further be significantly improved. However, the fundamental question of why alloying improves the NP properties is still poorly understood. Moreover, there is an ongoing debate on the mixing patterns of these systems. While theory predicts core-shell NPs, homogeneously mixed NPs are observed in experiment. In this contribution we address structural and electronic properties of Au-Pt NPs using density functional theory and semi-empirical molecular dynamics simulations. We show that the discrepancy between theory and experiment might have its reason in a misinterpretation of x-ray diffraction patterns. Furthermore, we discuss that special catalytic properties of Au-Pt NPs are expected based on general considerations, i.e., inherent properties of the Au and Pt component, respectively.

O 20.12 Mon 18:45 WIL B321

**Nanooxidation - Oxidation kinetics of small Rh nanoparticles** — •Patrick Müller[1,2], Heshmat Noei[1,2], Thomas F. Keller[1], Björn Arndt[1,2], Peter Wochner[3], Roberto Felici[4], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchrotron, 22603 Hamburg, Germany — [2]Fachbereich Physik, Universität Hamburg, 20355 Hamburg, Germany — [3]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [4]European Synchrotron Radiation Facility, 38043 Grenoble, France

Metal nanoparticles (NPs) are used in many technical fields such as heterogeneous catalysis and biosensors. Although the oxidation behaviour of transition metal surfaces was studied in depth in the past, the oxidation kinetics of small NPs is poorly understood. The traditional oxidation theory proposes different growth laws for single crystal surfaces, but does not take into account the properties of NPs like their shape. In recent studies the oxidation theories were modified to also comprise geometrical aspects as the curvature of the NP by using a spherical model [1,2]. Our experiments focused on the systematic study of the size dependence of the oxidation kinetics of half spherical Rh NPs with particles sizes from 2 to 12 nm on sapphire at 573 K and $10^{-3}$ mbar oxygen pressure. The experiments were carried out at the MPI beamline at ANKA and beamline ID03 at the ESRF. We employed x-ray reflectivity and grazing incidence small angle x-ray scattering. Our results demonstrate a dramatic change in the oxidation kinetics for the smallest NPs. [1] A. Ermoline, E. L. Dreizin, Chem. Phys. Lett. 505, 47 (2011);[2] A. T. Fromhold Jr., J. Phys. Chem. Solids 49, 10 (1988)

O 20.13 Mon 19:00 WIL B321

**Structural Changes of Cobalt Nanoparticles during Chemical Reactions: A RHEED Study** — •Stephan Bartling, Ingo Barke, Hannes Hartmann, Steve Jäger, and Karl-Heinz Meiwes-Broer — University of Rostock, Institute of Physics, 18051 Rostock, Germany

Size-selected cobalt oxide clusters deposited on amorphous alumina films can act as selective and efficient nanocatalysts for the dehydrogenation of cyclohexane [1]. In this contribution we present a new setup for reflection high energy electron diffraction (RHEED) under reactive conditions up to a pressure of $10^{-3}$ mbar. Soft-landed Co clusters of sizes in the nm range are exposed to oxygen and heated during the experiment. The evolution of RHEED patterns shows that the particles significantly change their structure at a critical temperature. The contributing phases are discussed in view of expected cobalt oxide stoichiometries and morphologies.

[1] E.C. Tyo et al., ACS Catalysis **2 (11)**, 2409 (2012)

## O 21: Transport: Quantum Dots, Quantum Wires, Point Contacts II (TT jointly with O)

Time: Monday 16:00–18:30 Location: HSZ 204

O 21.1 Mon 16:00 HSZ 204

**A two-atom electron pump** — Benoit Roche[1], Roman-Pascal Riwar[1], Benoit Voisin[1], Eva Dupont-Ferrier[1], Romain Waquez[3], Maud Vinet[3], Marc Sanquer[1], •Janine Splettstoesser[2], and Xavier Jehl[1] — [1]SPSMS, UMR-E, CEA Grenoble, INAC, Grenoble, France — [2]MC2, Chalmers University of Technology, Göteborg, Sweden — [3]CEA, LETI, MINATEC, Grenoble, France

In recent years there has been a lot of interest in time-dependently driven quantum systems, such as quantum-dot pumps, both in the adiabatic regime of slow driving as well as in the high-frequency regime. However, all experiments so far were carried out in either one of these regimes, but were not subsequently tuned to both. I will present an experimental realization [1] of electron pumping through two phosphorus donors in series implanted in a silicon nanowire. While quantized pumping is achieved in the low-frequency adiabatic regime, remarkable features are observed at higher frequency, when the charge transfer is limited either by the tunnelling rates to the electrodes or between the two donors. We model the transitions between quantum states involving a Landau-Zener transition, allowing to reproduce in detail the characteristic signatures observed in the non-adiabatic regime. Interestingly, the breakdown of the adiabatic limit can thus accurately be associated to the relation of the respective time-scales of tunneling to the electrodes or between the donors, compared to the time-scales of the driving. Consequently, information on the time-scales can be extracted from a detailed inspection of the pumping signal.

[1] B. Roche, *et al.*, Nat. Commun. 4, 1581 (2013)

O 21.2 Mon 16:15 HSZ 204

**Functional renormalization group in Floquet space and its application to periodically driven quantum dots** — •Katharina Eissing[1,2], Stefan Göttel[1,2], Dante Marvin Kennes[1,2], and Volker Meden[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, 52074 Aachen, Germany — [2]JARA Fundamentals of Future Information Technology, 52056 Aachen, Germany

The functional renormalization group (RG) was recently extended to study interacting, low-dimensional systems out of equilibrium. This includes correlated quantum dot setups with explicitly time-dependent Hamiltonians as e.g. realized in quantum quenches or in the presence of time-dependent bias voltages [Phys. Rev. B 85, 085113 (2012), Phys. Rev. B 85, 245101 (2012)]. However, following this route periodic pumping processes, which are of particular interest in e.g. nanoelectronics and quantum information science, can only be described in an inefficient way. Taking advantage of the periodicity, we combine the Floquet theorem with the functional RG. This allows us to transform the double-time self-energy and Green functions in the Floquet basis [J. Phys.: Condens. Matter 20 085224] and the functional RG treatment resembles the stationary formalism. This makes it feasible to study transport in periodically driven systems. In my talk, I will shortly introduce this Floquet theorem based functional RG and present first results on transport through a quantum dot described by the interacting resonant level model.

O 21.3 Mon 16:30 HSZ 204

**Interplay of edge state polarization and a Zeeman split quantum dot** — •Benedikt Probst[1], Pauli Virtanen[2], and Patrik Recher[1] — [1]Institute for Mathematical Physics, TU Braunschweig, Braunschweig, Germany — [2]O.V. Lounasmaa Laboratory, Aalto University, Finland

Topological insulators are a novel state of matter showing interesting physics. One of the effects realized in these materials is the quantum spin Hall effect in which electrons with different spin propagate in different directions on the edge of the system. Applying a bias to the system therefore leads to a spin bias for the edge state. We consider a system in which a quantum dot in the Coulomb blockade regime is attached to a helical Luttinger liquid. This quantum dot is treated as a localized spin, which can be manipulated by a magnetic field. The dynamics of the dots are described by setting up a general master equation. From the steady state of the system the polarization of the dot and the differential edge conductance is calculated. We discuss a regime in which the dot polarization exhibits a strong bias dependence and a regime in which the transport shows a characteristic bias asymmetry which allows to identify the relative orientation of the spin polarization in the edge state with respect to the magnetic field.

**15 min. break.**

O 21.4 Mon 17:00 HSZ 204

**Entanglement detection in an interacting beam-splitter device** — •Alexander Schroer[1], Bernd Braunecker[2], Alfredo Levy Yeyati[3], and Patrik Recher[1] — [1]Institute for Mathematical Physics, TU Braunschweig, Germany — [2]Department of Theoretical Condensed Matter Physics, Universidad Autónoma de Madrid, Spain — [3]School of Physics & Astronomy, University of St Andrews, UK

We investigate a tunnel contact between two Luttinger liquids, e.g. realized as two crossed one-dimensional nanowires. When injecting one of two electrons with opposite spin in each wire, the current measured behind the crossing differs for singlet, triplet or product states. This is an apparent non-Fermi liquid feature because the current has been shown to be independent of spin-entanglement for Fermi liquid beam-splitters before. It can be understood in terms of collective excitations and by taking spin-charge separation into account. This behavior may offer an easier alternative to traditional entanglement detection schemes based on current noise, which turns out to be suppressed by the electron-electron interaction.

O 21.5 Mon 17:15 HSZ 204

**Hierarchical Equation of Motion Investigation of Decoherence and Relaxation Dynamics in Nonequilibrium Transport through Interacting Quantum Dots** — •Rainer Härtle[1,2], Guy Cohen[3], David R. Reichman[3], and Andrew J. Millis[2] — [1]Institut für theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Department of Physics, Columbia Universtiy, New York, USA — [3]Department of Chemistry, Columbia Universtiy, New York, USA

A recently developed hierarchical quantum master equation approach [1,2] is used to investigate nonequilibrium electron transport through an interacting double quantum dot system in the regime where the inter-dot coupling is weaker than the coupling to the electrodes. The corresponding eigenstates provide tunneling paths that may interfere constructively or destructively, depending on the energy of the tunneling electrons [3]. Electron-electron interactions are shown to quench these interference effects in bias-voltage dependent ways, leading, in particular, to negative differential resistance, population inversion and an enhanced broadening of resonances in the respective transport characteristics [2]. Relaxation times are found to be very long, and to be correlated with very slow dynamics of the inter-dot coherences. The ability of the hierarchical quantum master equation approach to access very long time scales is crucial for the study of this physics.

[1] J. Jin *et al.*, J. Chem. Phys. 128, 234703 (2008).
[2] R. Härtle *et al.*, arXiv:1309.1170 (2013)
[3] R. Härtle *et al.*, Phys. Rev. B 87, 085422 (2013)

O 21.6 Mon 17:30 HSZ 204

**Detection of the decay rates in interacting quantum dots** — •Jens Schulenborg[1,2], L. Debora Contreras- Pulido[3], Michele Governale[4], and Janine Splettstoesser[1,2] — [1]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Göteborg, Sweden — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [3]Institut für Theoretische Physik, Universität Ulm, Germany — [4]School of Physical and Chemical Sciences, Victoria University of Wellington, New Zealand

Over the past years, potential applications in nanoelectronics, metrology and quantum information sparked great interest in studying the *dynamics* of time-dependently driven quantum dots. Recently, the relaxation rates in the dynamical response of an interacting single-level quantum dot, weakly tunnel coupled to an electronic reservoir and brought out of equilibrium by a step pulse, have been investigated [1].

This theoretical work focuses on the readout of these relaxation rates with a capacitively coupled sensor quantum dot (SQD). Using a generalized master equation approach for the combined system of dot and SQD, we investigate the measurability of the dot relaxation behavior via the SQD current, especially accounting for back-action effects.

Our results reveal parameter regimes in which back-action leads to a decrease of the dot decay rates and to a mixing of relaxation modes that decay independently in the absence of a measurement. However, avoiding these regimes, we show that the original dot rates can still be extracted from the SQD current.

[1] L. D. Contreras-Pulido et al., Phys. Rev. B **85**, 075301 (2012).

O 21.7 Mon 17:45 HSZ 204

**Hybrid Microwave Cavity Heat Engine** — Christian Bergenfeldt[1], Peter Samuelsson[1], •Björn Sothmann[2], Christian Flindt[2], and Markus Büttiker[2] — [1]Physics Department, Lund University, Box 118, SE-22100 Lund, Sweden — [2]Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

We propose and analyze the use of hybrid microwave cavities as quantum heat engines. A possible realization consists of two macroscopically separated quantum dot conductors coupled capacitively to the fundamental mode of a microwave cavity. We demonstrate that an electrical current can be induced in one conductor through cavity-mediated processes by heating up the other conductor. The heat engine can reach Carnot efficiency with optimal conversion of heat to work. When the system delivers the maximum power, the efficiency can be a large fraction of the Carnot efficiency. The heat engine functions even with moderate electronic relaxation and dephasing in the quantum dots. We provide detailed estimates for the electrical current and output power using realistic parameters.

[1] C. Bergenfeldt, P. Samuelsson, B. Sothmann, C. Flindt and M. Büttiker, arXiv:1307.4833v1 (2013).

O 21.8 Mon 18:00 HSZ 204

**Vibration-induced thermoelectric effects in quantum dots** — •Matti Laakso and Volker Meden — Institut für Theorie der Statistischen Physik, RWTH Aachen, Aachen, Germany

We study the thermoelectric transport through a quantum dot coupled to a single vibrational mode described by the Anderson-Holstein model. We use analytical methods in the linear response regime as well as the functional renormalization group (FRG) in the non-linear regime. We predict relatively large thermoelectric effects in the parameter regime where the phonon-mediated electron-electron interaction dominates over the bare Coulomb repulsion.

O 21.9 Mon 18:15 HSZ 204

**Superexchange transport and blockade in triple quantum dots** — •Rafael Sánchez[1], Ghislain Granger[2], Fernando Gallego-Marcos[1], Sergei A. Studenikin[2], Andrew S. Sachrajda[2], and Gloria Platero[1] — [1]Instituto de Ciencia de Materiales de Madrid, CSIC, E-28049 Madrid, Spain — [2]National Research Council Canada, Ottawa, ON K1A 0R6 Canada

We present recent experimental evidence of long range transport in triple quantum dots. Superexchange is responsible for the spin-dependent indirect coupling of the two outer quantum dots, mediated by virtual transitions through the middle one. They are manifested in the form of sharp current resonances at the degeneracy points of states with left-right symmetric charge distributions [1,2]. The transition can take two paths: two electrons in different dots tunnel simultaneously [1] or a single electron tunnels twice [2].

We analyze a configuration where the two paths with different virtual intermediate states are possible and lead to quantum interference. Remarkably, we find conditions where the destructive interference of these transitions completely cancels the transport, what we call superexchange blockade [3]. Spin correlations play an essential role by avoiding certain transitions. This effect, known as spin blockade, leads to the suppression of certain resonances whose observation gives a measure of spin decoherence times.
[1] M. Busl et al., Nature Nanotech. 8, 261 (2013).
[2] R. Sánchez et al., submitted.
[3] R. Sánchez, F. Gallego-Marcos and G. Platero, submitted.

## O 22: Organic Electronics and Photovoltaics II (CPP jointly with DS, HL, O)

Simulations, Polymers, Solar Cells

Time: Monday 15:00–18:00 Location: ZEU 222

O 22.1 Mon 15:00 ZEU 222

**Quantumchemical Calculation of Zn-Porphyrine-Indolocarbazole-Conjugates** — •Ksenia Korshunova and Wichard J. D. Beenken — Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

We have investigated the structure of Zn-porphyrin-indolocarbazole conjugates with a different number of indolocarbazol meso-substituents without and with THF and DMF axial ligands by quantumchemical methods in order to interpret experimental data such as Absorption spectra, fluorescence lifetime and quantum yields in different solutions. Contrarily to our expectations, we found very weak deformation the Zn-porphyrin macrocycle under the in uence of axial THF and DMF ligands, which only tend to pull the central Zn-atom out of its equilibrium position in the macrocycle plane. This means that the very different fluorescence yields for Zn-porphyrin-indolocarbazoles in toluole, THF, and DMF cannot be explained by a conformational change.

O 22.2 Mon 15:15 ZEU 222

**Estimating Coulomb model parameters in organic molecules from first principles** — •Irina Petreska[1,2], Ljupco Pejov[2], Ljupco Kocarev[3,4], and Gertrud Zwicknagl[1] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, 38 106 Braunschweig, Germany — [2]Faculty of Natural Sciences and Mathematics, Ss. Cyril and Methodius University, 1 000 Skopje, Republic of Macedonia — [3]Macedonian Academy of Sciences and Arts, Skopje, Republic of Macedonia — [4]Faculty of Computer Science and Engineering, Ss. Cyril and Methodius University, 1 000 Skopje, Republic of Macedonia

The Coulomb parameters are estimated from electronic structure calculations based on Density Functional Theory (DFT). Of particular interest are phenylene ethynylene oligomers exhibiting electric-field controlled conductance switching. The charge transport properties are analyzed adopting a simplified two-site model accounting for Coulomb correlation effects. The Coulomb parameters are deduced from a population analysis. The DFT calculations employ a combination of the Becke's three parameter adiabatic connection exchange functional (B3) with the Lee-Yang-Parr correlation one (LYP). The Kohn-Sham SCF equations are iteratively solved using the LANL2DZ basis set, for orbital expansion, on an "ultrafine" grid for numerical integration.

O 22.3 Mon 15:30 ZEU 222

**Theoretical Study of Simultaneous Electron- and Excitation Energy Transfer in a Fullerene-Chromophore Complex** — •Thomas Plehn, Jörg Megow, and Volkhard May — Humboldt-Universität zu Berlin, Germany

Mainly during the last decade fullerene based molecular systems have been of increasing interest with regard to future components in dye sensitized solar cells and artificial photosynthetic systems. This theoretical study focuses on the characteristic photoinduced charge separation process in a supramolecular complex containing a single fullerene and six pyropheophorbide-a molecules. For this purpose the excitation energy transfer processes are treated among the six chromophores. Simultaneously electron transfer takes place from the excited chromophores to the fullerene. The whole investigation uses molecular dynamics simulations of the highly flexible complex in explicit solvent environment. The transfer phenomena are described in terms of a special mixed quantum-classical version of the Förster- [1] and the well-known classical Marcus rate. Finally the charge separation process is computed concerning an ensemble of complexes. The resulting dynamics are in very good agreement with appropriate experimental data [2].

[1] J. Megow et al., ChemPhysChem 2011, 12 645-656
[2] M. Regehly et al., J. Phys. Chem. B 2007, 111, 998

**Invited Talk** O 22.4 Mon 15:45 ZEU 222

**Controlled crystallization of semiconducting polymer thin films** — •Sabine Ludwigs — Institute for Polymer Chemistry, University of Stuttgart, Germany

The talk will give an overview over current activities in my team on the morphological control of semiconducting polymers for applications in polymer electronics. Different methods to induce and control crystalline order over large areas in thin films will be presented. These include swelling and deswelling in defined solvent vapour atmospheres of good solvents and crystallization under confinement and with external fields. Regarding polymer materials we are currently extending our studies from conventional p-type semiconductors based on pure thiophenes like P3HT[1] to high performance p-type low bandgap polymers such as PCPDTBT[2] and n-type polymers such as PNDI2OD-2T[3]. The control of molecular orientation over macroscopic distances allows us to study the relationship between the polymer microstructure and the resulting charge transport properties along specific crystallographic directions.

[1] E. Crossland, K. Tremel, F.S.U. Fischer, K. Rahimi, G. Reiter, U. Steiner, S. Ludwigs, Adv. Mater. 2012, 24, 838. [2] F.S.U. Fischer, K. Tremel, A.-K. Saur, S. Link, N. Kayunkid, M. Brinkmann, D. Herrero-Carvajal, J. T. López Navarrete, M. C. Ruiz Delgado, S. Ludwigs, Macromolecules 2013, 46, 4924. [3] K. Tremel, F.S.U. Fischer, N. Kayunkid, R. DiPietro, R. Tkachov, A. Kiriy, D. Neher, S. Ludwigs, M. Brinkmann, Charge Transport Anisotropy in Highly Oriented Thin Films of the Acceptor Polymer P(NDI2OD-T2), submitted.

**15 min break**

O 22.5 Mon 16:30 ZEU 222

**Conjugated oligomers near surfaces with different physical and chemical nature: MD simulation of adsorption layers** — •Olga Guskova[1] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, D-01069 Dresden — [2]Techische Universität Dresden, Institut für Theoretische Physik, Zellescher Weg 17, D-01062 Dresden

Atomistic molecular dynamics simulations are used to explore some general principles of 2D supramolecular organization of conjugated oligomers on adsorbing substrates. Two systems are studied: (i) terminally substituted dicyanovinyl quaterthiophenes, prototypic absorbers for small molecule organic solar cells on a silica surface [1] and (ii) 2,5-dialkoxy-phenylene-thienylene-based oligomers on epitaxial monolayer graphene [2]. We demonstrate that the driving force of molecular orientation on substrate is embodied by the chemical nature of the surface and the character and position of functional groups the conjugated molecule bearing, i.e. the underlying balance of forces defines the spatial orientation - standing upright or lying-down molecules on substrates. This force balance clearly allows isolated molecules to explore flat, bent or twisted molecular conformations and to exploit force anisotropies to maximize their interactions when crystals are growing.
[1] O.A. Guskova et al. // J. Phys. Chem. C 2013. V. 117. P. 17285.
[2] R. Shokri et al. // J. Am. Chem. Soc. 2013. V. 135. P. 5693.

O 22.6 Mon 16:45 ZEU 222

**Frank elastic constants in nematic mesophases of polymeric semiconductors** — •Patrick Gemünden, Kurt Kremer, and Kostas Ch. Daoulas — Max Planck Institute for Polymer Research, Mainz

Liquid crystalline (LC) mesophases of polymeric semiconductors[1] can facilitate material processing. We develop a particle-based modeling approach considering poly(alkylthiophenes) as a test system for studying nematic mesophases. The method uses "soft tube" representations of chains where non-bonded potentials are defined by soft, directional interactions.[2,3] Here, we focus on Frank elastic constants (FC). Calculating FCs is important for comparing material properties from the soft model with experiments, studying theoretical questions related to FCs in polymer nematics and linking particle-based and continuum descriptions of LCs. We calculate FCs related to bend, splay and twist deformations from the fluctuations of the local nematic director. Indeed, the magnitudes of the FCs from our simulations agree with experiments on polymer nematics. We study the dependence on system parameters, e.g. chain length, and compare with predictions by analytical field theory.[4] Eventually we study local density fluctuations in the nematic samples, which, as predicted by theory, lead to an anisotropic scattering pattern and can be related to the elastic properties.

[1] Ho et al., Macromolecules 43, 7895 (2010) [2] Gemünden et al., Macromolecules 46, 5762 (2013) [3] Daoulas et al., J. Phys.: Condens. Matter 24, 284121 (2012) [4] Le Doussal & Nelson, Europhys. Lett. 15, 161 (1991)

O 22.7 Mon 17:00 ZEU 222

**Modeling LC mesophases in polymeric semiconductors with soft directional interactions** — Patrick Gemünden, Carl Poelking, Kurt Kremer, Denis Andrienko, and •Kostas Daoulas — Max Planck Institute for Polymer Research, Mainz

Often in Soft Matter mesoscale behavior couples across a hierarchy of scales to details of molecular architecture and interactions. When modeling such materials, features accounting for the latter must be included even in drastically coarse-grained (CG) representations. Focusing on liquid crystalline (LC) mesophases of polymeric semiconductors, we highlight a top-down strategy for developing such models, projecting classical density functionals on particle-based representations. Poly(3-alkylthiophenes) (P3AT) are considered as an example. Two different CG models are developed, representing: a) the polymer chain with a "soft" flexible tube [1] and b) each alkylthiophene as a plate-like object [2]. The first describes uniaxial nematics and the second captures biaxial nematic ordering, mimicking effects of anisotropy in microscopic interactions and chain architecture. We demonstrate that the model reproduces realistic material properties in nematic mesophases. In biaxial morphologies we discuss how collective orientation and planarization of molecules affects the lengths of conjugated segments, defined via conjugation-breaking torsional defects [3]. First results on the interplay between nematic ordering and phase separation in blends of P3AT with nanoparticles are presented.[1] Daoulas et al, J. Phys.: Condens. Matter (2012) 24, 284121 [2] Gemünden et al, Macromolecules (2013) 46, 5762 [3] Rühle et al, J. Chem. Phys. (2010) 32, 134103.

O 22.8 Mon 17:15 ZEU 222

**Correlating structural order and morphology with transport properties in donor-acceptor block copolymers for organic photovoltaics** — •Gaurav Gupta[1], Chetan Raj Singh[2], Ruth Lohwasser[3], Peter Muller Buschbaum[4], Mukundan Thelekkat[3], Harald Hoppe[2], and Thomas-Thurn Albrecht[1] — [1]Martin-Luther-Universität Halle-Wittenberg,Germany — [2]Technische Universität Ilmenau, Germany — [3]University of Bayreuth,Germany — [4]Technische Universität München,Germany

Microphase separated donor-acceptor block copolymers are promising systems for morphology control in OPV's. A nanostructure on exciton diffusion length scale, crystalline order and percolating pathways for charge transport are pre-requisites for obtaining good device properties. We here present a systematic study of the correlation between structure and charge transport in thin films of P3HT-b-PPerAcr after different thermal treatments. Combining AFM, microscopy and GISAXS we show that films annealed in the melt state above the melting temperatures of both components form typical microphase separated structures oriented parallel to the substrate, while films crystallized from the disordered state as obtained from spin coating show no well-defined microphase separated structures. GIWAXS measurements reveal that crystallization from the ordered state leads to strongly textured samples. Charge carrier mobilities as measured by SCLC were improved by 2 orders of magnitude in films crystallized from the disordered state, the unfavorable orientation of the microphase morphology in melt annealed films resulted in poor device performance.

O 22.9 Mon 17:30 ZEU 222

**Origins of Reduced Nongeminate Recombination in P3HT:PCBM Organic Solar Cells** — •Michael C. Heiber[1], Julien Gorenflot[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Understanding the nongeminate recombination processes that are the dominant loss mechanisms in organic solar cells is critical to improving device performance. In P3HT:PCBM blends, nongeminate recombination has been found to be significantly slower than expected from Langevin theory and also exhibits super-second order kinetics. Several theories for this behavior have been proposed, but a complete model has not yet been reached. To shed light on this problem, we have used a combination of transient absorption spectroscopy experiments and kinetic Monte Carlo simulations. By modeling the temperature dependence of the polaron transients measured in both neat P3HT films and annealed P3HT:PCBM blend films, we demonstrate the effects of phase separation, carrier trapping, and charge transfer states on the magnitude of the recombination rate. Furthermore, we show that while neat P3HT films exhibit second order recombination and mobility behavior indicating a Gaussian density of states (DOS), P3HT:PCBM blends are complicated by super-second order recombination that is indicative of an exponential DOS and mobility measurements that are consistent with a Gaussian DOS. To unify these observations, we show that a separate distribution of charge transfer states must be included.

O 22.10 Mon 17:45 ZEU 222

**Model systems for interchromophoric interactions in conjugated polymer materials** — •Thomas Stangl[1], Daniela Schmitz[2], Klaas Remmerssen[2], Dominik Würsch[1], Florian Steiner[1], Sigurd Höger[2], Jan Vogelsang[1], and John Lupton[1] — [1]Universität Regensburg, Regensburg, Deutschland — [2]Universität Bonn, Bonn, Deutschland

A set of pi-conjugated oligomer dimers templated in molecular scaffolds is presented as a model system of the interactions between chromophores in conjugated polymers. Single-molecule spectroscopy was used to reveal electronic aggregation between two oligomers with different well-defined distances and single polymer chains. It is concluded that the model systems can be used to investigate the impact of H-aggregation as a function of interchromophoric distance by simultaneous measurement of lifetime and single-molecule spectra. This reveals a strong heterogeneity in coupling strengths even for identical single molecules. Further, it is shown that the coupling strength varies over time on a single molecule, leading to the conclusion that electronic aggregation has to be understood as a dynamic property. In bulk polymer films, such interchromophoric coupling impacts the functionality, e.g. the emission color and the migration of excitation energy to quenching sites. Realizing the presence and dynamics of such interactions is crucial for understanding limitations in quantum efficiency of larger conjugated polymer materials.

# O 23: Organic Electronics and Photovoltaics III (DS jointly with CPP, HL, O)

Time: Monday 18:00–19:45 Location: CHE 91

O 23.1 Mon 18:00 CHE 91

**Studying the electric potential of organic solar cells** — •Michael Scherer[1,2,3], Tobias Jenne[1,2,3], Rebecca Saive[1,2,3], Felix Schell[1,2,3], Robert Lovrincic[1,2,3], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab GmbH, Heidelberg — [2]TU Braunschweig — [3]Universität Heidelberg

Despite steadily increasing efforts in the research on organic semiconductors, many of the models applied in the field are restricted to small clusters of molecules or model systems only, thus lacking prediction when it comes to full devices. With scanning Kelvin probe microscopy (SKPM) accompanied by device simulations we try to access the physics of entire OSC devices and bridge the gap between the molecular and the macroscopic understanding.

Our scanning probe station is placed within the vacuum of a scanning electron microscopy (SEM)/focused ion beam (FIB) cross beam system. We prepare OSC cross sections with the FIB and place the cantilever under SEM observation right at the cross section. Thus we are able to investigate the potential distribution of OSCs in situ with SKPM.

The SKPM measurements are backed by IV characterization and device simulations. Varying the parameter of the active layer/contact interface, we investigate their impact on the potential distribution and the device characteristics of the OSC. In IV measurements and cross sectional SKPM measurements we check the validity of the applied models and identify loss mechanisms and their localization in the solar cell device.

O 23.2 Mon 18:15 CHE 91

**Correlation of electric properties and interface band alignment in organic light-emitting diodes** — •Maybritt Kühn[1,2], Eric Mankel[1,2], Christof Pflumm[3], Thomas Mayer[1,2], and Wolfram Jaegermann[1,2] — [1]Technische Universität Darmstadt, Institute of Materials Science, Surface Science Division — [2]InnovationLab GmbH, Heidelberg — [3]Merck KGaA, Darmstadt

Organic light-emitting diodes consist of several functional organic layers sandwiched between two electrodes with different work functions. At the current onset voltage the applied electric field is high enough that charge carrier injection and transport begins. In some device structures the onset voltage increases with increasing thickness of the emission layer. We present a detailed study on this up to now unpredictable phenomenon by combining IV-measurements and interface investigations using photoelectron spectroscopy (XPS/UPS). We focus on two isomers synthesized by Merck that serve as matrix material in the emission layer-one showing the changes in onset voltage the other not. The complex device architecture was reduced to a model device system using NPB as hole-transport layer and the undoped isomers as emission layer. The shift in onset voltage can still be observed in the model devices as well in hole-only devices derived from the model system. By stepwise evaporation of the respective isomer onto NPB we performed PES-interface experiments and analyzed the band alignment between NPB and the isomers in an integrated UHV system. It was found that the hole injection barrier is larger by about 200 meV in case of the isomer showing the observed shift in onset voltage.

O 23.3 Mon 18:30 CHE 91

**Temperature dependent exciton diffusion length in ZnPc** — •Bernhard Siegmund[1], Johannes Widmer[1], Simone Hofmann[1], Moritz Riede[2], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Dresden, Germany — [2]Current address: Clarendon Laboratory, Oxford, England

The photo-current of organic solar cells is the result of a multi-step process. It includes the generation and diffusion of excitons as well as their separation into free charge carriers, the transport to the electrodes, and their final extraction. One bottleneck for highly efficient devices is the short exciton diffusion length in organic materials.

In this work, the singlet exciton diffusion length $\ell_{\mathrm{diff}}$ in the absorber material ZnPc is studied. For this purpose, the photo-current of organic solar cells, incorporating ZnPc and $C_{60}$ in a flat heterojunction architecture, is measured and modelled as a multi-step process. $\ell_{\mathrm{diff}}$ is extracted from a thickness variation of the absorber layer, as not yet encountered in the context of modelling the photo-current to determine $\ell_{\mathrm{diff}}$ before. Measurements at varying temperature between 200 K and 370 K reveal a thermal activation of the diffusion length above 310 K. This is interpreted as promotion of the excitons to higher energies with a density of states allowing for enhanced hopping transport. The activation energy is considered as a measure for the energetic disorder of the excitonic states. These investigations aim for a better understanding of exciton migration in order to design materials with longer exciton diffusion lengths for highly efficient organic solar cells.

O 23.4 Mon 18:45 CHE 91

**The effect of gradual fluorination on the opto-electronic properties of $F_n$ZnPc/$C_{60}$ bilayer cells** — •M. Brendel[1], A. Steindamm[1], A. Topczak[1], and J. Pflaum[1,2] — [1]Exp. Phys. VI, JMU Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

The respective position of energy levels at the donor/acceptor heterojunction is crucial for the resulting parameters of an organic solar cell. For instance the open circuit voltage ($V_{oc}$) is correlated to the energy difference between the highest occupied molecular orbital (HOMO) of the donor and the lowest unoccupied molecular orbital (LUMO) of the acceptor, the so-called effective band gap ($E_{g,eff}$). To gain insights into this correlation, tailoring of energy levels by chemical modification is a powerful approach. In this contribution, we investigate the impact of gradual fluorination of zinc phthalocyanine on the opto-electronic properties of $F_n$ZnPc/$C_{60}$ (n=0,4,8,16) bilayer cells. Upon fluorination, HOMO and LUMO levels are shifted towards lower energies. The gain in $V_{oc}$ for $F_4$ZnPc/$C_{60}$ and $F_8$ZnPc/$C_{60}$ by 11% and 23% respectively, compared to ZnPc/$C_{60}$, confirms qualitatively the expected energy level scheme. Besides, the differences between $e \cdot \Delta\ V_{oc}$ and $\Delta E_{g,eff}$ hint at the occurrence of dipoles and their gain in strength with increasing degree of fluorination. As will be shown, this dipol can be correctly accounted for in a plate capacitor geometry, considering image charges at the interface induced by electronegative fluorine in the immediate vicinity of $C_{60}$ molecules. We thank S. Sundarray and P. Erk from BASF for providing $F_4$ZnPc. Financial support by the DFG (program SPP1355) and the BMBF (GREKOS program).

O 23.5 Mon 19:00 CHE 91

**Effect of Counter-Anions During Electrodeposition on the Charge Transport Dynamics in Sensitized *ZnO* Solar Cells** — •Christoph Richter, Max Beu, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Thin porous *ZnO*/*EosinY* films have been electrochemically deposited from oxygen-saturated aqueous solution. During the electrochemical deposition chloride or perchlorate as different counter-anions have been used. After the removal of *EosinY* with *KOH* the films have been sensitized with the indoline dye D149. These electrodes were used in dye-sensitized solar cells (DSCs) and the charge transport dynamics were studied with electrochemical impedance spectroscopy (EIS), intensity modulated current/voltage spectroscopy (IMPS/IMVS) and IV-curves. Doping of the *ZnO* films by *Cl* alters the charge transfer dynamics by filling of otherwise unoccupied states in *ZnO* and changing the concentration of available trap states. By changing the counteranion to perchlorate well-reproducible results could be obtained which open the way to further improvements in DSCs.

O 23.6 Mon 19:15 CHE 91

**Efficiency roll-off in organic light-emitting diodes: influence of emitter position and orientation** — •Caroline Murawski[1], Philipp Liehm[1,2], Simone Hofmann[1], Karl Leo[1], and Malte C. Gather[1,2] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]present address: SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS (UK)

In this contribution, we study the efficiency decrease of organic light-emitting diodes (OLEDs) at high brightness (so-called roll-off).[1] We find a strong influence of the emitter-cathode distance and the transition dipole orientation of the emitter molecules on the roll-off by comparing two phosphorescent emitters (Ir(MDQ)2(acac) and Ir(ppy)3).[2] The measurements are modeled using triplet-triplet-annihilation (TTA) theory. A comparison of experiment and theory reveals the critical current density and the TTA rate constant and shows that the differences in roll-off behavior are predominantly caused by a change of the decay rates inside the OLED cavity. In order to provide guidelines for designing OLEDs with optimal high-brightness efficiency, we model the roll-off as a function of the emitter-cathode distance, emitter dipole orientation, and radiative efficiency.

[1] C. Murawski, K. Leo, and M.C. Gather, Adv. Mater. 10.1002/adma.201301603 (2013).

[2] C. Murawski, P. Liehm, K. Leo, and M.C. Gather, Adv. Funct. Mater. 10.1002/adfm.201302173 (2013).

O 23.7 Mon 19:30 CHE 91

**Solution-based planarization layers for organic solar cells on flexible silver nanowire transparent electrodes** — •Jan Ludwig Bormann[1], Franz Selzer[1], Nelli Weiss[2], Lars Müller-Meskamp[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, TU Dresden — [2]Physikalische Chemie, TU Dresden

Flexible transparent electrodes made of silver nanowires (AgNWs) are an emerging research field for different optoelectronic devices such as organic transistors, organic light emitting diodes (OLED) and organic photovoltaics (OPV). They exhibit excellent electrical and optical properties (sheet resistance of 11 Ohm/sq at 85% transmittance) and are suitable for the application on flexible substrates. These transparent electrodes show high roughness and therefore require a planarization layer for fabricating efficient small molecule devices.

In this work, solution-based organic materials are processed with spin coating to planarize the AgNW electrode. A solution processed small molecule layer acts as planarizing layer and as hole transport layer in organic solar cells with a bulkheterojunction comprising the fullerene C60 as acceptor and different small molecule donor layers (oligothiophenes and phtalocyanines) . The efficiency of these devices is comparable or even better to reference devices with indium tin oxide (ITO) as transparent electrode.

## O 24: Invited Talk (Swetlana Schauermann)

Time: Tuesday 9:30–10:15 Location: TRE Phy

**Invited Talk** O 24.1 Tue 9:30 TRE Phy

**Elementary Steps in Surface Reactions: Mechanisms, Kinetics and Thermodynamics** — •Swetlana Schauermann — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Atomistic-level understanding of surface processes is a key prerequisite for rational design of new catalytic and functional materials. In our studies, we investigate mechanisms, kinetics and thermodynamics of heterogeneously catalyzed reactions and adsorption processes on nanostructured model supported catalysts to provide fundamental insights into the surface chemistry. By employing pulsed multi-molecular beam techniques, IRAS and synchrotron-based spectroscopies on Pd/Fe3O4/Pt(111) model surfaces, we study mechanistic details of complex multi-pathway surface reactions, such as hydrocarbon transformation in presence of hydrogen or selective hydrogenation of multi-unsaturated hydrocarbons. The ultimate goal of our research is obtaining detailed correlations between reactivity, selectivity and the particular atomistic structure of the catalytic surface. Complementary, single crystal adsorption calorimetry is employed to address thermodynamics of adsorption processes and surface reactions, such as e.g. adsorption and reaction of oxygen and CO. Specifically, we focus on the particle size dependence of adsorption and reaction energies to obtain a fundamental-level understanding of how the nanometer scale confinement of matter effects the energetics of surface reactions.

## O 25: Symposium Spin Properties of Graphene (HL jointly with DS, MA, O, TT)

Time: Tuesday 9:30–12:15 Location: HSZ 02

**Invited Talk** O 25.1 Tue 9:30 HSZ 02

**Intrinsic magnetism in graphene** — •Irina Grigorieva — School of Physics and Astronomy, University of Manchester, UK

I will review our recent experiments on inducing and controlling magnetic response in graphene via introduction of point defects such as vacancies and adatoms. Graphene is hailed as potentially an ideal material for spintronics due to its weak spin-orbit interaction and the ability to control its electronic properties by the electric field effect. We have demonstrated that point defects in graphene - both vacancies and adatoms - carry magnetic moments, leading to pronounced paramagnetic behaviour that dominates graphene's low-temperature magnetism. Even better, we show that the defect magnetism is itinerant (i.e. due to localisation of conduction electrons) and can be controlled by doping, so that the induced magnetic moments can be switched on and off. This not only adds important functionality to potential graphene devices but also has important implications for spin transport.

**Invited Talk** O 25.2 Tue 10:00 HSZ 02

**Defect Induced Magnetic Moments in Graphene** — •Roland Kawakami — The Ohio State University, Columbus, OH, USA — University of California, Riverside, CA, USA

We utilize non-local spin transport measurements to detect the presence of defect induced magnetic moments in graphene. As shown in this talk, point defects such as hydrogen adatoms and lattice vacancies generate magnetic moments in graphene that have substantial exchange coupling with the conduction electrons. Therefore, this exchange coupling produces spin relaxation in the conduction electrons. Specifically, a characteristic field dependence of the non-local spin transport signal identifies the presence of the magnetic moments. Furthermore, Hanle spin precession measurements indicate the presence of an exchange field generated by the magnetic moments. The entire experiment including spin transport is performed in an ultrahigh vacuum chamber, and the characteristic signatures of magnetic moment formation appear only after hydrogen adatoms or lattice vacancies are introduced.

**Invited Talk** O 25.3 Tue 10:30 HSZ 02

**Role of MgO barriers for spin and charge transport in Co/MgO/graphene spin-valve devices** — •Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

We investigate the influence of MgO barriers on spin and charge transport in single (SLG) and bilayer (BLG) graphene spin-valve devices. Similar to previous studies on BLG [1], we observe a $1/\mu$ of the spin lifetime in SLG devices. This general trend is only observed in devices with large contact resistance area products $R_cA > 1\text{k}\Omega\mu\text{m}^2$. In devices with long spin lifetimes, we furthermore observe a second Dirac peak, which results from charge transport underneath the contacts. In contrast, all devices with $R_cA < 1\text{k}\Omega\mu\text{m}^2$ only exhibit a single Dirac peak. Additionally, the spin lifetime is significantly reduced indicating that an additional spin dephasing occurs underneath the electrodes. In the latter devices we achieve a gradual increase of $R_cA$ values by successive oxygen treatments. With this manipulation of the contacts both spin lifetime and amplitude of the spin signal can significantly be increased by a factor of seven in the same device. Finally, we present a new method to fabricate graphene-based lateral spin valves on hexagonal boron nitride yielding spin lifetimes above 3 ns, spin diffusion length above 10 $\mu$m and large charge carrier mobilities above 30.000 cm$^2$/Vs.

This work was supported by DFG through FOR 912.

[1] T.-Y. Yang *et al.*, Phys. Rev. Lett. 107, 047206 (2011).

[2] F. Volmer *et al.* Phys. Rev. B 88, 161405(R)(2013).

**Coffee break (15 min.)**

**Invited Talk** O 25.4 Tue 11:15 HSZ 02

**Defect-Mediated Spin Relaxation and Dephasing in Graphene** — Mark Lundeberg[1,2], Silvia Folk[1], and •Joshua Folk[1] — [1]University of British Columbia, Vancouver, Canada — [2]Institute of Photonic Sciences, Barcelona, Spain

This talk will describe a series of transport measurements that disentangle mechanisms of spin and orbital phase relaxation in graphene. The measurements are based on well-known quantum interference phenomena–weak localization and universal conductance fluctuations. We show that a careful analysis of the in-plane magnetic field and temperature dependences of these effects can separately quantify spin-orbit and magnetic scattering rates; this technique works especially well in graphene due to its single-atom thickness. Spin relaxation in exfoliated graphene on $SiO_2$ is found to be dominated by magnetic scattering (scattering off of magnetic defects), with a smaller contribution from spin-orbit interaction. A similar measurement performed in graphene on SiC suggests that both magnetic scattering and spin-orbit interaction are a factor of 10 stronger than in exfoliated graphene.

**Invited Talk** O 25.5 Tue 11:45 HSZ 02

**Electron spin relaxation in graphene: resonant scattering off local magnetic moments** — •Jaroslav Fabian, Denis Kochan, and Martin Gmitra — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Dirac electrons in graphene should have large spin relaxation time, some microseconds, due to the weak spin-orbit coupling of its itinerant electrons. Yet experiments show spin lifetimes as short as 100 ps. Traditional spin relaxation mechanisms, Elliott-Yafet and Dyakonov-Perel, seem incapable to explain such short lifetimes, even though some external influences such as hydrogen adatoms seem to induce giant local spin-orbit coupling [1] and so enhance spin-orbit induced spin flips. We believe that the culprit may instead be local paramagnetic moments due to vacancies and some adatoms. As the local moments sit on resonance sites, the spin flip is resonantly enhanced. These resonant local moments are acting as spatial spin hot spots: they may contribute little to momentum relaxation of graphene, but dominate the spin relaxation. This new mechanism explains the observed 100 ps spin lifetimes with as little as 1 ppm of local moments [2]. We acknowledge support from DFG SFB 689, SPP 1285, GRK 1579, and EC under Graphene Flagship (Contract No. CNECT-ICT-604391). [1] M. Gmitra, D. Kochan, and J. Fabian, Spin-orbit coupling in hydrogenated graphene, Phys. Rev. Lett. 110, 246602 (2013);[2] D. Kochan, M. Gmitra, and J. Fabian, Spin relaxation mechanism in graphene: resonant scattering by magnetic impurities, arXiv:1306.0230.

## O 26: Transport: Graphene (TT jointly with O)

Time: Tuesday 9:30–13:15 Location: WIL C107

**Topical Talk** O 26.1 Tue 9:30 WIL C107

**A First-Principles Perspective on Two-Dimensional Transition-Metal Dichalcogenides** — •Udo Schwingenschlögl — KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

Layered transition-metal dichalcogenides recently are attracting great attention, because of the possibility to achieve two-dimensional (2D) materials, similar to the exfoliation of graphene from graphite. Using first-principles calculations, we study prototypical monolayer $MoS_2$ to obtain insight into the influence of defects and substitutional doping, for a wide range of transition-metal dopants. We also address polar transition-metal dichalcogenide monolayers with respect to their structural stability and the effects of the spin-orbit coupling. Heterojunctions of $MoS_2$ with unsaturated and saturated MXenes are studied; such hyrid systems are interesting for application in all-2D devices.
[1] Phys. Rev. B 87, 100401(R) (2013)
[2] EPL 102, 57001 (2013)
[3] Phys. Rev. B 87, 245307 (2013)

O 26.2 Tue 10:00 WIL C107

**Ab-initio simulations of local current flows in functionalized graphene flakes and ribbons** — •Michael Walz, Alexei Bagrets, and Ferdinand Evers — Institute of Nanotechnology (INT) and Institut für Theorie der Kondensierten Materie (TKM), Karlsruhe Institut of Technologie (KIT), D-76131 Karlsruhe, Germany

Using our DFT-based transport framework AITRANSS [1,2], we calculate the transmission and the local current density in graphene flakes functionalized by adsorbed atoms, such as nitrogen or hydrogen.

We find that even a single nitrogen atom can almost completely suppress the conductance of a (gated) graphene armchair nano-ribbon. In this situation local ring currents emerge that result in local (orbital) magnetic moments.

As one expects, very wide ribbons (flakes, $W \gg L$) exhibit the bulk conductance $G = \frac{2e^2}{h}\frac{W}{\pi L}$ in the absence of adsorbants. With 20% hydrogen absorbants, we observe very complicated patterns of streamlines with many eddies and a broad distribution of local magnetic fields, $\mathbf{B}(\mathbf{r})$, that are induced by the dc-current flow. We plan to study the statistics of the conductance and $\mathbf{B}(\mathbf{r})$ of such large flakes and its dependency on the impurity concentration. Performing such calculations starting from first principles is challenging because of high computational costs. On this account, we parallelized our transport module AITRANSS using standard MPI and OpenMP techniques, also including Scalapack to treat systems up to 10.000 carbon atoms.
[1] A. Arnold *et al.*, J. Chem. Phys. **126**, 174101 (2007).
[2] J. Wilhelm, MW, *et al.*, Phys. Chem. Chem. Phys. **15**, 6684 (2013).

O 26.3 Tue 10:15 WIL C107

**Quantum transport simulations and Fabry-Perot interference patterns in multiple pn-junctions on graphene** — •Fedor Tkatschenko[1], Ming-Hao Liu[1], Klaus Richter[1], Martin Drienovsky[2], Jonathan Eroms[2], and Dieter Weiss[2] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg

Advancements in experimental techniques have led to an amazing progress towards excellent graphene samples and to graphene devices with fascinating properties, ranging from narrow pnp junctions below 100 nm to large mean free paths up to micron scales. In such devices the charge carriers undergo multiple reflections at pn or np interface leading to interesting Fabry-Perot-type interference patterns in the conductance map[1,2]. We address the peculiar features of Fabry-Perot resonances in graphene. To this end we calculate the potential profiles for typical experimental setups[3] with the quantum capacitance model and perform transport calculations using the recursive Green's function technique. The numerical results are in good agreement with the experimental data. We further show that the leading contribution to the Fabry-Perot resonances in the conductance map originates from the first two pn junctions.
[1] A.F. Young and Ph. Kim, Nat. Phys. **5** (2009)
[2] P. Rickhaus, R. Maurand, M. H. Liu, M. Weiss, K. Richter and C. Schönenberger, Nat. Comm. **4** 2342 (2013)
[3] M. Drienovsky, F.-X. Schrettenbrunner, M. H. Liu, F. Tkatschenko, K.Richter, D. Weiss and J. Eroms, in preparation

O 26.4 Tue 10:30 WIL C107

**Ballistic interferences in suspended graphene** — •Ming-Hao Liu[1], Peter Rickhaus[2], Romain Maurand[2], Markus Weiss[2], Klaus Richter[1], and Christian Schönenberger[2] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Complex Fabry-Pérot interferences in ultraclean suspended graphene have been recently observed, with the ballistic origin confirmed by transport calculations well agreeing with experiment [1]. The observed conductance oscillations account for quantum interference of electron waves propagating ballistically over distances exceeding 1 $\mu$m. The complex interference patterns stem from Fabry-Pérot resonances within different cavities defined by electrically controlled pn junctions and the graphene-contact interfaces. In this talk, the theoretical part of this work [1], namely, the full modeling of the ballistic transport from contact to contact through the suspended graphene, will be illustrated at an appropriate depth.
[1] P. Rickhaus, R. Maurand, M.-H. Liu, M. Weiss, K. Richter, and C. Schönenberger, Nat. Commun. **4**, 2342 (2013)

O 26.5 Tue 10:45 WIL C107

**Ballistic transport in graphene nanoconstrictions** — •Danny J. M. Jörger[1,2], Bernat Terrés[1,2], Stephan Engels[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], Slava V. Rotkin[1,4], and

Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan — [4]Physics Department, Lehigh University, Bethlehem, Pennsylvania 18015, USA

Graphene nanodevices, such as for example nanoconstrictions are interesting systems for studying mesoscopic phenomena. Recent developments in the fabrication of graphene devices have revealed a significant increase in carrier mobility (e.g. 200.000 $\mathrm{cm}^2/\mathrm{Vs}$ in bulk samples), making mean free path in the order of device dimensions accesible. This allows to investigate quantum interference effects and ballistic transport in nanostructured graphene. We discuss the differences in electrostatic coupling ($\alpha \approx 9.4 \times 10^{10}$ $\mathrm{cm}^{-2}\mathrm{V}^{-1}$) at high and low magnetic fields and the width-dependency of the overall conductance level at zero magentic field. Results confirm the Dirac fermion nature of confined charge carriers in graphene. We report on the observation of quasi one-dimensional subband transport characteristics in graphene nanoconstrictions encapsulated in hexagonal boron nitride. The ballistic nature of the transport in our devices ($l_m \geq 500$ nm) allows to study the interplay between confinement and Landau quantization and its crossover.

**15 min. break.**

O 26.6 Tue 11:15 WIL C107

**Optical conductivity of graphene** — •Julia Link, Peter P. Orth, and Jörg Schmalian — Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Graphene is a two-dimensional crystal of carbon atoms with a honeycomb structure, which has many fascinating optical and electronical properties. It has a high mobility of electrons at room temperature and a high transparency of light with 97.7%. In the optical domain, the value of the transparency does not depend on the frequency of white light being transmitted and is thus universal. This universality is linked to the fine structure constant $\alpha = 1/137$ and can be derived using non-interacting Dirac fermions.

We aim to understand the correction of the optical transparency due to Coulomb interaction. Since there is a long dispute about this correction in the literature [1-6], we try to resolve this controversy. Therefore we combine two different regularization schemes: dimensional regularization and a deformation of the Coulomb potential. We discuss the physical implication of the choice of the regularization.

[1] Herbut, Juricic, Vafek, Phys. Rev. Lett. **100**,046403 (2008)
[2] Mishchenko, Europhys. Lett. **83**, 17005 (2008)
[3] Sheey, Schmalian, Phys. Rev. B **80**, 193411 (2009)
[4] Juricic, Vafek, Herbut, Phys. Rev. B **82**, 235402 (2010)
[5] Rosenstein et al., Phys. Rev. Lett. **110**, 066602 (2013)
[6] Gazzola, Cherchiglia, Cabral, Nemes, Sampaio, Europhys. Lett. **104**, 27002 (2013)

O 26.7 Tue 11:30 WIL C107

**Polycrystalline graphene: mechanical, electrical and thermal properties** — •Thomas Lehmann[1,2], Arezoo Dianat[1,2], Frank Ortmann[1,2], Dmitry Ryndyk[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, Germany

Large-area samples of graphene tend to be polycrystalline (PC) on some substrates. Grain boundaries with structural defects are expected to alter the structural and electronical properties of graphene. In this work, the mechanical properties of PC graphene are studied by means of density-functional theory and furthermore the electrical and thermal transport properties are addressed. To construct grain boundaries of zigzag and rotated armchair graphene sheets, molecular dynamics simulations are performed. The critical strain leading to structural failure of PC graphene nanoribbons is only half the value of pristine armchair nanoribbons. However we show that it can be significantly enhanced by the reaction of the chemically active grain boundaries with atmospheric gases. The transport properties of those systems are investigated, both parallel and perpendicular to the grain boundary, using an ab initio based atomistic model combined with Landauer transport theory and recursive Green function method. The electronic part is calculated within a tight-binding model and a force-constant approach has been applied for phonon transport.

O 26.8 Tue 11:45 WIL C107

**Electric field control of spin-polarized electron transport through zigzag graphene nanosheets** — •Dirk Wiedmann[1], Marius Bürkle[2], and Fabian Pauly[1] — [1]Department of Physics, University of Konstanz, Germany — [2]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

We study the spin-polarized transport through a finite zigzag graphene nanoribbon, contacted by carbon-nanotube electrodes [1]. The electronic structure is determined from density functional theory, and Green's functions are used to compute the phase-coherent electric current within the Landauer scattering theory. We observe antiferromagnetically coupled edge states in the graphene nanosheet, which may lead to spin-polarized currents. We analyze how they depend on the position of the electrodes and on applied transverse electric fields. Our ab-initio results are rationalized with the help of a Hubbard model.

[1] D. Wiedmann, M. Bürkle, and F. Pauly, in preparation.

O 26.9 Tue 12:00 WIL C107

**Radiative damping and synchronization in a graphene-based terahertz emitter** — •Andrey Moskalenko and Sergey Mikhailov — Institute of Physics, University of Augsburg, Germany

We investigate the collective electron dynamics in a recently proposed graphene-based terahertz emitter [1] under the influence of the radiative damping effect, which is included self-consistently in a molecular dynamics approach. We show that under appropriate conditions synchronization of the dynamics of single electrons takes place, leading to a rise of the oscillating component of the charge current. The synchronization time depends dramatically on the applied dc electric field and electron scattering rate, and is roughly inversely proportional to the radiative damping rate that is determined by the carrier concentration and the geometrical parameters of the device. The emission spectra in the synchronized state, determined by the oscillating current component, are analyzed. The effective generation of higher harmonics for large values of the radiative damping strength is demonstrated.

[1] S. A. Mikhailov, Phys. Rev. B 87, 115405 (2013)

O 26.10 Tue 12:15 WIL C107

**Non-vanishing Coulomb drag in clean double-layer graphene at the Dirac point** — •Sven Aeschlimann[1], Michael Schütt[2], Igor Gornyi[1,2,3], Boris Narozhny[1], and Alexander Mirlin[1,2,4] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]A. F. Ioffe Physica-Technical Institute, St. Petersburg, Russia — [4]Petersburg Nuclear Physics Institute, St. Petersburg, Russia

Coulomb drag is the frictional effect of simple Coulomb interaction onto two currents driven through two spatially separated conducting layers. Initiating a current through one layer, causes a current or a voltage drop in the other.

Recent experiments revealed a suprising nonvanishing resistance at the Dirac point that was expected to be zero for symmetry considerations. We focus on the possibility of a non-vanishing resistance in clean samples due to third order interaction contributions to drag.

O 26.11 Tue 12:30 WIL C107

**Linear Magnetoresistance in bilayer graphene** — •Ferdinand Kisslinger, Christian Heide, Christian Ott, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, ferdinand.kisslinger@physik.uni-erlangen.de

We investigate the magnetoresistance in bilayer graphene obtained by hydrogen intercalation of monolayer graphene grown on the SiC(0001) surface. Whereas in monolayer graphene electron-electron-interaction and weak localization can be observed at low temperatures, a strong linear contribution dominates the magnetoresistance for bilayer graphene. It is found to be nearly temperature independent.

A variation of charge carrier density using a bottom gate and the comparison of different samples is carried out. The entity of data agrees well with a theoretical model [1] that describes a resistance network of Van-der-Pauw resistors. Consistency with the experiment is achieved when a network of resistors with different resistances is assumed. There are several possibilities where such inhomogeneities may originate from. We can exclude some of them and propose dislocations recently found in bilayer graphene [2] as a good candidate causing this effect.

[1] M.M. Parish and P.B. Littlewood , Nature 426 (2003) 162
[2] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber,

B. Meyer and E. Spiecker, Nature (2013), accepted, DOI: 10.1038/nature12780

O 26.12 Tue 12:45 WIL C107

**Wigner Crystal phases in bilayer graphene** — •Peter Silvestrov and Patrik Recher — Institut für Mathematische Physik, TU Braunschweig, Germany

It is generally believed that Wigner Crystal in single layer graphene can not exist because the magnitudes of the electron interaction and the kinetic energy scale similarly with the decreasing electron density. This scaling argument however does not work for the low energy states in bilayer graphene. We consider the Wigner Crystal in slightly doped bilayer graphene with a gap in spectrum opened by applying a perpendicular electric field. We argue that in this system the formation of the Wigner Crystal is not only possible, but a different phases of the crystal with very peculiar properties may exist here depending on the parameters.

O 26.13 Tue 13:00 WIL C107

**Half-metallic bilayer graphene** — •Jie Yuan — Raum 26 A 407 RWTH Aachen Sommerfeldstrasse 26, D-52056, Aachen

Charge neutral bilayer graphene has very likely a gapped ground state, as transport experiments have demonstrated. The nature of the ground state is undertermined yet. One plausible ground state is the layered antiferromagnetic spin density wave (LAF) state, where the spins in the top and bottom layers have the same magnitude with opposite directions. We propose that lightly doped bilayer graphene in an electric field perpendicular to the graphene plane may be a half-metal where only one spin direction lis conducting. By the special properties of the half-metal deriving from the LAF state, the primary source of the gap at charge neutrality may be distinguished from other competing ground states like the quantum spin-Hall state. We study this explicitly by using a mean-field theory on a two-layer Hubbard model.

## O 27: Organic/bio Molecules on Metal Surfaces III

Time: Tuesday 10:30–13:15 Location: TRE Phy

O 27.1 Tue 10:30 TRE Phy

**Kondo effect in PTCDA/Au(111) induced by doping with single gold atoms** — •Taner Esat[1], Christian Wagner[1], Ruslan Temirov[1], Stefan Tautz[1], Thorsten Deilmann[2], Peter Krüger[2], and Michael Rohlfing[2] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany — [2]Institut für Festkörpertheorie, Universität Münster, D-48149 Münster, Germany

Interest in molecular magnets has been growing rapidly for the last few years. Understanding and gaining control over their properties might open a route to nanospintronics and quantum computing. One of the interesting possibilities to tune the magnetic properties of molecules is by controlled charge transfer from other molecules [1] or metal surfaces [2]. In this work we show another approach by doping non-magnetic molecules physisorbed on metal surfaces with single metal atoms.

By means of LT-STM and STS we have investigated the adsorption of single Au adatoms on a PTCDA monolayer adsorbed on a Au(111) surface.

We find two different types of Au adatoms on PTCDA which differ in their STS spectra and apparent size in the STM images. Both types show a pronounced peak in dI/dV conductance at zero bias. Temperature dependent measurements of FWHM and height of the zero-bias conductance peak confirm that the peak originates from the Kondo effect with a corresponding Kondo temperature of $37.5 \pm 6.5$ K.

[1] I. Fernández-Torrente et al.,Phys. Rev. Lett. 108, 036801 (2012)
[2] R. Temirov et al., Nanotechnology 19 (6), 065401 (2008)

O 27.2 Tue 10:45 TRE Phy

**A single Au adatom on PTCDA:Au(111) – results from abinito calculations** — •Thorsten Deilmann[1], Peter Krüger[1], Michael Rohlfing[1], Taner Esat[2], Christian Wagner[2], Ruslan Temirov[2], and Stefan Tautz[2] — [1]Institut für Festkörpertheorie, Universität Münster, D-48149 Münster, Germany — [2]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany

The electronic properties of organic adsorbates on a noble-metal surface depend on structural and environmental details [1].

Here we investigate the influence of an additional Au adatom on a PTCDA monolayer that is adsorbed on a Au(111) surface. Adsorption structures, electronic spectra and scanning tunneling microscopy (STM) images are calculated within density-functional theory.

The weak binding of PTCDA on Au(111) leads to a large bond distance of more than 3 Å between the molecule and the substrate. We investigate different conceivable adsorption sites for the Au adatom above PTCDA. The most favorable adatom position is about 2 Å above the PTCDA molecule. Alternatively, an Au adatom can be located in the region between the molecules. The electronic structure around $E_F$ shows distinct differences for the two absorption sites. If the adatom is above a PTCDA molecule a dominant maximum above the Au adatom is visible in the calculated STM image.

[1] A. Greuling et al., *Physica Status Solidi B* **250**, 2386 (2013).

O 27.3 Tue 11:00 TRE Phy

**Gold-Adatom-Mediated Bonding and Molecular Orbital Redistribution in Metal-Organic Chains** — •zechao yang[1], martina corso[1,2], christian lotze[1], elena mena-osteritz[3], peter bäuerle[3], katharina j. franke[1], and jose i. pascual[1,2] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]CIC nanoGune, 20018 Donostia-San Sebastián, Spain — [3]Institute of Organic Chemistry II and Advanced Materials, University of Ulm, Germany

Dicyanovinyl-quinquethiophenes (DCV5T-Me2) is a prototype molecule for organic electronics. Here, we investigated the structural and electronic properties of DCV5T-Me2 molecules on Au(111) using low temperature scanning tunneling microscopy and atomic force microscopy. DCV5T-Me2 self-assembles in chains, stabilized by intercalated Au atoms. The spectroscopic fingerprint of the incorporation of Au adatoms is an energetic downshift of the lowest unoccupied molecular orbital of the molecules within the chains with respect to uncoordinated molecules due to metal-ligand hybridization. An asymmetric coordination of the molecule by gold atoms from only one side, leads to an asymmetric orbital shape along the molecule. It is attributed to a redistribution of charge over the molecule as a consequence of a localized coordination bond to the gold atom, as confirmed by density functional theory calculations. Our study demonstrates that one can manipulate molecular orbital alignments and distribution simultaneously within individual molecules by contacting metal atoms.

O 27.4 Tue 11:15 TRE Phy

**Porphyrin metalation providing an example of a redox reaction facilitated by a surface reconstruction** — •Jan Nowakowski[1], Christian Wäckerlin[1], Jan Girovsky[1], Dorota Siewert[1], Thomas A. Jung[1], and Nirmalya Ballav[2] — [1]PSI, Villigen, Switzerland — [2]IISER, Pune, India

Recently, significant attention has been drawn to on-surface reactions [1], including on-surface redox chemistry [2], of which the metalation of free-base porphyrins is an interesting example [3, 4]. The on-surface metalation can be realized in three ways: (i) by picking up free heteroatoms from a surface [5]; (ii) by depositing metal atoms on top of molecules predeposited on an intert substrate (e.g. Au or Ag); or (iii) self-metalation, i.e. by coordination with atoms of a crystalline substrate. The temperature of on-surface metalation depends on the method chosen and on the element used [5]. We show [5] that, surprisingly, passivating a Cu(001) surface with an oxygen- surface reconstruction lowers the self-metalation temperature of 5,10,15,20-Tetraphenylporphin (2HTPP) from 450 K on native Cu(001) surface to 285 K on the oxygen-reconstructed Cu(001) surface. In the presented study X-Ray Photoelectron Spectroscopy (XPS) and Scanning Tunneling Microscopy (STM) methods have been used.

[1] C. Diaz et al., Science, 2009, 326, 832;
[2] D.-T. Pham et al., New J. Chem., 2006, 30, 1439;
[3] W. Auwärter et al., ChemPhysChem, 2007, 8, 250;
[4] J. M. Gottfried et al., J. Am. Chem. Soc., 2006, 128, 5644;
[5] J. Nowakowski et al., Chem. Commun., 2013, 49, 2347.

O 27.5 Tue 11:30 TRE Phy

**NTCDA and CuPc heteroorganic phases on Ag (111)** — •Sonja Schröder, Benjamin Stadtmüller, Francois C. Bocquet, Caroline Henneke, Christoph Kleimann, Serguei Soubatch, Frank Stefan Tautz, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany and Jülich Aachen Research Alliance Fundamentals of Future Information Technology, Jülich, Germany

While in the last decade most studies of organic adsorbates on metal surfaces concentrated on homomolecular systems, recently also heteromolecular thin films moved into the focus of interest. In particular, acceptor-donator systems have considerable potential for future organic devices. Here we report on the heteroorganic system NTCDA and CuPc on Ag(111). In comparison to the system PTCDA+CuPc/Ag(111) investigated earlier [1], the acceptor strength of the charge accepting molecule is weakened by replacing PTCDA by NTCDA. We have investigated the consequences of this manipulation by means of SPA-LEED, NIXSW, UPS and ARPES. As for the PTCDA-CuPc system three mixed structures with different stoichiometric ratios were found: A NTCDA-rich, a *1:1*, and a CuPc-rich phase. In this presentation we concentrate on the lateral and vertical structure formation and show some results from our electron spectroscopic investigations. [1] B. Stadtmüller, D. Lüftner, M. Willenbockel, E.M. Reinisch, T .Sueyoshi, G. Koller, S. Soubatch, M.G. Ramsey, P. Puschnig, F.S .Tautz, C .Kumpf, to be published.

O 27.6 Tue 11:45 TRE Phy

**Interaction of a Kondo impurity with its molecular ligand** — •Jörg Meyer, Anja Nickel, Robin Ohmann, Loka Mani, Cormac Toher, Dmitry Ryndyk, Francesca Moresco, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany

We investigated a Co containing organic molecule on different metal surfaces by STM and STS. On Ag(100) the molecule showed a prominent asymmetric peak at the Fermi level. To verify the Kondo nature of this peak, temperature dependent STS was applied and the resulting spectra were fitted with the Fano formula. Afterwards, we measured a grid of spectra with submolecular resolution to determine the shape of the Kondo resonance in different spots of the molecule. Interestingly, the asymmetry/Fano parameter q strongly changed around the molecule in a clearly non-radialsymmetric fashion, representing the influence of the molecular ligand on the resonances appearance. This is interpreted as signal transduction of the Kondo resonance via the molecular orbitals. Simulations to support this hypothesis are still ongoing. The strong influence of the local environment is further illustrated by the disappearance of the Kondo resonance on Cu(110). Instead of the asymmetric peak at the Fermi level we found a symmetric peak at -0.2 V. A dI/dV map of these states show the same spatial distribution like the Kondo resonance at the Fermi Level obtained from the specgrid measurements.

O 27.7 Tue 12:00 TRE Phy

**Structural and optical investigation of ultra-thin layers of potassium doped PTCDA on Ag(111)** — •Marco Gruenewald, Christian Zwick, Roman Forker, and Torsten Fritz — Friedrich-Schiller University Jena, Institute of Solid State Physics, Max-Wien-Platz 1, Jena 07743, Germany

Here we report on the influence of potassium doping on highly-ordered ultra-thin layers of the dye molecule 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on Ag(111). The doped thin films have been structurally characterized by LEED and LT-STM as well as optically by in-situ differential reflectance spectroscopy (DRS) [1,2]. We found that potassium doping of submonolayers of PTCDA on Ag(111) induces different highly ordered phases of PTCDA-potassium complexes depending on the doping concentration. Consequently, the electronic and thus optical characteristics of the thin film changes dramatically. For instance, by applying DRS during the film growth and the subsequent doping process we found distinct optical fingerprints which can be partially assigned to anionic features of PTCDA showing different doping stages (as investigated in detail on an inert mica substrate in ref. [3]). Furthermore, structural relaxation of PTCDA-potassium complexes due to annealing will be discussed.

References: [1] R. Forker et al., Annu. Rep. Prog. Chem., Sect. C: Phys. Chem., 2012, 108, 34-68. [2] R. Forker and T. Fritz, Phys. Chem. Chem. Phys., 2009, 11, 2142-2155. [3] T. Dienel et al., Adv. Mater., 2010, 22, 4064-4070.

O 27.8 Tue 12:15 TRE Phy

**Temperature-induced Structural and Chemical Changes of Ultrathin Ethylene Carbonate Films on Cu(111)** — •Florian Buchner[1], Maral Bozorgchenani[1,2], Hanieh Farkhondeh[1,2], Benedikt Uhl[1,2], and R. Jürgen Behm[1,2] — [1]Helmholtz Institute Ulm (HIU), Ulm, Germany — [2]Ulm University, Institute of Surface Chemistry and Catalysis, Ulm, Germany

Ethylene Carbonate (EC) is a key component in Li-ion battery electrolyte. A molecular scale understanding of the solid-electrolyte interphase (SEI) is crucial to improve the Li-ion battery performance. The adsorption and reaction of EC on Cu(111), as a model system, was investigated with scanning tunnelling microscopy (STM) and X-ray photoelectron spectroscopy (XPS) under ultrahigh vacuum (UHV) conditions. Highly ordered 2D EC islands were obtained on Cu(111) at submonolayer and monolayer coverage by STM for adsorption at around 100 K. The adsorption behaviour is discussed in terms of intermolecular interactions and mobility on the surface. The XP C1s and O1s core level spectra prove the adsorption of intact EC molecules. Between 80 K and 420 K, significant structural and chemical changes were detected. Upon heating to room temperature, a highly mobile molecular adlayer is detected by STM. Upon post annealing and cool down to around 100 K a transformation from 2D EC islands into islands with arbitrary shapes is observed. Variable temperature XPS resolves chemical changes of the adlayer upon heating, including desorption of molecular species and decomposition of EC into new surface species.

O 27.9 Tue 12:30 TRE Phy

**Resonant tunnelling observed in metal-PTCDA-metal junction** — •Matthew Green, Alexander Grötsch, Ruslan Temirov, and Stefan Tautz — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany

Understanding of charge transport in single molecule junctions is of fundamental importance, especially for future molecular electronics applications. Single molecules have been shown to conduct electric current, but there is relatively little understanding of the precise charge transport mechanisms responsible for conductance in single molecule junctions. Here we describe a new insight into quantum transport through a single PTCDA molecule suspended between two metal electrodes, namely an atomically clean metal surface and the tip of a combined NC-AFM/STM [1][2]. We are able to probe transport characteristics across a wide range of applied bias voltages. In particular, resonant tunnelling through the lowest unoccupied molecular orbital is observed. Our findings open up the possibility to a more detailed understanding of different charge transport regimes present in single molecule junctions.

[1] N. Fournier et al., Phys. Rev. B 84(3) 035435 (2011)
[2] C. Wagner et al., Phys. Rev. Lett. 109(7) 076102 (2012)

O 27.10 Tue 12:45 TRE Phy

**Stiffness and Electronic Properties of a Single-Molecule Wire** — •Christian Lotze[1], Martina Corso[2], Jingcheng Li[2], Gunnar Schulze[1], Thomas Niehaus[3], Alessandro Pecchia[4], Katharina J. Franke[1], and Nacho Pascual[2,5] — [1]Freie Universität Berlin — [2]CIC nanoGune, Donostia-San Sebastian, Spain — [3]Universität Regensburg — [4]CNR-ISMN, Rome, Italy — [5]IKERBASQUE, Bilbao, Spain

Understanding and controlling charge transport properties in single-molecule devices is of great interest, for example to realize future molecular electronic circuits. These properties may change under external stimuli, e.g. light irradiation, electric field or mechanical stress [1]. In our experiments we measure the stiffness and electronic properties of a wire consisting of a single molecule by means of combined Scanning Tunneling and Atomic Force Microscopy (STM/AFM) [2]. With our STM tip we contact a functionalized polyphenyl molecule in one side and lift it up from the surface, while the other side remains attached to the substrate [3]. During lift up we observe characteristic features in the molecule's conductance and find these correlated with plastic changes of the molecular junction. In agreement with DFT simulations we identify the creation of bonds as their origin and can draw a detailed picture of the lifting process of a single-molecule wire. [1] Briechle *et al.*, Beilstein J. Nanotechnol. 2012, 3, 798 [2] Giessibl, Reviews of Modern Physics, 75, 949 (2003) [3] F. Pump *et al.*, Appl. Phys. A 93, 335 (2008)

O 27.11 Tue 13:00 TRE Phy

**Force and Conductance in a Single Molecule Junction: SnPc on Ag(111)** — •Nuala M. Caffrey, Cesar Lazo, Paolo Ferriani, and Stefan Heinze — Institut für Theoretische Physik und Astrophysik, Christian-Albrecht-Universität zu Kiel, D-24098 Kiel, Germany

Characterisation of the relationship between chemical force and electronic transport in an atomic scale junction is now possible with the combination of scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) (e.g. [1]). Recent work in this area has concentrated mainly on atomic point contacts [2]. In this contribution, we determine, using density functional theory (DFT), the force experienced by an STM tip as it approaches the bistable tin-phtalocyanine (SnPc) molecule adsorbed on a Ag(111) surface. This molecule has been experimentally shown to have one of two possible conformations upon adsorption – either with the central Sn atom pointing away from (SnPc-up) or towards (SnPc-down) the surface [3]. We calculate the electronic transport through both conformations as a function of tip-molecule distance, i.e., in both the tunnelling and contact regime. We calculate the extent of the structural relaxations' contribution to both the force and conductance and furthermore extract the correlation between the two.

[1] Hauptmann et al., New J Phys. **14**, 073032 (2012)
[2] Ternes et al., Phys. Rev. Lett. **106**, 016802 (2011)
[3] Wang et al., J. Am. Chem. Soc. **131**, 3639 (2009)

## O 28: Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale III

Time: Tuesday 10:30–13:15 Location: TRE Ma

**Topical Talk** O 28.1 Tue 10:30 TRE Ma
**Ultrafast relaxation dynamics of Hubbard nanoclusters** — •Michael Bonitz[1], Sebastian Hermanns[1], Christopher Hinz[1], and Denis Lacroix[2] — [1]Institut für Theoretische Physik und Astrophysk, CAU Kiel, Leibnizstr. 15, 24098 Kiel — [2]IPN Orsay, 15 Rue Georges Clemenceau, 91406 Orsay

With the growing availability of intense short-pulse radiation sources it becomes possible to drive interacting many-particle or few-particle systems out of equilibrium in a controlled way. The subsequent relaxation and equilibration dynamics is still poorly understood. From a theory point of view these processes are complicated due to the simultaneous dynamics of the occupation functions and of binary correlations. The problem becomes even more complicated when the system has finite size and is spatially inhomogeneous [1]. The Hubbard model is a prototype for treating correlation effects in condensed matter or molecular systems fully including finite size and inhomogeneity effects. We, therefore, concentrate on the relaxation dynamics of small 1D, 2D and 3D Hubbard clusters that contain from a few to several hundred electrons. We observe a complex multi-stage relaxation behavior that depends on the external excitation, on the coupling strength and on the geometry of the system. In this talk we present results from two complementary theoretical approaches: first, from nonequilibrium Green functions where we apply the Generalized Kadanoff Baym ansatz [1] and, second, from a stochastic mean field approach.

[1] K. Balzer, and M. Bonitz, "Nonequilibrium Green's Functions Approach to Inhomogeneous Systems", Lect. Notes Phys. **867** (2013)

O 28.2 Tue 11:00 TRE Ma
**Exact adiabatic approximation in TDDFT** — •Jeiran Jokar and Nicole Helbig — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The use of functionals from static density functional theory in an adiabatic way in a time-dependent framework is known to cause various problems due to the resulting exchange-correlation kernel being frequency independent. In order to isolate the effects which are due to the adiabatic approximation we calculate the exact static potential for two electron systems. Before using this potential in an adiabatic way in a time propagation we need to ensure that the potential is well defined also at those parts of space where the density is small as they might become more populated at a later time. We use the exact adiabatic approximation to describe Rabi oscillations, i.e. the oscillation between the ground state and an excited state when a monochromatic laser with a frequency close to the resonance is applied.

O 28.3 Tue 11:15 TRE Ma
**Real-time propagation of coupled Maxwell-Schrödinger and time-dependent Kohn-Sham-Maxwell systems** — •René Jestädt[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Based on the Riemann-Silberstein vector of the electromagnetic field, we formulate Maxwell's equations in a symplectic spinor representation similar to the Dirac equation. This spinor representation allows us to use standard unitary propagation techniques developed for the Schrödinger equation [1] also for Maxwell's equations and simplifies a coupled solution of Maxwell's and Schrödinger's equations. To illustrate our approach, we present the real-time evolution of atomic systems embedded in optical waveguides and dielectric nanostructures. The coupling of Maxwell's equations to the time-dependent Kohn-Sham equations is a basic ingredient for the development of a time-dependent density functional theory formulation of quantum electrodynamics [2]. As an extension of our work on coupled Maxwell-Schrödinger systems, we show first steps of an implementation of Maxwell's equations coupled to the time-dependent Kohn-Sham equations in the first principles real-space real-time code octopus [3].

[1] A. Castro et al., J. Chem. Phys. **121** (2004).
[2] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011); I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).
[3] X. Andrade et al., J. Phys. Cond. Mat. **24** (2012).

O 28.4 Tue 11:30 TRE Ma
**Nonlinear optics by means of the dynamical Berry phase: Application to second- and third-harmonic generation** — •Claudio Attaccalite[1] and Myrta Gruning[2] — [1]Univ. Grenoble Alpes/CNRS, Institut Neel, F-38042 Grenoble, France — [2]School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK

We present an real-time approach to study nonlinear optical properties in Condensed Matter systems that is especially suitable for crystalline solids. The equation of motions and the coupling of the electrons with the external electric field are derived from the Berry phase formulation of the dynamical polarization. Many-body effects are introduced by adding single-particle operators to the independent-particle Hamiltonian. Specifically we include crystal local field effects, renormalization of the energy levels and excitonic effects. The approach is validated by calculating the second and third harmonic generation of bulk semiconductors. Finally we present second-harmonic generation spectrum of h-BN or MoS2 monolayers and show that correlation effects double the signal intensity at the excitonic resonances with respect to the contribution from independent electronic transitions.

References: [1] Nonlinear optics from ab-initio by means of the dynamical Berry-phase http://arxiv.org/abs/1309.4012 [2] Second Harmonic Generation in h-BN and MoS2 monolayers: the role of electron-hole interaction http://arxiv.org/abs/1310.7459

### 15 min. break

O 28.5 Tue 12:00 TRE Ma
**Accurate Correlation Energies from Adiabatic Time-Dependent Density Functional Theory with Renormalized Kernels** — •Thomas Olsen[1] and Kristian S. Thygesen[2] — [1]Universidad del Pais Vasco — [2]Center for Atomic-scale Materials Design (CAMD), Technical University of Denmark

We demonstrate the accuracy of electronic correlation energies obtained from the adiabatic connection and Time-Dependent Density Functional Theory (TDDFT) using a non-empirical renormalized gradient-corrected exchange-correlation kernel. The method can be viewed as a natural step beyond the Random Phase Approximation (RPA) and captures the short-range correlation effects which are poorly described in RPA. In particular, we show that for molecules and solids the renormalized kernel gives a four and five fold improvement in binding energies respectively when compared to RPA. We also consider examples of barrier heights in chemical reactions, molecular adsorption and graphene interacting with metal surfaces, which are three examples where RPA has provided highly accurate results. In these cases, our novel kernel provides results that are of equal quality or even slightly better than RPA, with a similar computational cost. We finally note that the renormalization procedure can be applied to any known semi-local exchange-correlation functional and thus defines an entire new class of adiabatic non-local functionals for ground state calculations within TDDFT.

O 28.6 Tue 12:15 TRE Ma

**Low scaling algorithm for the random phase approximation** — •Merzuk Kaltak, Jiri Klimeš, and Georg Kresse — University of Vienna, Computational Material Physics

The computationally most expensive step in conventional RPA implementations is the calculation of the independent particle polarizability $\chi$. We present an RPA algorithm that calculates $\chi$ using the Green function $G$ in real space and imaginary time. The systematic construction of optimized time and frequency grids for $G$ is obtained by means of solving a fitting problem. Furthermore a non-uniform discrete Fourier transform between the two grids is introduced, which converges exponentially. We show that the usage of the Green function approach in combination with the optimized grids can be used for the calculation of the RPA correlation energy for large systems.

O 28.7 Tue 12:30 TRE Ma

**Long range correlation energy from coupled atomic response functions** — •Alberto Ambrosetti and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Faradayweg 4-6 14195 Berlin, Germany

Electron correlation is an elusive and ubiquitous energy contribution that arises from transient collective electron fluctuations. Its reliable (accurate and efficient) modeling is central to the correct description of cohesive, structural, and response properties of molecules and solids. In this regard, the main challenge is to model the long-range correlation energy beyond (semi-)local density-functional approximations. Here we propose a very efficient method to compute the long-range correlation energy for non-metallic molecules and solids within a density functional theory framework, by using coupled atomic response functions (ARF). Extending the recent MBD method [1], we separate the coupling between ARFs into short and long range, allowing for a seamless many-body treatment of weakly and strongly polarizable systems. Thorough benchmarking on large data sets including small molecules (S22, S66x8), large supramolecular complexes (S12L), molecular crystals (X23) and bulk graphite shows consistently good agreement with high level theoretical and experimental reference binding energies (within the order of 6%). The uniform accuracy for molecules and solids represents a strong validation of our method, and further confirms the importance of modeling the truly collective nature of the long-range correlation energy. [1] A. Tkatchenko et al. PRL **108** 236402 (2012).

O 28.8 Tue 12:45 TRE Ma

**The exact Hohenberg-Kohn functional for a lattice model** — •Tanja Dimitrov[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Standard local exchange-correlation and semi-local functionals in ground-state density functional theory are known for their shortcomings in describing correct charge transfer, dissociation energies of molecular ions, and barriers of chemical reactions [1,2]. To understand the failures of approximate functionals and to gain insight into the behavior of the exact functional, we investigate the exact solution of the many-body Schrödinger equation for a lattice model. Using exact diagonalization, we explicitely construct the exact Hohenberg-Kohn functional and the mapping from densities to wavefunctions. Besides the normal inter-system derivative discontinuity widely discussed in the density-functional theory community, we observe a new feature of the exact functional in the low-density limit. This ”intra-system derivative discontinuity” resembles the inter-system derivative discontinuity, but is within the system (work in progress [3]). The description of many physical phenomena linked to charge-transfer processes (both in the static and dynamical regimes) require a proper account of this ”intra-system derivative discontinuity”.

[1] A. J. Cohen et al. Science **321**, 792 (2008).
[2] P. Mori-Sanchez et al., Phys. Rev. Lett. **100**, 146401 (2008).
[3] T. Dimitrov, H. Appel, A. Rubio to be published

O 28.9 Tue 13:00 TRE Ma

**Incorporating static correlation effects into density functional theory** — Nektarios N. Lathiotakis[1], •Nicole Helbig[2], Nikitas I. Gidopoulos[3], and Angel Rubio[4,5] — [1]Theoretical and Physical Chemistry Institute, NHRF Athens, Greece — [2]Peter-Grünberg Institut, Forschungszentrum Jülich, Germany — [3]Department of Physics, Durham University, United Kingdom — [4]Nano-Bio Spectroscopy group, Universidad del Pais Vasco and DIPC, San Sebastian, Spain — [5]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We present a novel idea that builds on the knowledge acquired in Reduced density matrix functional theory (RDMFT) to construct a density-functional scheme which accurately incorporates static and left-right correlation effects. At the same time, the new scheme preserves the high quality of a density functional description at the equilibrium and keeps the computational costs at an acceptable level comparable to the costs when using hybrid functionals. Within this scheme the natural orbitals, i.e. the eigenfunctions of the one-body density matrix, are constrained to be solutions of a single-particle Schrödinger equation with a local effective potential. This provides a natural way to connect an energy eigenvalue spectrum to the natural orbitals. This energy spectrum is found to reproduce the ionization potentials of different atoms and molecules very well. In addition, the dissociation limit of diatomic molecules is well described without the need to break any spin symmetry, i.e. this attractive feature of RDMFT is preserved. The present scheme can be easily implemented in all first principles codes for electronic structure calculations.

## O 29: Topological Insulators

Time: Tuesday 10:30–13:15 Location: GER 38

O 29.1 Tue 10:30 GER 38

**Topological Insulator goes Elemental: $\alpha$-Sn on InSb** — •M. R. Scholz[1], A. Barfuss[1], L. Dudy[1], A. Fleszar[2], G. Bihlmayer[3], D. Wortmann[3], J. H. Dil[4], G. Landolt[4], M. Radovic[4], G. Li[2], R. Claessen[1], and J. Schäfer[1] — [1]Phys. Inst. and RCCM, Univ. Würzburg — [2]Inst. f. Theo. Physik u. Astronomie, Univ. Würzburg — [3]Peter Grünberg Inst. a. Inst. f. Advanced Simulation, FZ Jülich — [4]Swiss Light Source, Paul-Scherrer-Institut Villigen

We report on the topological insulator phase of epitaxially grown $\alpha$-Sn on InSb substrates where compressive strain is induced by a slight lattice mismatch. The topological surface state (TSS) forms in the presence of an unusual band order not based on direct spin-orbit coupling, as shown in DFT and GW slab-layer calculations. Angle-resolved photoemission probes how the TSS emerges from the second highest bulk valence band. By means of spin-resolved photoemission we show that the surface state is highly spin-polarized with a counter-clockwise helicity below the Dirac point. The band situation in $\alpha$-Sn closely resembles that of strained HgTe. Quantum well films of HgTe sandwiched between CdTe are a system where the topological properties have been successfully probed in DC transport [1]. The similarities to HgTe make $\alpha$-Sn a promising candidate to exhibit the quantum spin Hall effect as well, if the film thickness is reduced to the 2D limit. Particularly, as a nontoxic elemental system, $\alpha$-Sn is easier to fabricate which opens various pathways to access and manipulate the topological surface state. As a first step, we demonstrate the precise control of the Fermi level by dopants. [1] M. König et al., Science 318, 766 (2007).

O 29.2 Tue 10:45 GER 38

**Temperature effects in soft and hard x-ray photoemission from topological insulators** — •Jürgen Braun, Jan Minar, and Hubert Ebert — Dept. Chemie, LMU Universität München, Germany

A brief introduction to the theory of temperature-dependent soft and hard x-ray angle-resolved photo electron spectroscopy (SARPES, HARPES) of solid materials is given with an emphasis on the so-called one-step-model of photoemission. The main aspects of the theory [1,2] and its implementation within the Munich SPR-KKR program package [3] will be reviewed. Our method, which is based on the Coherent Potential Approximation (CPA) alloy theory (alloy analogy model), goes well beyond the simple, but standard Debye-Waller approach to photoemission by including in particular the temperature dependence of the effective photoemission matrix elements as well. This allows among others to reproduce the so called XPS- or density of states limit in angle-resolved photoemission which occurs for high photon energies and/or high temperatures due to a full Brillouin zone averaging caused by phonon scattering. First examples of soft- and hard x-ray ARPES calculations at finite temperature for W(110), $Sb_2Te_3$ and $Bi_2Se_3$ will be presented.

1. A. Gray, J. Minár, J. Braun, H. Ebert, C. S. Fadley et al., Nature Materials, **10**, 759 (2011) and Nature Materials **11**, 957 (2012) 2. J. Braun, J. Minár, H. Ebert et al. Phys. Rev. B **88** 005400 (2013) 3. H. Ebert et al., The Munich SPR-KKR package, version 6.3, http://olymp.cup.uni-muenchen.de/ak/ebert/

O 29.3 Tue 11:00 GER 38

**Reorganization of a Topologically Protected Surface State: Theory for Au-Covered $Bi_2Te_3$(111)** — Francisco Muñoz[1,2], •Jürgen Henk[2], and Ingrid Mertig[2] — [1]Facultad de Ciencias, Universidad de Chile, Chile — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

The electronic structure of Au-covered $Bi_2Te_3$ is investigated by first-principles calculations. The Dirac surface state of the topological insulator $Bi_2Te_3$ hybridizes with the Au sp states, which gives rise to strong reorganization of the surface electronic structure. Striking features of the modified Dirac surface state are (i) the introduction of new Dirac points within the fundamental band gap of $Bi_2Te_3$, (ii) an extremely weak dispersion, and (iii) an anisotropic number of conducting channels in the fundamental band gap of $Bi_2Te_3$ which leads to a complicated Fermi surface. Our findings have impact for spin-dependent surface transport.

O 29.4 Tue 11:15 GER 38

**Barrier-free sub-surface incorporation of magnetic impurities into the Bi(111) surface: Manipulation of the protected surface state - Experiment** — •C. Klein[1], P. Zahl[2], N. Vollmers[3], U. Gerstmann[3], D. Lückermann[4], G. Jnawali[1], H. Pfnür[4], C. Tegenkamp[4], W.-G. Schmidt[3], P. Sutter[2], and M. Horn-von Hoegen[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, DE — [2]Center for Functional Nanomaterials, Brookhaven National Laboratory, New York, USA — [3]Department of Physics, University of Paderborn, DE — [4]Institut for Solid State Physics, University of Hannover, DE

Due to the large spin orbit coupling, electron backscattering within the Bi(111) surface states is strongly suppressed. In order to identify possible scattering mechanisms we performed low temperature scanning tunneling microscopy (LT-STM) measurements in which submonolayer amounts of 3d-metals (Fe, Co, Ni, Cu) were deposited at 5K. The metal atoms become immediately embedded in a sub-surface site, as they are not present in STM topography. They only become apparent in STS at tunneling conditions close to the Fermi-energy, as they are surrounded by a pronounced anisotropic threefold electronic scattering pattern with lateral dimensions of more than 10 nm. DFT calculations indeed confirm a barrier free incorporation of the 3d-metal impurities into the first Bi-Bilayer even at such low temperatures. This incorporation effect is limited to 3d-metals, as screening effects of the s- and p- orbitals are of great importance and leads to an effective reduction of the free surface energy of about 5 eV.

O 29.5 Tue 11:30 GER 38

**Efficient full-relativistic DFT calculations for large systems: Application to Bi-related surface states** — •Uwe Gerstmann[1], Nora Jenny Vollmers[1], Wolf Gero Schmidt[1], Claudius Klein[2], Michael Horn-von Hoegen[2], Philipp Kröger[3], Daniel Lückermann[3], Herbert Pfnür[3], and Christoph Tegenkamp[3] — [1]Department of Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn — [2]Center for Nanointegration CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — [3]Institut for Solid State Physics, University of Hannover, Appelstr. 2, 30167 Hannover

Spin-orbit coupling is well-known to be the driving force behind ferromagnetism and can be used to control the functionality of electronic devices in spintronics. In asymmetric quantum wells and at surfaces spin-split electron gases may form and give rise to the Rashba-effect. In some cases, e.g. Bi(111) bilayers, the bandstructures are furthermore affected by k-point dependent shifts in the order of several eV. This effect may become crucial if adatoms are incorporated or adsorbed at the surface, strongly influencing the occupancy of the adatom-induced states and by this the magnetic moments and further magneto-transport properties of the resulting structures. In this work, we present an efficient pseudopotential-based method that allows a full-relativistic description of large systems containing several hundreds of atoms. The approach is used to describe the incorporation of a wide range of atomic species (3d-transition, coin-metal as well as rare-earth ions) into Bi(111) surfaces, where supercells with more than 200 atoms are needed to describe the resulting extended magnetic structures correctly.

O 29.6 Tue 11:45 GER 38

**Magnetic impurities on Bi thin films - Conductivity and surface diffusion** — •Philipp Kröger[1], Daniel Lükermann[1], Sergii Sologub[2], Nora Vollmers[3], Uwe Gerstmann[3], Wolf Gero Schmidt[3], Herbert Pfnür[1], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Inst. für FKP, Appelstr. 2, 30167 Hannover — [2]Inst. of Ph., Nat. Acad. of Sc., Nauky Av. 46, 03028 Kyiv, Ukraine — [3]Universität Paderborn, Theoretische Physik, 33098 Paderborn

The semimetal bismuth has attracted a lot of interest because of its unique electronic properties such as a low carrier concentration and a large mobility. The surface states reveal a pronounced Rashba splitting and the conductivity can be well discriminated from bulk contributions if thin films are grown epitaxially on Si(111) substrates, making surface related effects accessible even in macroscopic conductance measurements.

In this context the adsorption of the magnetic atom Cr (4,8 $\mu_B$) on the Bi(111) surface will be discussed. In comparison to other adsorbates (Fe, Co, Tb) Cr exhibits the strongest scattering effect, accompanied by a transition from Weak Anti- to Weak Localization. This transition indicates strong impurity scattering, which lifts all spin-dependent selection rules. Furthermore, a significant increase of electron concentration due to hybridization effects has been found. For Tb and Cr surface diffusion of adsorbate-atoms even at $T \approx 10$ K needs to be considered.

O 29.7 Tue 12:00 GER 38

**Magnetic interaction and magnetic fluctuations in topological insulators with ordered and disordered magnetic adatoms** — •MAIA G. VERGIORY[1,4], LEVAN CHOTORLISHVILI[2], ARTHUR ERNST[1], VITALI DUGAEV[1], ANDREAS KOMNIK[3], MIJAIL OTROKOV[4], EVGUENI CHULKOV[4], and JAMAL BERADKAR[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Institut fr Physik, Martin-Luther-Universitat Halle-Wittenberg, Germany — [3]Institut fr Theoretische Physik, Universitt Heidelberg, Germany, — [4]Donostia International Physics Center, Donostia - San Sebastian, Spain

Using a first-principles Green's function approach we study magnetic properties of the magnetic binary topological insulators Bi2Se3, Bi2Te23 and Sb2Te3 doped with 3d transition metals. We analyze the magnetic phase for each dopant, the exchange interaction, the Curie temperature and the Bloch spectral function. Furthermore, we observe that the interaction of magnons with surface electrons essentially renormalizes the electron energy spectrum. The renormalized spectrum is nonlinear and can be characterized by a negative effective mass of electrons and holes for any k point different from 0. The electron velocity near the Dirac point depends on the electron-magnon coupling.

O 29.8 Tue 12:15 GER 38

**The edge state at the dark side of the weak topological insulator $Bi_{14}Rh_3I_9$ probed by STM** — •Christian Pauly[1], Bertold Rasche[2], Marcus Liebmann[1], Marco Pratzer[1], Klaus Koepernik[3], Manuel Richter[3], Michael Ruck[2], Jeroen van den Brink[3], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University and Jara Fit, Germany — [2]Departement of Chemistry and Food Chemistry, TU Dresden, Germany — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Germany

Using scanning tunneling microscopy (STM) and spectroscopy (STS) at 6 K, we probe the local atomic and electronic structure of the weak topological insulator $Bi_{14}Rh_3I_9$ [1]. In [001]-direction, the material is built from stacks of intermetallic planes with non-trivial 2D topology and spacer layers in between. Thus, the surfaces of the intermetallic planes, which are the natural cleaving planes of the material, exhibit a trivial band gap however with topologically protected states at each step edge [1]. Bi$_{14}$Rh$_3$I$_9$ is cleaved at a base pressure of $10^{-10}$ mbar giving rise to several hundreds of nm large terraces of the intermetallic layer interrupted by step edges. Using STS, we identified the band gap on top of the intermetallic layer, which is in agreement with ARPES data, whereas at the step edges we directly mapped the edge state. The edge state appears continuously through the band gap and exhibits a spatial distribution of 0.4 nm FWHM. The observed spatial periodicity along the step edge is in line with the atomic structure confirming the Bloch type of this state. Partially, dispersive features appear which will be discussed. [1] B. Rasche et al., Nature Mater. 12, 422 (2013)

O 29.9 Tue 12:30 GER 38

**Evidence for topological band inversion of the phase change material Ge$_2$Sb$_2$Te$_5$** — •Marcus Liebmann[1], Christian Pauly[1], Alessandro Giussani[2], Jens Kellner[1], Sven Just[1], Jaime Sanchez-Barriga[3], Emile Rienks[3], Oliver Rader[3], Raffaella Calarco[2], Gustav Bihlmayer[4], and Markus Morgenstern[1] — [1]II. Inst. Phys. B, RWTH Aachen University — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin — [3]Helmholtz-Zentrum für Materialien und Energie, BESSY, Berlin — [4]Peter-Grünberg-Institut and Institute für Advanced Simulation, Forschungszentrum Jülich

We present an angle-resolved photoemission study of the ternary phase change material Ge$_2$Sb$_2$Te$_5$, epitaxially grown on Si(111) in the metastable cubic phase. This material serves, e.g., in DVDs as a fast switchable material (1 ns) between the metallic cubic and an insulating amorphous phase. The observed upper bulk valence band shows a minimum at $\bar{\Gamma}$ being 0.3 eV below the Fermi level $E_\mathrm{F}$ and a circular Fermi contour around $\bar{\Gamma}$ with a dispersing diameter of $0.27-0.36$ Å$^{-1}$. This is in agreement with density functional theory calculations of the Petrov stacking sequence of the cubic phase which is topologically non-trivial. Moreover, the results are in line with all previous calculations of Ge$_2$Sb$_2$Te$_5$ exhibiting the valence band maximum at $\Gamma$ for a trivial $\mathbb{Z}_2$ topology and away from $\Gamma$ for a non-trivial one. Scanning tunneling spectroscopy exhibits a band gap of 0.4 eV around $E_\mathrm{F}$. Our finding opens the perspective of ns-switching between a topological crystalline and an insulating amorphous phase.

O 29.10 Tue 12:45 GER 38

**Step wise variation of the electrochemical potential at step edges of the Bi$_2$Se$_3$ surface** — •Christian A. Bobisch, Sebastian Bauer, and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

Bi$_2$Se$_3$ is a 3D topological insulator (TI) whose surface states are protected from direct backscattering by time reversal symmetry [1]. However, step edges on a Bi$_2$Se$_3$ surface are predicted to work as an electron scatterer for other scattering angles than 180° backscattering [2]. We studied the electron transport on the surface of a 14.5 QL (quintuple layer) thick Bi$_2$Se$_3$ film grown on Si(111). By a distance dependent resistance measurement [3] in the $\mu m$ range, we found a metallic character of the film with a sheet conductance of $2\times10^{-3}\Omega^{-1}$ which agrees well with recent literature [4]. By scanning tunneling potentiometry (STP) [5], we simultaneously analyzed the topography and the electrochemical potential $\mu_{ec}$ under real transport conditions. We observe on the microscopic scale a potential gradient which corresponds well the macroscopic conductance. In the vicinity of step edges we find a step-like variation of $\mu_{ec}$ which is a fingerprint of electron scattering at the step edge. For the given sample the electrical conductivity of a 1 QL step could be deduced to $3800\pm500\Omega^{-1}\mathrm{cm}^{-1}$.

[1] M. Z. Hasan et al., Rev. Mod. Phys. 82, 3045 (2010). [2] W. Jing et al., Chin Phys. B 22, 067301 (2013). [3] P. Jaschinsky et al., J. Appl. Phys. 104, 094307 (2008). [4] A. A. Taskin et al., Phys. Rev. Lett. 109, 066803 (2012). [5] P. Muralt et al., Appl. Phys. Lett. 48, 514 (1986).

O 29.11 Tue 13:00 GER 38

**Quantum phase transitions of a disordered antiferromagnetic topological insulator** — •Paul Baireuther[1], Jonathan M. Edge[1], Ion C. Fulga[1], Carlo W.J. Beenakker[1], and Jakub Tworzydlo[2] — [1]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — [2]University of Warsaw, Hoza 69, 00-681 Warsaw, Poland

We have studied the effect of electrostatic disorder on the conductivity of a three-dimensional antiferromagnetic insulator (a stack of quantum anomalous Hall layers with staggered magnetization). The phase diagram contains regions where the increase of disorder first causes the appearance of surface conduction (via a topological phase transition), followed by the appearance of bulk conduction (via a metal-insulator transition). The conducting surface states are stabilized by an effective time-reversal symmetry that is broken locally by the disorder but restored on long length scales. A simple self-consistent Born approximation reliably locates the boundaries of this socalled "statistical" topological phase.

## O 30: Surface Chemical Reactions and Heterogeneous Catalysis II

Time: Tuesday 10:30–12:45 Location: PHY C 213

O 30.1 Tue 10:30 PHY C 213

**Recent mechanistic insights into the electrochemical CO2 reduction at platinum electrodes in pyridine containing electrolytes** — •Katrin R. Bickel, Simon Filser, Qi Li, Konrad Schönleber und Katharina Krischer — Nonequilibrium Chemical Physics, Physics Department, Technical University Munich, Germany

The development of suitable energy storage concepts is essential for the efficient use of renewable energy sources. One promising approach is the electrochemical conversion of CO2 to liquid or gaseous fuels. However, due to the large activation barrier for the reduction of CO2, such a process is challenging.

In the 1990s, Bocarsly et al. reported that in the presence of pyridine CO2 can be electrochemically reduced to methanol on palladium or platinum electrodes at a comparably low overpotential [1]. Despite various electrochemical and theoretical studies, the mechanism of this reduction process is still unclear. In particular, the role of the metal surface and the occurring reaction intermediates are under dispute.

We present recent results of a mechanistic study of the CO2 reduction in the presence of pyridine, amongst others by rotating disk electrode measurements. We found strong indications for the presence of an adsorbed pyridine species at the metal electrode. Therefore, a particular focus is placed on the nature of this surface species and its role in the reduction process.

[1] G. Seshadri, C. Lin, A. B. Bocarsly; J. Electroanal. Chem., 1994, 372, 145

O 30.2 Tue 10:45 PHY C 213

**Anodization of aluminum surfaces** — •Florian Bertram[1], Jonas Evertsson[1], Fan Zhang[2], Jinshan Pan[2], Francesco Carlà[3], and Edvin Lundgren[1] — [1]Lund University, Division of Synchrotron Radiation Research, Lund, Sweden — [2]KTH Royal Institute of Technology, Department of Chemistry, Division of Surface and Corrosion Science, Stockholm, Sweden — [3]ESRF, Grenoble, France

Aluminum and Aluminum alloys are used in a broad range of everyday commercial products. For many of these products an efficient corrosion protection is critical. In oxygen or aqueous environment aluminum forms a passivating surface oxide layer with a typical thickness of 2-4.3 nm. This surface oxide already offers some corrosion protection. By increasing the thickness of the surface oxide it is possible to increase the corrosion resistivity. One way to increase the thickness widely used in today's industry is anodization.

Here, we present the results of the anodization of an aluminum single crystal and an aluminum alloy studied by in-situ x-ray reflectivity. The reflectivity studies have been complemented by electrochemical impedance spectroscopy. Both single crystal as well as alloy samples show a linear increase of film thickness with increasing anodization voltage. However, the slope is much higher in the single crystal case.

O 30.3 Tue 11:00 PHY C 213

**Improvement of the electrical conductivity of bipolar plates for fuel cells by plasma etching in carbon dioxide environment** — •Tatiana Fedosenko, Nicolas Wöhrl, and Volker Buck — Faculty of Physics, University of Duisburg-Essen, Carl-Benz-Str. 199, 47057 Duisburg, Germany

Bipolar plates for the fuel cells, made of carbon-polymer composites, are one way to distribute the fluid and to conduct the current from the anode of one cell to the cathode of the adjacent cell. However, polypropylene (PP) significantly decreases the contact conductivity between the plates in a stack. It is possible to improve the contact conductivity by etching the PP at the surface in microwave plasma. A microwave plasma source is used in remote mode (CYRANNUS by iplas) that allows plasma treatments up to atmospheric pressure, making the process scalable for industrial applications.

In this study the bipolar plates are etched in carbon dioxide plasma, varying the etching time. SEM and Fourier transform infrared spectroscopy (FTIR) is used to analyze the changes in the surface chemistry. Plasma etching is more advanced than the deposition of the coating of electrocatalytic materials onto the surface of the bipolar plates, since such coating must meet many criteria: a very good adhesion, the coating should not be degraded by high temperatures and water.

Contact resistivity measurements are interpreted with respect to the etching of the surface and rearrangements of the chemical bonds in the PP due to plasma irradiation of the surface.

O 30.4 Tue 11:15 PHY C 213

**Photo-catalytic water splitting with co-catalysts: beyond proton-coupled electron transfer** — •Harald Oberhofer, Markus Sinstein, Ran Jia, and Karsten Reuter — Technische Universität München, Germany

Efficient, sustainable production of molecular hydrogen—a promising alternative to batteries in terms of energy storage—is still an unsolved problem. Recently, we presented [1] a novel screening method for viable combinations of photocatalysts and metal co-catalysts based on the computational hydrogen electrode approach pioneered by Nørskov and Rossmeisl.[2] In this thermodynamic approach charge-neutral proton-coupled electron transfer (PCET) pathways are generally assumed. Any screening approach resting on this assumption may therefore falsely rule out viable catalysts following other, uncoupled pathways.

Using an implicit solvent model we recently implemented into the FHI-aims DFT package,[3] we extend our screening scheme to uncoupled reaction paths, where due to the occurrence of charged intermediates solvent screening effects can no longer be neglected. We present first results of our screening efforts and show that even for charge-neutral PCET pathways solvent effects can not be neglected.
[1] H. Oberhofer, K. Reuter, J. Chem. Phys. **139**, 44710 (2013).
[2] A. Valdes *et al.*, J. Phys. Chem. C **112**, 9872 (2008).
[3] V. Blum *et al.*, Comp. Phys. Commun. **180**, 2175 (2009).

O 30.5 Tue 11:30 PHY C 213

**Towards Heterogeneous Catalysis Beyond the Born-Oppenheimer Approximation: LDFA and beyond** — •Simon P. Rittmeyer[1], J. Iñaki Juaristi[2], Karsten Reuter[1], and Jörg Meyer[1] — [1]TU München, Germany — [2]Depto. & Centro de Física de Materiales (CSIC-UPV/EHU), San Sebastián, Spain

Inspired by the need of a more efficient and thus responsible use of energy, an age of light-enhanced heterogeneous catalysis is dawning. Even photons from sunlight can be used to accelerate surface reactions, if their energy is selectively and efficiently transferred into distinct nuclear degrees of freedom [1]. However, on metal catalysts resulting athermal mode populations are generally challenged by rapid energy dissipation in particular into the continuum of easily accessible electron-hole pair excitations. *Ab initio* molecular dynamics simulations beyond the Born-Oppenheimer approximation can assess corresponding lifetimes and therewith answer important questions as to the feasibility and efficiency of such light enhancement of catalytic reaction steps. On the way to establishing a numerically tractable approach even for complex surface processes we pursue the local density friction approach (LDFA) [2] and extend it beyond the hitherto inherent independent-atom and frozen-surface approximation. We apply this new scheme to the non-adiabatic damping of adsorbate vibrations on transition metal surfaces and critically discuss it by comparing the results to other theoretical approaches as well as experimental data.
[1] S. Linic *et al.*, Acc. Chem. Res. **46**, 1890 (2013).
[2] J. I. Juaristi *et al.*, Phys. Rev. Lett. **100**, 116102 (2008).

O 30.6 Tue 11:45 PHY C 213

**Ligand-controlled electrocatalytical response in the oxygen reduction reaction in iron-based 2D metal-organic structures** — Doris Grumelli[1], •Benjamin Wurster[1], Sebastian Stepanow[1], Rico Gutzler[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

In this work we present the electrochemical characterization of single iron atoms coordinated by either tetracyanoquinodimethane (TCNQ), bis-pyridyl-bipyrimidine (PBP) or phythalocyanine (Pc) on Au(111).

The samples were prepared under ultra-high vacuum (UHV) conditions by evaporating either FePc or the organic ligands together with iron, which subsequently self-assemble and form two-dimensional metal-organic coordination networks. By scanning tunneling microscopy in UHV the composition and structure of the networks and FePc layer were controlled and characterized. The sample is brought from UHV to the electrochemical cell through a transfer chamber in a controlled environment, in which the catalytic activity towards the oxygen reduction reaction in alkaline media is studied. Linear voltammetry experiments show that depending on the coordination environment of Fe the mechanism of the reduction of $O_2$ is changed. TCNQ-Fe catalyzes the reduction towards $H_2O_2$ on a $2e^-$ pathway. For PBP-Fe and FePc the complete reduction to $H_2O$ is observed. PBP-Fe catalyzes on a $(2+2)e^-$ pathway, while FePc on a direct $4e^-$ pathway.

O 30.7 Tue 12:00 PHY C 213

**Non-adiabatic effects in the oxidation of ultrathin crystalline Mg films: quantum size effects and hot charge carrier distribution** — •Ulrich Hagemann and Hermann Nienhaus — Faculty of Physics and Center for Nanointegration (CeNIDE), University of Duisburg-Essen, D-47048 Duisburg, Germany

The low-temperature oxidation of ultrathin Mg films in the thickness range between 5 and 30 monolayers (ML) epitaxially grown on Si(111)-7x7 substrates is studied applying the chemicurrent method. The well-ordered films are characterized by electron diffraction and quantum well photoelectron spectroscopy. The exothermic reaction of $O_2$ molecules with Mg surfaces creates electron-hole pairs which are detected in the Mg:*p*-Si Schottky diodes as a chemicurrent. For metal layer thicknesses of approximately 8 and 12 ML the chemically induced current is significantly enhanced by a factor of up to three. We show that this result can be explained by an increased initial reactivity due to the normal confinement of the electrons. The resulting quantum well states lead to larger electron densities of states at the Fermi level for 8 and 12 ML. By fabricating different Mg/Si Schottky diodes with varying barrier heights the energy distribution of the excited hot charge carriers for the Mg oxidation is probed. The distribution exhibits an exponential behaviour which may be described by a Boltzmann-type function with an effective temperature of approximately 1600K.

O 30.8 Tue 12:15 PHY C 213

**Kinematic effects in the non-adiabatic energy dissipation during oxidation of Al surfaces** — •Achim Gerstenberg, Ulrich Hagemann, and Hermann Nienhaus — University of Duisburg-Essen and Center for Nanointegration (CENIDE), Duisburg, Germany

There is a long-standing controversial debate on the nature of the low initial sticking of oxygen molecules on Al(111) surfaces [1]. In the present study, the reaction is investigated for low substrate temperatures with respect to the kinetic energies of the impinging oxygen molecules using the chemicurrent method. The released reaction energy is partly dissipated non-adiabatically by generation of electron-hole pairs in the metal surface. The created hot charge carriers are detected as a chemicurrent in large-area Al/*p*-Si (111) Schottky diodes with Al films of 4 to 20 nm thickness. The homogeneous Schottky barrier height is determined to be 0.45 eV. Upon exposure to a hyperthermal molecular beam of oxygen molecules seeded in He gas the temporal evolution of the chemicurrent exhibits a maximum in agreement with the low initial reaction probability and in accordance to a nucleation and growth kinetics. When the kinetic energy of the molecules is raised from 50 to 250 meV the respective chemicurrent increases strongly. This kinematic current enhancement is still observed after longer exposures for the partially oxidized Al(111) surface.
[1] M.Kurahashi and Y.Yamauchi, PRL 110 (2013) 246102 and ref. therein.

O 30.9 Tue 12:30 PHY C 213

**Temperature programmed desorption from chemoelectronic nanodiodes** — •Jan Philipp Meyburg, Ievgen Nedrygailov, Eckart Hasselbrink, and Detlef Diesing — Fakultät für Chemie, Universität Duisburg-Essen, Essen, Germany

Chemoelectronic nanodiodes based on metal–oxide–semiconductor thin film structures allow the in-situ detection of energy release on the top metal electrode of the devices when a surface reaction takes place. This energy can be transported through the nanodiode by hot charge carriers that lead to a detectable current. While the contribution of hot carriers during oxidation and adsorption processes is already reported, the involvement of hot carriers during desorption processes is still to be observed. In this context, temperature programmed desorption from the surface of Pt–$SiO_2$–$n$-Si chemoelectronic nanodiodes is demonstrated using a heating method that allows for desorbing locally from the Pt top electrode. For this purpose, the 5 nm Pt top electrode is directly heated from 80 to 300 K by a current flow. Simultaneously the temperature is monitored by measuring the Pt film resistance. Reproducible results for water desorption are obtained using this method.

## O 31: Molecular Films: Properties and Preparation

Time: Tuesday 10:30–13:00 Location: WIL A317

O 31.1 Tue 10:30 WIL A317

**Ultrathin poly(ethylene glycol) films as flexible platform for plasmonics and nanofabrication** — Nikolaus Meyerbröker and •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

We present a novel approach to prepare ultrathin, biocompatible, hydrogel films based on cross-linking of multi-functionalized, star-branched poly(ethylene glycols) (STAR-PEGs) with tunable film thicknesses of 4-200 nm. The films revealed pronounced swelling behavior, which was fully reversible and could be precisely controlled. Additionally, they provided a high affinity to citrate-stabilized gold nanoparticles (AuNP) that could be adsorbed with high densities into the PEG matrix from an aqueous solution. These novel PEG/AuNP composite films offer interesting and potentially useful optical properties. Controlling the accessibility, swelling behavior, and biorepulsive properties of the PEG films lithographically, we prepared nanocomposite patterns of metal nanoparticles and fluorophores imbedded into the PEG matrix as well as protein-affinity patterns in protein-repelling background. Further, using electron beam lithography, we succeeded to fabricate a variety of different nanostructures. Finally, we demonstrated that the PEG films can be separated from the substrate and exist as ultrathin, biocompatible, free-standing membranes. These membranes possess high stability and exceptional elasticity. They can be used in transmission electron microscopy experiments on sensitive biological targets and as a new type of support for the characterization of nanoparticles.

O 31.2 Tue 10:45 WIL A317

**X-ray spectroscopic analysis of the electronic structure of aqueous salt solutions** — •Yekkoni Jeyachandran[1], Frank Meyer[2], Andreas Benkert[2,3], Marcus Bär[4,5], Regan Wilks[4], Monika Blum[5], Wanli Yang[6], Friedrich Reinert[2], Clemens Heske[3,5], Lothar Weinhardt[3,5], and Michael Zharnikov[1] — [1]Angew. Phys. Chemie, Universität Heidelberg. — [2]Exp. Phys. VII, Universität Würzburg. — [3]Inst. Photon Sci. Synchr. Rad., Karlsruhe Institute of Technology. — [4]Sol. Energy Res., Helmholtz-Zentrum Berlin. — [5]Dept. Chem., University of Nevada Las Vegas. — [6]Advanced Light Source, Lawrence Berkeley National Laboratory.

Modification of the molecular structure of water in the presence of ionic salts is of primary importance for a variety of chemical and biochemical processes. Advanced soft X-ray spectroscopic techniques, which provide information on the local electronic structure of molecules, can be used to probe such a modification. In this work, using a specially designed experimental setup, we studied the electronic structure of water molecules in aqueous alkali halide and calcium chloride solutions by non-resonant and resonant X-ray emission spectroscopy (XES). Significant changes in the characteristic emission spectra of water were observed at the variation of the salt concentration, with the extent and character depending on the size and valence state of the involved anions and cations. The observed spectral changes are discussed in terms of the disturbances of the hydrogen bond network of water molecules induced by the salts. These changes are accompanied by the changes in the electronic structure of water, which can be traced by XES.

O 31.3 Tue 11:00 WIL A317

**Thermally induced defects in Langmuir-Blodgett films** — Jan Weber, Eckart Hasselbrink, and •Thorsten Balgar — Fakultät für Chemie, Universität Duisburg-Essen, Germany

In recent years organic monolayers of long-chain aliphatic molecules are intensively discussed in the context of heterogeneous catalysis, microelectronics or biosensing since they allow for chemical tailoring of various surfaces.[1-3] In this context the inner structure of the monolayer regarding a proper chain alignment is of considerable interest. We have utilized vibrational sum-frequency generation spectroscopy (VSFG) to monitor the creation of conformational chain defects at elevated temperatures. Our study is focused on Langmuir-Blodgett monolayers of long-chain carboxylic acids on glass substrates.

[1] A. Corma and H. Garcia, Adv. Synth. Catal. 348 (2006) 1391

[2] T. Balgar, S. Franzka, E. Hasselbrink and N. Hartmann, Appl. Phys. A 82 (2006) 15

[3] F. Schreiber, Prog. Surf. Sci. 65 (2000) 151

O 31.4 Tue 11:15 WIL A317

**Molecular level insights into diatom biomineralization** — •Helmut Lutz[1], Joe Baio[2], Adrienne Roehrich[3], Mischa Bonn[1], Gary Drobny[3], and Tobias Weidner[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz — [2]Oregon State University, Merryfield South 102A, Corvallis OR 97331 — [3]University of Washington, Seattle, Washington 98195, United States

The nano-patterned silica shells of diatoms represent a remarkable example for biomineralization, a process controlled by protein*mineral interactions. Within the unicellular algae Cylindrotheca fusiformis, the silaffin proteins play a crucial role in the molecular biomineralization machinery. A specific repeat unit within the silaffin precursor protein, SSKKSGSYSGSKGSKRRIL (R5), precipitates silica-peptide nanoparticles out of a solution of silicic acid. We found that artificial peptides consisting of lysine and leucine (LK peptides) can mimic this capability of forming various biosilica structures. These peptides were designed to adopt helical or beta-sheet structures due to their hydrophobic periodicities and represent simple model systems to study the effect of protein folding on mineralization. In order to propose rational protein- and surface design rules it is essential to elucidate the driving force of the biosilification process. By means of surface sensitive techniques, e.g. sum frequency generation (SFG) we have studied the interactions of R5 and the LK peptides within biosilica composites and on silica surfaces.

O 31.5 Tue 11:30 WIL A317

**Core-Level Spectroscopy Studies on Self-Assembly and Switching of Mixed Azobenzene Monolayers** — •Daniel Przyrembel[1], Thomas Moldt[1], Daniel Brete[1], Joel R. Goldman[2], Rafal Klajn[2], Cornelius Gahl[1], and Martin Weinelt[1] — [1]Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]Department of Organic Chemistry, Weizmann Institute of Science, 76100 Rehovot, Israel

We have prepared mixed self-assembled monolayers (SAMs) containing photochromic azobenzene derivatives.[1] Besides this, our approach allows creating layers of, *e.g.*, an 11-(4-(phenyldiazenyl)phenoxy)alkyl-1-thiol diluted with a $C_{12}$ alkane thiol on Gold(111) substrates from solution in a controlled way. Like this we obtained monolayers with tuneable packing density of the azobenzene units that are stable and durable under ambient conditions. Moreover, the attained increase in free volume around the chromophores in combination with efficient decoupling from the substrate yields reversibly switchable SAMs, responsive to ultraviolet and visible light. Here we present our results from investigating by means of core-level spectroscopies the self-assembly process and the photoswitching. The samples exhibit a complex mixing behaviour with preferential adsorption of one component; and we observed a changing degree of ordering depending on the time the samples are immersed during preparation. The measured changes due to photoswitching vary for different surface component ratios.

[1] D. Brete, D. Przyrembel, C. Eickhoff et al. *J. Phys.: Condens. Matter* **24**, 394015 (2012).

O 31.6 Tue 11:45 WIL A317

**Molecular Orientation and Excitonic Coupling in Photoswitchable Azobenzene-Based SAMs on Gold**(111) — •Thomas Moldt[1], Daniel Brete[1], Daniel Przyrembel[1], Joel R. Goldman[2], Rafal Klajn[2], Cornelius Gahl[1], and Martin Weinelt[1] — [1]Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Department of Organic Chemistry, Weizmann Institute of Science, 76100 Rehovot, Israel

We present results of polarization-dependent UV/vis Differential Reflectance Spectroscopy (DRS) and Near Edge X-Ray Fine Structure (NEXAFS) spectroscopy measurements performed on mixed self-assembled monolayers (SAMs). The layers consist of 11-(4-(-phenyldiazenyl)phenoxy)undecane-1-thiol (Az11) and dodecane-1-thiol (C12). The average orientation of the azobenzene moieties and the strength of the excitonic coupling between the chromophores depend on the component ratio in the SAM. Likewise, this influences the efficiency of the reversible photoswitching of the layer.

O 31.7 Tue 12:00 WIL A317

**New Chemistry of Metal-Protein Systems: S-Layer Protein Interaction with Copper and Iron under Ultra-High Vacuum** — •Anna A. Makarova[1,2], Vera S. Neudachina[3], Elena V. Grachova[2], Lada V. Yashina[3], Anja Blüher[1], Michael Mertig[1], Serguei L. Molodtsov[4], Clemens Laubschat[1], and Denis V. Vyalikh[1] — [1]Technische Universität Dresden, Dresden, Germany — [2]St.Petersburg State University, St.Petersburg, Russia — [3]Moscow State University, Moscow, Russia — [4]European XFEL GmbH, Hamburg, Germany

In recent years an increasing interest in the design of bio-metal hybrid structures and their application in electronics and robotics has lead to a need of understanding of the mechanisms involved in chemical interaction between metals and biosystems under vacuum conditions. Herein by means of photoelectron spectroscopy we characterize interaction occurring between protein and technologically essential metals (copper and iron).

O 31.8 Tue 12:15 WIL A317

**Hybrid organic-inorganic systems: metal nanoparticles (Au, Al and Ag) embedded into organic semiconductor thin film** — •Olga Molodtsova[1], Irina Aristova[2], Oleg Vilkov[3], Anetta Pietzsch[3,4], Maxim Tchaplyguine[4], Sergey Babenkov[1], Vitaly Kveder[2], and Victor Aristov[1,2] — [1]HASYLAB at DESY, D-22607 Hamburg, Germany — [2]Russian Acad. Sci, ISSP, Chernogolovka 142432, Russia — [3]HZB für Materialien und Energie, BESSY II, D-12489 Berlin, Germany — [4]Lund Univ, MAX-lab, S-22100 Lund, Sweden

Materials with a high on-off resistance ratio could become the basis for resistive random-access memory (RRAM). Such a storage class memory would revolutionize the information technology industry. One type of RRAM can be based on hybrid organic*inorganic systems, mainly consisting of inorganic nanoparticles (NP) blended into an organic matrix. The evolution of the morphology and the electronic properties of the hybrid organic-inorganic systems composed of aluminum, silver and gold NPs distributed in an organic matrix, CuPc and CuPcF4, as a function of nominal metal content was studied by TEM and PES using synchrotron radiation. Strong difference in morphology and electronic properties were observed for aluminum nanoparticles self-assembled in a wide-gap organic semiconductor matrix if compare to gold and silver NPs in the same matrix. E.g., on the very first stage of aluminum deposition, aluminum atoms show strong chemical interaction with substrate atoms. Supported by RFBR grant N 13-02-00818.

O 31.9 Tue 12:30 WIL A317

**The influence of annealing temperature on molecular structure on HOPG** — Peng Jiang and •Michael Hietschold — Solid Surfaces Analysis Group, Institute of Physics, D-09107 Chemnitz, Germany

As an n-type organic molecule, F16CoPc film on HOPG is investigated by UV STM. The ultrathin molecular film is prepared by OMBE, and then annealed at 375K for 20min. The influence of temperature on molecular adsorbate structure is investigated in this work.

At submonolayer coverage, molecules form large areas with ordered arrangement, where the structure of HOPG can be considered as the template: F16CoPc employs hexagonal structure, with a unit cell of about 1.5nm.

After annealing at 375K, there are two new structures observed: unidirectional row structure and near-square structure with molecular unit cells characterized by side lengths of 1.3nm*2.2nm and 1.4nm*1.7nm and angles 91° and 95°, respectively. In addition, a new effect is found simultaneously: smaller protrusions appear at the original sites of some molecules, which form only after annealing; and some of them disappear later again after scanning. This effect happens only to single molecules in closed packed structures, such as hexagonal and square structure.

O 31.10 Tue 12:45 WIL A317

**Biomimetic solid-supported polymer bilayer incorporated with natural membrane proteins** — •xiaoyan zhang[1], wangyang fu[2], cornelia g. palivan[1], and wolfgang meier[1] — [1]Department of Chemistry, University of Basel, Klingelbergstrasse 80, CH-4056 Basel, Switzerland — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Lipid cell membrane is the most important interface in biological systems, which is able to selectively control the transport by their specific proteins. Reconstitution of membrane proteins in artificial membranes creates a platform for exploring their potential for pharmacological or biotechnological applications. Previously, we demonstrated amphiphilic block copolymer is a relatively stable substitute for a lipid and is able to be used as promising building blocks for artificial membranes with long-term stability and tailorable structural parameters. However, the insertion of membrane proteins has not previously been realized in a planar large-area, stable, and solid-supported artificial membrane. Herein we present our recent work on the first, preliminary model of a channel protein that is incorporated in block copolymer, tethered, solid-supported bilayer membrane (TSSBM). Unprecedented ionic transport characteristics that differ from previous results on protein insertion into planar, free-standing membranes, are identified. For the unique variation in conductance in a TSSBM, a model describing channel protein mediated ion transport was introduced. Our findings mark a change in understanding protein insertion and ion flow within natural channel proteins when inserted in an artificial TSSBM.

# O 32: Organic Semiconductors: Photovoltaics (HL jointly with CPP, DS, O)

Time: Tuesday 10:00–12:30 Location: POT 081

O 32.1 Tue 10:00 POT 081

**Analytical transmission electron microscopy on hybrid solar cells based on perovskites** — •Diana Nanova[1,2,4], Anne Katrin Kast[1,3,4], Christian Müller[1,4], Rasmus R. Schröder[3,4], Robert Lovrincic[1,4], and Wolfgang Kowalsky[1,4] — [1]Institut für Hochfrequenztechnik, TU Braunschweig — [2]Kirchhoff Insitut für Physik, Universität Heidelberg — [3]Cryo-EM, CellNetworks, Bioquant, Universität Heidelberg — [4]InnovationLab GmbH, Heidelberg

Hybrid solar cells based on metal-organic perovskite absorbers are of major interest due to their remarkable power conversion efficiencies of up to 15%. Recently, it has been shown that the morphology of the perovskite itself as well as the interplay between the absorber and the mesostructured electron acceptor strongly affects the electrical properties of the device. We present a combined study of the structure-function relationship of solution processed solar cells based on mesostructured perovskites. The morphology of the solar cells was studied by analytical transmission electron microscopy (ATEM). In ATEM electron energy loss spectroscopy (EELS) and electron spectroscopic imaging (ESI) are applied in order to obtain material contrast. To be able to classify the TiO2 and the perovskite rich areas in the corss-section of the device a series of monochromatic images in the low-loss regime was acquired. We observed significant changes in pore size, pore filling and pore distribution of the mesostructured layer depending on the annealing conditions of the perovskite. Furthermore, we correlated our results to the I-V characteristics of the solar cells.

O 32.2 Tue 10:15 POT 081

**Alloyed zinc sulfide - copper indium disulfide nanocrystals for application in hybrid photovoltaics** — •Björn Kempken, Nikolay Radychev, Christopher Krause, Jie Li, Holger Borchert, Joanna Kolny-Olesiak, and Jürgen Parisi — Carl von Ossietzky University of Oldenburg, 26111 Oldenburg

Semiconductor nanocrystals (NCs) continue to attract immense attention because of their size-dependent optical, physical, and chemical properties which causes them to be a favourable material for hybrid solar cell applications. A promising candidate for the inorganic/organic active layer is alloys of ZnS and CuInS2 (ZCIS NCs), which on the one hand strongly absorb in the visible range up to 800 nm, and, on the other hand, belongs to the "green" type of semiconductor NCs. In the present work, high quality ZCIS NCs were synthesized and subjected to hexanethiol ligand exchange procedures. Laboratory solar cells based on blends of treated ZCIS NCs and poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)-alt-4,7(2,1,3-benzothiadiazole)] (PCPDTBT) as active layer were prepared and investigated by current-voltage and electron spin resonance measurements. Hybrid ZCIS/PCPDTBT laboratory solar cells demonstrate well pronounced diode behavior with outstanding characteristics of the open-circuit voltage which reached up to 1.2 V.

O 32.3 Tue 10:30 POT 081

**Improving efficiency of solar power generation by combination of a sensitized mesoscopic solar cell with a thermoelectric generator** — •Hans-Fridtjof Pernau, Jana Heuer, Karina Tarantik, Alexandre Jacquot, Jan D. König, Martin Jägle, and Kilian Bartholomé — Fraunhofer IPM, Freiburg, Germany

Standard photovoltaic(PV) solar cells use only about half of the light spectrum provided by the sun. The infrared part is not used for producuction of electrical energy. Even further, the infrared light heats up the pv cell and decreases thereby its efficiency. The basic idea for a combined pv and thermoelectric solar cell has been published in 2008 [1]. The improvements in thermoelectric materials and scientific work on thermoelectrics lead to new ideas for those systems [2] which will be investigated in the EU-FP7-Projekt Globasol. Within the project, a hybrid solar cell made of a sensitized mesoscopic solar cell and a thermoelectric generator (TEG) will being developed. The light of the sun is split at about 800nm. The visible and ultra violet part is transfered to the sensitized mesoscopic solar cell, the infrared part illuminates the TEG cell. With the hybrid solar cell, the full solar spectrum is exploited. We present the first modeling results of the project and the first evaluation version of the hybrid cell.

[1] T.M. Tritt, H. Böttner and L. Chen, *Thermoelectric: Direct Solar Thermal Energy Conversion*, MRS Bulletin, vol.33 (2008) pp. 366-368; [2] D. Kraemer et al., *High-performance flat panel solar thermoelectric generator with high thermal concentration*, Nature materials vol.10 (2011) pp. 532-538.

O 32.4 Tue 10:45 POT 081

**Spin dynamics in organic solar cells measured by pulsed electrically detected magnetic resonance** — •Alexander J. Kupijai, Konstantin M. Behringer, Martin Stutzmann, and Martin S. Brandt — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching

Organic photovoltaics are of great interest in the development of sustainable energy sources. To investigate the recombination and transport processes in organic solar cells we use the technique of pulsed electrically detected magnetic resonance (EDMR) where we measure the change of the photocurrent caused by resonant X-band microwave pulses in the presence of an external magnetic field. As test devices, we use bulk heterojunction P3HT/PCBM (poly(3-hexylthiophene-2,5-diyl) / [6,6]-phenyl $C_{61}$ butyric acid methyl ester) solar cells. At temperatures of 10K we are able to observe both positively and negatively charged polarons in the pulsed EDMR spectrum and can identify them as partners in a spin-dependent pair process by experiments using two microwave frequencies. Using the time resolution and sensitivity of pulsed EDMR we are able to quantify the spin dynamics of the system and measure the lifetime of parallel spin pairs, the lifetime of antiparallel spin pairs, the spin decoherence time and the coupling strength between the spin partners. All of these microscopic parameters provide valuable information for an optimization of overall solar cell efficiencies.

O 32.5 Tue 11:00 POT 081

**Imaging the origin of S-shaped current-voltage characteristics of organic solar cells by scanning Kelvin probe microscopy** — •Christian Müller[1,2,3], Rebecca Saive[1,2,3], Janusz Schinke[1,3], Robert Lovrincic[1,3], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab GmbH, Heidelberg, Germany — [2]Kirchhoff-Institut für Physik, University Heidelberg, Germany — [3]Institut für Hochfrequenztechnik, Technische Universität Braunschweig, Germany

We investigated organic bilayer solar cells consisting of poly(3-hexylthiophene)/1-(3-methoxycarbonyl)propyl-1-phenyl[6,6]C61 (P3HT/PCBM). Scanning Kelvin probe microscopy (SKPM) was performed on the solar cell cross sections which were exposed with a focused ion beam. We prepared the P3HT/PCBM bilayer solar cells by solution processing. These bilayer solar cells showed normal and anomalous, S-shaped current-voltage characteristics. Using SKPM on the device cross sections, we found that in normal bilayer solar cells the potential dropped at the ITO/PEDOT:PSS contact and over the active area, whereas in S-shaped bilayer solar cells the potential dropped exclusively at the aluminium contact. This behavior confirms the assumption that S-shaped curves are caused by hindered charge transport at electrode interfaces.

### Coffee break (15 min.)

O 32.6 Tue 11:30 POT 081

**Improving the Charge Transport Parameters of Near-Infrared Absorbers** — •Sebastian Radke[1,2], Frank Ortmann[1,2], Reinhard Scholz[2,3], and Gianaurelio Cuniberti[1,2,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, Germany — [3]Institut für Angewandte Photophysik, TU Dresden, Germany — [4]Center for Advancing Electronics Dresden, TU Dresden, Germany

For an improved performance of organic tandem solar cells, efficient organic infrared absorber materials are necessary. A promising class already used successfully in organic solar cells are 4,4'-difluoro-4-bora-3a,4a-diaza-s-indacenes (BODIPYs). Based on a comparative study of the intramolecular electronic properties as well as the intermolecular coupling in the crystal phase of three potential candidates, we find that the benzannulation of the molecular core improves both electron and hole transfer. As the frontier molecular orbitals are delocalized over the entire molecule also by attaching additional functional groups to the molecular core, the intermolecular coupling and especially the performance in amorphous phase can be optimized further. However, an immobilization of these substituents is necessary to regulate an increase in the reorganization energy for hole transfer. Based on these design rules, BODIPYs with optimized charge transfer properties can be synthesized increasing also the performance of the devices.

O 32.7 Tue 11:45 POT 081

**Qualitative und quantitative Auswertung von komplementären bildgebenden Methoden zur Degradationsuntersuchung und Qualitätskontrolle von Polymersolarzellen** — •Roland Rösch, Marco Seeland, Daniel Fluhr, Burhan Muhsin, Peter Fischer, Rolf Öttking und Harald Hoppe — Institut für Physik, TU Ilmenau, Deutschland

Wir berichten über beschleunigte Alterungstests an modernen organischen und polymeren Solarzellen, ergänzt durch bildgebenden Methoden, wie z.B. bildgebende Lumineszenz, Lock-in Thermographie und lichtinduziertes Kurzschlussstrommapping. Neben einer qualitativen Interpretation der Daten, ist es durch die Kombination der verschiedenen Methoden möglich, auch eine quatitative Auswertung der Dynamiken der verschiedenen Degradationsmechanismen zu erhalten. Desweiteren vergleichen wir die experimentellen Ergebnisse mit theoretischen Modellen des Ladungsträgerflusses und -Rekombination. Daraus lassen sich intrinsische Paramter der Bauelemente, wie Elektrodenwiderstand und Diodenidealitätsfaktor bestimmen. Die wichtigste Erkenntnis aus diesen Untersuchungen ist, dass die Stabilität von modernen organischen Solarzellen vor allem durch die Elektrodendegradation und die Qualität der Versiegelung begrenzt ist. Diese Arbeit liefert einen Leitfaden für weitere Verbesserungen hin zu stabilen organischen Solarzellen.

O 32.8 Tue 12:00 POT 081

**Visualization of Lateral Phase Separation in Polymer: Fullerene Solar Cells by Quantitative Evaluation of Luminescence Imaging Measurements** — •Marco Seeland, Christian Kästner, and Harald Hoppe — Institut für Physik, TU Ilmenau, Ilmenau, Germany

Luminescence imaging has evolved to a versatile characterization method for studying the laterally resolved behavior of polymer solar cells. Especially in degradation studies the use of luminescence imaging is beneficial as it is non-invasive and offers short measurement times. By either electrical or optical excitation separate characterization of the electrical contacts and the active layer is feasible. However, the data analysis so far is mainly qualitative, i.e. interpretation of the measured luminescence image by comparison with other techniques. In this work we present a quantitative analysis of electroluminescence images of laterally inhomogeneous polymer solar cells. By decoupling the local parameters within an iteration procedure this analysis allows calculation of the local current flow through and the local voltage applied to the active layer. Furthermore quantitative images of the local series resistance and the saturation current-density are achieved. The local saturation current-density contrast was found to correlate perfectly with the strong lateral phase separation occurring in PPE-PPV:PCBM based devices. Further analysis of the lateral difference in the saturation current-densities delivers information on the thermal activation of charge carriers at the donor/acceptor-interface and in the phase separated bulk.

O 32.9 Tue 12:15 POT 081

**The influence of fullerene loading on the photogeneration in intercalated polymer: fullerene bulk heterojunction solar cells** — •Andreas Zusan[1], Koen Vandewal[2], Benedikt Allendorf[1], Nis Hauke Hansen[1], Jens Pflaum[1], Martin Heeney[3], Alberto Salleo[2], Vladimir Dyakonov[1,4], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Department of Materials Science and Engineering, Stanford University, Stanford, California 94305, USA — [3]Department of Chemistry, Imperial College, London, SW7 2AZ, UK — [4]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

The conjugated polymer, pBTTT, allows a systematic tuning of the blend morphology by varying the acceptor material and blend ratio, making it a well-suited structural model for studying the fundamental processes in organic BHJ solar cells. To analyze the correlation between photogeneration and intercalation, we have performed time delayed collection field (TDCF) measurements and Fourier-transform photocurrent spectroscopy (FTPS) on pBTTT:PCBM devices in various stoichiometries. An increased PCBM loading resulted in a less field dependent dissociation, which we attribute to enhanced electron delocalization along extended PCBM nanophases and energetically driven spatial separation of polarons due to the presence of pure acceptor domains. The highly efficient transfer of charge carriers from the intercalated phase into the pure phase has been studied further by extending TDCF measurements to include segregated pBTTT:bisPCBM blends.

## O 33: Invited Talk (Guy Le Lay)

Time: Tuesday 15:00–15:45 Location: TRE Phy

**Invited Talk** O 33.1 Tue 15:00 TRE Phy

**Beyond graphene: silicene and germanene, its silicon and germanium cousins** — •Guy Le Lay — Aix-Marseille University, France

Silicene and germanene are the silicon and germanium analogues of graphene, hosting also Dirac fermions [1]. They are predicted to be two-dimensional topological insulators, up to nearly room temperature for germanene. The mobilities of their charge carriers are expected to be very high, potentially exceeding those of graphene for the latter. After describing our breakthrough realization of epitaxial silicene on silver (111) substrates [2] we will present hints of the synthesis of single layer epitaxial germanene, a novel germanium allotrope that does not exist in the nature [3]. If confirmed, this new achievement might open the way to tantalizing applications. [1] G. Brumfiel, Nature, 495, 153 (2013); Nature 485, 9 (2012). [2] P. Vogt et al., Phys. Rev. Lett., 108, 155501 (2012). [3] A. Resta et al., to be published

## O 34: Magnetic Adatoms on Surfaces (MA jointly with O)

Time: Tuesday 15:00–16:00 Location: BEY 118

**Invited Talk** O 34.1 Tue 15:00 BEY 118
**Manipulating the magnetic properties of single atoms on surfaces** — •Alexander Ako Khajetoorians — Institute of Applied Physics, Hamburg University, Hambury, Germany

With the development of sub-Kelvin high-magnetic field STM, two complementary methods, namely spin-polarized scanning tunneling spectroscopy (SP-STS) [1] and inelastic STS (ISTS) [2-3], can address single spins at the atomic scale. While SP-STS reads out the projection of the impurity magnetization, ISTS detects the excitations of this magnetization as a function of an external magnetic field. They are thus the analogs of magnetometry and spin resonance measurements pushed to the single atom limit. We have recently demonstrated that it is possible to reliably combine single atom magnetometry with an atom-by-atom bottom-up fabrication to realize complex atomic-scale magnets with tailored properties [4-6] on metallic surfaces [1,7]. In this talk, I will address recent developments in probing the spin excitations and magnetization curves of atoms on a multitude of non-magnetic surfaces, and the effects of hydrogenation on the magnetic state of such atoms. Finally, I will discuss investigations of the magnetization dynamics [6] of coupled spins as probed with spin-resolved STM. [1] A.A.K., et al. , PRL, 106, 037205 (2011); [2] A. J. Heinrich, et al. , Science, 306, 466 (2004); [3] A.A.K, et al. ,Nature, 467, 1084 (2010); [4] A.A.K., et al., Nature Physics, 8, 497 (2012) [5] A.A.K., et al. , Science, 332, 1062 (2011), [6] A.A.K., et al.,Science, 339, 55 (2013), [7] A.A.K., et al, PRL, 111, 126804 (2013).

**Invited Talk** O 34.2 Tue 15:30 BEY 118
**Spin Interaction of Atoms studied with Ultrafast STM** — •Sebastian Loth — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg — Max Planck Institute for Solid State Research, Stuttgart

Spin-dependent interaction between magnetic atoms produces a variety of quantum phenomena ranging from superposition ground states and magnetic tunneling to quantum criticality. In this talk we will show that time-resolving scanning tunneling microscopy (STM) makes it possible to study these effects experimentally.

We engineer experimental representations of different Spin Hamiltonians by assembling transition metal atoms into arrays of different shape and elemental composition on the surface of a thin insulator/metal substrate. Inelastic electron tunneling and all-electronic pump-probe spectroscopy at GHz frequencies quantifies the energy level structure, energy loss mechanisms and spin lifetimes of the interacting spins [Science 329, 1628 (2010)]. Using this technique we identified a new approach to suppress magnetic tunneling in antiferromagnetic spin chains triggered by a phase transition from a singlet ground state to classical magnetic states [Science 335, 196 (2012)]. Magnetic tunneling can also be enhanced by combining atoms with different spin magnitude into chains that exhibit spin-correlated singlet ground states even at several nanometers length.

The time-domain information further enables non-local measurements of magnetic states shedding light onto possible pathways to controllably interact with atom-sized quantum spins.

## O 35: Transport: Topological Insulators I (TT jointly with O)

Time: Tuesday 14:00–16:00 Location: HSZ 304

O 35.1 Tue 14:00 HSZ 304
**All in-ultra-high-vacuum study of thin film topological insulators: $Bi_2Te_3$** — •Katharina Hoefer, Diana Rata, Christoph Becker, and Liu Hao Tjeng — Max Planck Institute for Chemical Physics of Solids

Thin films of topological insulators offer the possibility for the experimental study of the expected specular phenomena occurring at the surface or interface with these materials due to the increased surface to bulk ratio in comparison to bulk crystals. Bulk materials are always defective which leads to extra contributions in conductance.

To protect the surface integrity an all in- ultra-high-vacuum study is crucial. High quality thin films of $Bi_2Te_3$ were grown on well lattice matched $BaF_2$(111) substrates using Molecular Beam Epitaxy. The preparation, characterization by RHEED, LEED, XPS and ARPES and especially transport measurements, were performed all in-situ under ultra-high-vacuum conditions.

Results of this study and the effect of air exposure on the electronic structure and transport properties will be presented.

O 35.2 Tue 14:15 HSZ 304
**Finite width effect on weak antilocalization in MBE grown $Bi_2Te_3$ thin films** — •Christian Weyrich[1,2], Tobias Merzenich[1,2], Igor E. Batov[3], Gregor Mussler[1,2], Jörn Kampmeier[1,2], Jürgen Schubert[1], Thomas Schäpers[1,2], and Detlev Grützmacher[1,2] — [1]Peter Grünberg Institute (PGI-9) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Virtual Institute for Topological Insulators (VITI), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [3]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, 142432, Moscow Distr., Russia

The weak antilocalization effect is measured in $Bi_2Te_3$ layers under various tilt angles of the magnetic field with respect to the layer surface. The investigated $Bi_2Te_3$ layer was prepared by molecular beam epitaxy. For a magnetic field oriented perpendicularly to the layer the weak antilocalization effect at different temperatures can be well-fitted by the Hikami-Larkin-Nagaoka model. From the fit a phase coherence length of about 200 nm is obtained at a temperature of 2 K. A clear signature of weak antilocalization is also observed when the magnetic field is oriented parallel to the $Bi_2Te_3$ layer. This effect is compared to classical models as well as a recently developed theory, which takes into account the finite penetration depth of the surface or interface states into the bulk.

O 35.3 Tue 14:30 HSZ 304
**Band structure and magnetotransport in strained HgTe** — •Jan Böttcher and Ewelina M. Hankiewicz — Universität Würzburg, Faculty for Physics and Astronomy, Am Hubland, D-97074 Würzburg

Strained mercury telluride is a 3D topological insulator with negligible bulk conductivity [1]. Here we report on band structure calculations using a six-band Kane model with a self-consistent Poisson solver. We find that while the surface states lie within the band gap, the Dirac point lies deep in the heavy hole subbands. We study this system as a function of gate voltage and give possible explanations of exciting experimental observations of the Landau level structures in high magnetic fields as well as oscillations in the Shubnikov-de Hass data at low magnetic fields.

We acknowledge financial support via grant HA 5893/4-1 within SPP 1666.

[1] C. Brüne, C. X. Liu, E. G. Novik, E. M. Hankiewicz, H. Buhmann, Y. L. Chen, X. L. Qi, Z. X. Shen, S. C. Zhang, and L. W. Molenkamp, Phys. Rev. Lett. 106, 126803 (2011)

O 35.4 Tue 14:45 HSZ 304
**Photoemission investigation of the predicted topological Kondo insulator behavior of $SmB_6$** — •Peter Hlawenka[1], Emile Rienks[1], Konrad Siemensmeyer[1], Eugen Weschke[1], Andrei Varykhalov[1], Natalya Shitsevalova[2], Slavomir Gabani[3], Karol Flachbart[3], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin — [2]Institute for Problems of Material Science, Kiev, Ukraine — [3]IEP, Slovak Academy of Science, Kosice

The system $SmB_6$ is known for its unusual resistivity which increases exponentially with decreasing temperature and saturates below 3 K [1]. This has recently been attributed to topological-Kondo-insulator behavior where a topological surface state is created by Sm4$f$-5$d$ hybridization and is responsible for the transport [2]. The local-density-approximation + Gutzwiller calculations of the (100) surface predict the appearance of three Dirac cones in the surface Brillouin zone [2]. We perform angle-resolved photoemission (ARPES) below 1 K and do not observe the predicted Dirac cones at $\overline{\Gamma}$ or $\overline{\mathrm{X}}$. Moreover, the Fermi surface is made up of steeply dispersing bulk Sm5$d$ states. The $\mathrm{Sm}^{2+}$ 4$f$ band and the hybridization gaps where the surface states are expected [2] are too far ($\sim$ 20 meV) below the Fermi energy in order to contribute to the transport. These results will be discussed in comparison to other ARPES studies.

[1] J. C. Cooley, M. C. Aronson, Z. Fisk, P. C. Canfield, Phys. Rev. Lett. 74, 1629 (1995)

[2] F. Lu, J. Zhao, H. Weng, Z. Fang, Xi Dai, Phys. Rev. Lett. 110, 096401 (2013)

O 35.5 Tue 15:00 HSZ 304

**Excitations of surface and bulk states in spin orbit dominated materials** — •Peter Lemmens[1], Vladimir Gnezdilov[1,2], Dirk Wulferding[3], Patrik Recher[4], Helmuth Berger[5], Yoichi Ando[6], R Sankar[7], and Fang-Cheng Chou[7] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE, Kharkov, Ukraine — [3]POSTECH, Korea — [4]IMAPH, TU-BS, Braunschweig — [5]EPFL, Lausanne, Switzerland — [6]ISIR, Osaka, Japan — [7]CCMS, National Taiwan Univ., Taipei, Taiwan

Using Raman scattering experiments we probe inelastic processes in the giant Rashba material BiTeI, the topological semimetal $\mathrm{Cd_3As_2}$ and several topological insulators. By comparing surface with bulk scattering processes we notice the dominance of quantum well states. With exception to $\mathrm{Cd_3As_2}$ all materials show pronounced resonances in the Raman scattering cross section.

O 35.6 Tue 15:15 HSZ 304

**Josephson Effect in Topological Insulator Planar, Nanostep and Edge Junctions** — •Jennifer Nussbaum, Rakesh Tiwari, Thomas Schmidt, and Christoph Bruder — University of Basel, Switzerland

Topological insulators are states of quantum matter which are characterized by a full insulating gap in the bulk and gapless surface states which are protected by time-reversal symmetry. By using the superconducting proximity effect on a $\mathrm{Bi_2Se_3}$ topological insulator, a topological superconductor - topological insulator - topological superconductor (SIS) junction can be engineered. By solving the Dirac-Bogoliubov-De-Gennes equation in such a junction the maximal supercurrent that can flow through the surface of the $\mathrm{Bi_2Se_3}$ topological insulator with heavily doped superconducting electrodes is calculated. In this manner, short and wide nanostep Josephson junctions involving different side surfaces of the 3D topological insulator are investigated. The results are compared to the Josephson response of a junction involving only one side surface. The comparison reveals, for example, that a step setup leads to a non-trivial scaling of the Josephson current.

O 35.7 Tue 15:30 HSZ 304

**Parity measurement in topological Josephson junctions** — •François Crépin and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

We study the properties of a topological Josephson junction made of both edges of a 2D topological insulator. We show that, due to fermion parity pumping across the bulk, the global parity of the junction has a clear signature in the periodicity and critical value of the Josephson current. In particular, we find that the periodicity with the flux changes from $4\pi$ in a junction with an even number of quasi-particles to $2\pi$ in the odd sector. In the case of long junctions, we exhibit a rigorous mathematical connection between the spectrum of Andreev bound-states and the fermion parity anomaly, through bosonization. Additionally, we discuss the rather quantitative effects of Coulomb interactions on the Josephson current.

O 35.8 Tue 15:45 HSZ 304

**PN junctions of Topological Insulators** — •Sourin Das[1] and Disha Wadhawan[2] — [1]MPIPKS, Dresden, Germany & University of Delhi, India — [2]University of Delhi, India

Spin textures of surface states of topological insulators (TI) open up possibilities for designing ultra fast electrically controllable spin transistor. In this context I will discuss spin-valve effect associated with a gating induced PN junction designed on the surface state of 2D and 3D TI. I will show that *conduction to conduction* and *conduction to valence* band transport in a PN junction is topologically distinct resulting in asymmetric electrical transport. The topological distinction is shown to be quantifiable in term of the Pancharatnam geometric phase.

## O 36: Posters: Bio/organic Molecules on Surfaces, Graphene, Solid/liquid interfaces, Metal Substrates, Electronic Structure Theory

Time: Tuesday 18:30–22:00 Location: P1

O 36.1 Tue 18:30 P1

**Coverage-dependent metalation and dehydrogenation of tetraphenylporphyrin on Cu(111)** — •Michael Röckert, Matthias Franke, Quratulain Tariq, Michael Stark, Stefanie Ditze, Hubertus Marbach, Hans-Peter Steinrück, and Ole Lytken — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, 91058 Erlangen, Egerlandstraße 3, Germany

The coverage-dependent metalation and dehydrogenation of tetraphenylporphyrin (TPP) on Cu(111) was investigated with XPS, STM and TPD under UHV conditions. 2HTPP has two distinct adsorption structures on Cu(111) [1]: At low coverages ($<$ 0.36 molecules/nm$^2$) 2HTPP adsorbs in a disordered structure, but as the coverage is increased a checkerboard-like structure is formed and saturates at 0.55 molecules/nm$^2$. As 2HTPP layers on Cu(111) are heated, three distinct reactions take place: metalation, resulting in CuTPP, a partial dehydrogenation of the outer porphyrin-sphere, linking most likely the pyrrole and phenyl rings together, and upon further heating complete dehydrogenation [2]. The two first reactions, metalation and partial dehydrogenation, strongly depend on the structure of the 2HTPP layer. At low coverages, the temperatures for both processes are very close to each other, while at higher coverages metalation shifts down and dehydrogenation up in temperature.

[1] Stark, M. et al. Langmuir 2013, 29, 4104-4110. [2] Xiao, J.; Ditze, S. et al. J. Phys. Chem. C 2012, 116, 12275-12282.

O 36.2 Tue 18:30 P1

**Self organization driven structure formation of DIP molecules on Cu(111)** — Hazem Aldahhak, •Wolf Gero Schmidt, and Eva Rauls — Theoretische Physik, Universität Paderborn

Thin films of organic molecules like diindenoperylene (DIP) on metal substrates are of great interest for the further miniaturization of organic optoelectronic devices. DIP molecules show an interesting behavior on different terraces. While step edges have rare influence on the azimuthal molecular orientation of DIP-molecules on Cu(100) [1], they control the molecular crystallographic directions on Au(111) independently of the underlying surface symmetry [2]. On Cu(111), the self-assembly depends on the terrace width. On narrow terraces (<15 nm), the DIP molecules assemble in a co-directionally oriented adsorption pattern, the symmetry of which is not dictated by the hexagonal substrate symmetry [3]. On wider terraces, in contrast, completely different adsorption patterns with a short-range order determined by the underlying substrate are observed. We performed first principles calculations and investigated the balance between intermolecular and molecule-substrate interactions. Special focus is put on the role of step-edges to initiate the molecular self-assembly depending on the terrace width. Based on our investigations, we deduced a model which explains the experimental observations.

[1] Zhang et al., Surface Science, 603(2009) 3179. [2] De Oteyza et al., Journal of Physical Chemistry C 112, 18 (2008) 7168. [3] De Oteyza et al., Phys. Chem. Chem. Phys. 11, 8741 (2009).

O 36.3 Tue 18:30 P1

**STM Study of the structural formation of crystal violet on**

**Au(100) and Au(111) surfaces** — •Patrick Mehring, Lothar Brosda, and Carsten Westphal — Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund

The selective modification of metal surfaces offers a large variety of possible applications in different fields. Thus, the understanding of the adsorption and structural formation of molecules with well-known properties attracted large attention for different applications in the last years. Crucial parameters having strong influence on the assembly mechanism are the molecular coverage, temperature, and substrate interaction which are topics of many studies. The adsorption and structural formation of crystal violet on Au(100) and Au(111) was investigated by means of scanning tunneling microscopy for different coverages ranging from submonolayer to multilayer regime. The molecules are found forming ordered structures near a closed monolayer on both surfaces. Thus, the phases show similar structural features on both substrate orientations. Overall, two different molecule orientations can be identified. A structure model is presented for both Au(100) and Au(111) surfaces. When reaching the multilayer regime the long range order decreases and only isolated areas with alternating molecule orientation are found.

O 36.4 Tue 18:30 P1

**On the dynamics of molecular processes: STM investigations of porphyrins on Cu(111)** — •Stefanie Ditze, Michael Stark, Martin Drost, Florian Buchner, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen

For the controlled fabrication of molecular nanostructures it is important to understand dynamic processes such as surface diffusion, molecular rotation, conformational changes or chemical reactions on well-defined surfaces. Herein, we show that scanning tunneling microscopy (STM) can be a powerful tool to study the dynamics of porphyrins on Cu(111) under UHV conditions. The results of corresponding isothermal measurements at different temperatures are used for an Arrhenius type analysis to finally extract the energetics of the process. Following this route, the kinetic parameters for 2D surface diffusion and 2D molecular rotation of 2H-5,10,15,20-tetraphenylporphyrin (2HTPP) [1], the activation energy for the self-metalation reaction of 2HTPP with Cu substrate atoms [2] and finally even the energetics to conformational switch an individual 2H-5,10,15,20-tetrakis(3,5-di-tert-butyl)-phenylporphyrin can be determined.

This work has been funded by the DFG through SFB 583.

[1] F. Buchner et al., J. Phys. Chem. C 115 (2011) 24172-24177.

[2] S. Ditze et al., Angew. Chem., Int. Ed. 51 (2012) 10898-10901.

O 36.5 Tue 18:30 P1

**Coverage dependent adsorption behavior of Ni-TPBP on Cu(111): A scanning tunneling microscopy study** — •Michael Lepper, Liang Zhang, Michael Stark, Stefanie Ditze, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

In order to design self-assembled supramolecular architectures with specific functional properties it is necessary to understand the adsorption behavior of molecular building blocks on well-defined substrates. One very versatile class of adsorbates in this regard are porphyrins which offer not only a rigid molecular framework but also ligand functionality to bind metals. In this study, we investigate the coverage dependent supramolecular arrangement of Ni(II)-tetraphenylbenzoporphyrin (NiTPBP) on Cu(111) with scanning tunneling microscopy at room-temperature (RT) in ultra-high vacuum (UHV). At low coverage, we observed adsorption of the porphyrin molecules at the steps. By increasing the coverage island formation of NiTPBP is promoted. Interestingly, we were able to monitor three different molecular appearances of the NiTPBP islands at the same coverage and temperature.

O 36.6 Tue 18:30 P1

**Atomic Force Microscopy: The qPlus sensor applied to molecules on metal surfaces** — •Robin Ohmann[1,2], Anja Nickel[1,2], Jörg Meyer[1,2], Francesca Moresco[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Dresden, Germany — [2]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany

Atomic force microscopy invented in 1986 allows measuring forces between a probing tip and the surface. In 1998 the qPlus sensor was developed by Franz J. Giessibl which is comprised of a tuning fork found in watches and operates in frequency modulation mode (FM-AFM). By attaching a conducting tip on one of the prongs of the fork it allows to combine scanning tunneling microscopy and atomic force microscopy leading to atomic resolution images of the surface. In our lab, we have set up such an STM/AFM system operating at low temperatures (5 K) under ultra-high vacuum conditions. Our goal is to investigate single molecules and supramolecular structures on metal surfaces with the qPlus sensor. In this poster, I will present our first measurements on molecules on metal surfaces.

O 36.7 Tue 18:30 P1

**Vibrational properties and dynamic charge transfer of the CuPc/Ag(111)-system** — •Sebastian Thussing und Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany

The vibrational properties and thermal evolution of ultra thin films of copper-pthalocyanine (CuPc) grown on Ag(111) have been investigated using Fourier-transform infrared absorption spectroscopy (FTIRAS), spot-profile-analysis low energy electron diffraction (SPA-LEED) and thermal desorption spectroscopy (TDS). Thereby, various phases in the submonolayer regime could be distinguished and characterized. Bilayer and multilayer are largely decoupled from the Ag(111) substrate and display a distinctly different spectroscopic signature. Mono- and bilayers are orientated parallel to the Ag(111) surface whereas a slightly inclined geometry prevails for the multilayers. The monolayer phases are subject to a pronounced interfacial dynamical charge transfer (IDCT). Interestingly, this process is attenuated upon growth of the bilayer. TDS spectra reveal an incomplete desorption for the CuPc monolayer from the Ag(111) surface. At about 600K a second pathway becomes dominant with fragments desorbing in variable amounts.

O 36.8 Tue 18:30 P1

**Large pores and multiple active sites: a 2D metal-organic network employing a de-novo synthesized porphyrin linker** — •Yuanqin He[1], Felix Bischoff[1], Knud Seufert[1], Willi Auwärter[1], Daphné Stassen[2], Davide Bonifazi[2], and Johannes Barth[1] — [1]Technische Universität München, Department of Physics, E20, Garching, Germany — [2]University of Namur, Department of Chemistry, Namur, Belgium

Exploring principles for future single-molecule devices and developing new materials for catalysis using functional molecular building blocks are motivations for molecular nanoscience. Herein, the bottom-up fabrication of metal-organic networks is a promising approach, notably regarding temperature stability or controllable and tunable assembly protocols. We present a low-temperature scanning tunneling microscopy study of the de-novo synthesized porphyrin linker (5,10,15,20)tetra[4-(4-pyridyl)phenyl]porphyrin on Ag(111). This free-base tetrapyrrole species forms nanoporous, metal-organic networks via N-Cu-N coordination bonds when adding Cu atoms. Networks with large openings stabilized by directional coordination interactions present metal atoms as possible catalytically active sites, porphyrin macrocycles as "chemical pockets" and open pores for host-guest chemistry.

O 36.9 Tue 18:30 P1

**STM of functionalized platform molecules on Au(111)** — •Torben Jasper-Tönnies[1], Sandra Ulrich[2], Rainer Herges[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — [2]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel

The coupling to a metal substrate affects the electronic and geometric structure of molecules. To preserve their intrinsic properties it may be desirable to decouple functional groups from the substrate. This can be achieved by supporting a molecule by a molecular platform, conceivably via a spacer group. Using low temperature scanning tunneling microscopy we investigate the trioxotriangulenium (TOTA) platform molecule with various functional groups. In contrast to the similar platform molecule triazatriangulenium (TATA), functionalized TOTA can be thermally evaporated due to its higher thermal stability. Depending on the functional groups attached to the TOTA molecules we observe varying degrees of fragmentation. This will be discussed in terms of electronic properties of the functional groups. Financial support by the Deutsche Forschungsgemeinschaft via SFB 677 is gratefully acknowledged.

O 36.10 Tue 18:30 P1

**Surface Control of Alkyl Chain Conformations and Chiral Amplification** — •Katharina Scheil[1], Nadine Hauptmann[1], Thiruvancheril G. Gopakumar[2], Franziska L. Otte[3], Christian Schütt[3], Rainer Herges[3], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Department of Chemistry Indian Institute of Technology Kanpur, Uttar Pradesh 208 016, India — [3]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

For alkyl substituents and alkane chains in thin layers on surfaces it was found that adjacent alkyl chains align parallel to each other. We investigated Trioctyl-functionalized triazatriangulenium (TATA) deposited on Au(111) and Ag(111) surfaces by electrospray ionization using low-temperature scanning tunneling microscopy. The molecules surprisingly adsorb with a bent geometry of the octyl groups making them chiral with eight possible configurations. When arranged in hexagonal networks however only one configuration was found making islands homochiral. We suggest a model of the geometry and a mechanism leading to the observed chiral amplification. Financial support by the Deutsche Forschungsgemeinschaft via the SFB 677 is gratefully acknowledged.

O 36.11 Tue 18:30 P1

**Cyano-Functionalized Triarylamines on Au(111): Competing Intermolecular versus Molecule/Substrate Interactions** — •Stefano Gottardi[1], Kathrin Müller[1], Juan Carlos Moreno-López[1], Handan Yildirim[3], Ute Meinhardt[2], Milan Kivala[2], Abdelkader Kara[3], and Meike Stöhr[1] — [1]Zernike Institute of Advanced Materials, University of Groningen, AG, Groningen, The Netherlands — [2]Chair of Organic Chemistry 1, Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Erlangen, Germany — [3]Department of Physics, University of Central Florida, Orlando, FL, USA

The self-assembly of cyano-substituted triarylamine derivatives on Au(111) is studied with scanning tunneling microscopy and density functional theory calculations. Two different phases, each stabilized by at least two different cyano bonding motifs are observed. In the first phase, each molecule is involved in dipolar coupling and hydrogen bonding, while in the second phase, dipolar coupling, hydrogen bonding and metal-ligand interactions are present. Interestingly, the metal/ligand bond is already observed for deposition of the molecules with the sample kept at room temperature leaving the herringbone reconstruction unaffected. It is proposed that for establishing this bond, the Au atoms are slightly displaced out of the surface to bind to the cyano ligands. Despite the intact herringbone reconstruction, the Au substrate is found to considerably interact with the cyano ligands affecting the conformation and adsorption geometry, as well as leading to correlation effects on the molecular orientation.

O 36.12 Tue 18:30 P1

**Adsorption of HTMGT on Au(111): Influence of Surface Roughness** — •Jan Pischel[1], Anna Lebkücher[2], Hans-Jörg Himmel[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg — [2]Institut für anorganische Chemie, Im Neuenheimer Feld 270, D-69120 Heidelberg

Hexakis(tetramethylguanidinyl)triphenylene (HTMGT) is a guanidinyl-functionalized aromatic compound (GFA) recently synthesized in the group of H.-J. Himmel in Heidelberg. GFAs are strong electron donors and can be linked to semiconducting polymers under formation of coordinative bonds mediated, e. g., by copper and iodine [1]. Furthermore, due to appropriate HOMO and LUMO levels (calculation), HTMGT is an interesting material for application in active layers of organic field effect transistors.

We show here an infrared (IR) reflection absorption spectroscopic investigation of its adsorption on the Au(111) surface and focus especially on the influence of surface roughness. Roughness in the submonolayer region is introduced in a well-defined manner by evaporation of gold onto the pristine Au(111) surface cooled to 40K. The different regimes of substrate roughness are determined by using carbon monoxide as a probe for IR spectroscopy.

[1] H.-J. Himmel, Z. Anorg. Allg. Chem., **639**:1940–1952, 2013.

O 36.13 Tue 18:30 P1

**Exploring the cerium-directed assembly of porphyrin derivatives on Ag(111)** — •Felix Bischoff, Willi Auwärter, Knud Seufert, David Ecija, Saranyan Vijayaraghavan, and Johannes Barth — Technische Universität München, Department of Physics, E20, Garching, Germany

In the field of molecular nanoscience considerable effort is put in the bottom-up synthesis of novel interfacial compounds and architectures. In this domain, rare-earth metal complexes are particularly interesting regarding their function as single-molecule magnets, field effect transistors or molecular rotors. Among the series of rare-earth complexes, those incorporating cerium are especially versatile because cerium can be in a +III or +IV oxidation state. Here we assess the metal-directed assemblies afforded by adsorbed porphyrin derivatives (2H-TPP and 2H-P) and Cerium atoms on Ag(111) in an STM study. Depending on the preparation procedure, observed products were, amongst others, modified single molecules, highly ordered cerium-porphyrinato islands, extended double-decker chains and even triple-deckers. The multiple reaction products reveal that the understanding and control of the reaction parameters is a prerequisite for well-defined products. Thus we explored routes for the controlled synthesis of distinct cerium-porphyrinato arrangements.

O 36.14 Tue 18:30 P1

**Spontaneous change in molecular orientation at order-disorder transition of tetracene on Ag(111)** — •Tomoki Sueyoshi[1], Martin Willenbockel[1], Michael Naboka[2], Alexei Nefedov[2], Serguei Soubatch[1], Christof Wöll[2], and Stefan Tautz[1] — [1]Peter Grünberg Institut (PGI-3), JARA, Forschungszentrum Jülich, Germany — [2]Institute of Functional Interfaces, Karlsruhe Institute of Technology (KIT), Germany

Molecular orientation is not only correlated closely to the electronic properties of molecular layers but also related directly to formation of various molecular phases composed of the identical molecule(s). Here, we investigate the molecular orientation of tetracene in ordered and disordered layers on Ag(111) using near-edge X-ray absorption fine structure (NEXAFS) spectroscopy [1]. Quantitative analysis of NEXAFS intensities reveals that the compact monolayer $\alpha-$phase at 150 K consists of essentially flat-lying molecules with an average tilt angle $\alpha < 9^\circ$ with respect to the Ag(111) surface. At room temperature the tetracene monolayer is dynamically disordered with $\alpha = 15 \pm 4^\circ$ ($\alpha' -$ phase). The increase in the average tetracene tilt angle indicates that orientational degrees of freedom perpendicular to the surface drive the order-disorder transition in the tetracene monolayer on Ag(111). We argue that the phase transition can be explained by a delicate balance between the interfacial enthalpy and the orientational entropy.

[1] T. Sueyoshi, M. Willenbockel, M. Naboka, A. Nefedov, S. Soubatch, C. Wöll, and F. S. Tautz, J. Phys. Chem. C 117, 9212 (2013).

O 36.15 Tue 18:30 P1

**Self-assembling and electronic structure of metallocenes on Pb(111) and Pb(100)** — •Wibke Bronsch, Benjamin Heinrich, and Katharina Franke — Freie Universität Berlin, Germany

Metallocene molecules are promising candidates for future spintronic applications. However, in contact to metallic leads their stability has recently been discussed [1,2]. Employing low-temperature scanning tunneling microscopy, we show that ferrocene on Pb(111) and Pb(100) forms self-assembled islands, in which the molecular axis is almost parallel to the surface normal. Dissociation of the molecules occurs when the molecules are forced to closer distance, as e.g. at dislocation lines or higher molecular coverages. Tunneling spectroscopy reveals that the HOMO and LUMO are mainly localized on the cylcopentadienyl rings. In agreement with the spin singlet state of the free molecule, we do not find any indication of magnetic interaction with the substrate.

[1] Braun, K.-F. et al., Phys. Rev. Lett. **96**, 246102 (2006)

[2] Heinrich, B. W. et al., Phys. Rev. Lett. **107**, 216801 (2011)

O 36.16 Tue 18:30 P1

**Structural and optical investigation of K doping induced changes of PTCDA on Ag(111)** — •Christian Zwick, Marco Gruenewald, Roman Forker, and Torsten Fritz — Friedrich-Schiller University, Institute of Solid State Physics, Max-Wien-Platz 1, Jena 07743, Germany

We report on the impact of potassium doping on highly-ordered ultra-thin layers of the dye molecule 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on a Ag(111) surface under ultra-high vacuum conditions. The thin films were characterized optically by *in situ* differential reflectance spectroscopy (DRS) [1,2] as well as structurally by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). Depending on the doping concentration, distinct optical spectra could be observed. Except for one all could be assigned to the optical fingerprints of ionized PTCDA, showing different doping states ranging up to tetraanions. For the first three doping levels of PTCDA we were able to study the corresponding structures, which significantly differ from each other, referencing directly to the influence of the doping, i.e., doping induced phase transitions and the adsorption sites occupied by the dopants.

References:

[1] R. Forker *et al.*, *Annu. Rep. Prog. Chem., Sect. C: Phys. Chem.*, **2012**, *108*, 34-68.

[2] R. Forker and T. Fritz, *Phys. Chem. Chem. Phys.*, **2009**, *11*, 2142-2155.

O 36.17 Tue 18:30 P1

**Understanding the peptide folding on surfaces in UHV by electrospray ion beam deposition (ES-IBD)** — •Sabine Abb[1], Gordon Rinke[1], Stephan Rauschenbach[1], Ludger Harnau[2,3], and Klaus Kern[1,4] — [1]Max-Planck-Institute for Solid State Reserach, Heisenbergstr. 1, Stuttgart — [2]Max-Planck-Institute for Intelligent Systems, Heisenbergstr. 3, Stuttgart — [3]IV. Institute for Theoretical Physics, University Stuttgart, Pfaffenwaldring 57, Stuttgart — [4]Ecole Polytéchnique Fédérale de Lausanne, Switzerland

Specific functionality of peptides and proteins is reached by folding into a unique secondary and tertiary structure which is steered by intramolecular interactions as well as metal coordination. A new route to investigate the properties and structural formation of amino acid sequences on surfaces in low dielectric environments ( e.g. in vacuo) is possible with our home-built ES-IBD instrument which allows in-situ STM characterization of (bio)molecules. It also gives additional modes of control, for instance by using selected charge states and generating metal-peptide complexes which already form in solution.

Here we show preliminary results of STM investigations of the eight-amino acid peptide angiotensin II on various metal surfaces. We observe dimer to multimer self-assembled structures and present preliminary structural models. For a deeper understanding of the ongoing processes, special attention is paid to the structural differences and similarities between the protonated and coordinated angiotensin II as well as the comparison to the nine-amino acid peptide Bradykinin.

O 36.18 Tue 18:30 P1

**Ion beam-induced nanoscale surface modulations and their effect on protein-surface adsorption** — •Alexander von Müller, Jana Sommerfeld, and Carsten Ronning — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 3, 07743 Jena

Under specific experimental conditions, the irradiation of solid surfaces with ions can result in periodic surface modulations at the nanoscale. This effect of ripple formation is widely discussed in the literature and has been observed on many different types of materials - e.g. semiconductors, amorphous materials, graphite, and metals [1,2]. We will present results of experiments in which we have tested the biocompatibility of such ion beam-induced surface morphologies by studying their effects on the surface adsorption behaviour of human plasma fibrinogen (HPF) proteins. The nanopatterned surfaces have been created by irradiation of different substrates with low-energy ions (< 20 keV). Both the effects of the irradiations and the adsorption of the proteins have been studied by means of atomic force microscopy (AFM).

[1] Nanostructuring surfaces by ion sputtering, U. Valbusa, C. Boragno, F. Buatier de Mongeot, J. Phys: Condens. Matter, 2002, 14, 8153-8175

[2] Ion-Induced Nanoscale Ripple Patterns on Si Surfaces: Theory and Experiment, A. Keller, S. Facsko, Materials, 2010, 3, 4811-4841

O 36.19 Tue 18:30 P1

**STM and XPS Investigation of Ethylene Carbonate Monolayers on Cu(111) and Co-Adsorption of Lithium** — •Maral Bozorgchenani[1,2], Florian Buchner[1], Hanieh Farkhondeh[1,2], Benedikt Uhl[1,2], and R. Jürgen Behm[1,2] — [1]Helmholtz Institute Ulm (HIU), Ulm, Germany — [2]Ulm University, Institute of Surface Chemistry and Catalysis, Ulm, Germany

Ethylene Carbonate (EC) and Lithium (Li) are major components in Li-ion battery electrolytes. An understanding of the solid-electrolyte interphase (SEI) at a molecular level would be highly desirable to improve Li-ion batteries. The co-adsorption of both components, as a model system, is topic of the present work and will be investigated to mimic the situation at the SEI. In a first step, adsorption of the two materials on a Cu(111) surface was studied independently: (1) The adsorption behaviour of EC on Cu(111) was investigated by scanning tunnelling microscopy (STM) and X-ray photoelectron spectroscopy (XPS) under ultrahigh vacuum (UHV) conditions. At sub-monolayer coverage, the STM images show highly ordered 2D EC islands around 100 K. Evidence for intact EC adsorbed on Cu(111) is provided by the XP C1s and O1s core level spectra. Temperature induced structural and chemical changes will be highlighted. (2) After deposition of Li atoms on Cu(111) held at 80 K, objects with a circular shape were identified. The adsorption behaviour and interaction mechanism is discussed. Co-deposition of both materials together on Cu(111) will be explored in forthcoming experiments.

O 36.20 Tue 18:30 P1

**Comparison of the adsorption behavior of the ionic liquids [EMIM][TFSA] and [OMIM][TFSA] on Au(111) and Ag(111)** — •Benedikt Uhl[1,2], Hsinhui Huang[1], Dorothea Alwast[1,2], Florian Buchner[2], and R. Jürgen Behm[1,2] — [1]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany — [2]Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89069 Ulm, Germany

Ionic liquids (IL) have attracted high interest because of their special chemical and physical properties; e.g., the application in electrolytes of Li-ion batteries is a promising concept. To gain a better understanding of the fundamental molecular processes at the electrode|electrolyte interface, the interaction of 1-ethyl-3-methylimidazolium-bis(trifluoromethylsulfonyl)imide ([EMIM][TFSA]) and 1-octyl-3-methylimidazolium-bis(trifluoromethyl-sulfonyl)imide ([OMIM][TFSA]) with Au(111) and Ag(111) was investigated by scanning tunneling microscopy (STM) under UHV conditions at temperatures between 80 K - 293 K. Since both ILs differ only in the length of their alkyl chains, differences in structure formation on the same surface can solely be caused by this. For Au(111) as well as for Ag(111), both ILs show a very similar behavior: long-range ordered (2D crystalline) domains/islands coexist with a short-range ordered (2D glass) phase. The 2D crystalline structures of both IL adsorbates showed the same space requirement per adsorbed molecule, which points to an adsorption geometry of the molecule with the alkyl chain sticking up from the surface.

O 36.21 Tue 18:30 P1

**Molecular Aggregates for Photoemission Electron Microscopy (PEEM)** — •Hannes Hartmann, Ingo Barke, Karl-Heinz Meiwes-Broer, and Sylvia Speller — University of Rostock, Institute of Physics, 18051 Rostock, Germany

Molecular aggregates are of significant interest for applications in organic electronics and for photovoltaics. Our experiments aim at spatial and energy-resolved studies of excitations in molecular aggregates. The primary method is photoemission electron microscopy (PEEM), in combination with fluorescence- and scanning probe microscopy. The PEEM system is equipped with energy filters and different excitation sources. For time-resolved measurements a pump-probe setup is under construction. The current state of affairs is presented and discussed.

O 36.22 Tue 18:30 P1

**Structure and Fluorescence of Molecular Crystals** — Björn Vogler[1], Hannes Hartmann[1], Kai Wardelmann[1], Heinrich Behle[1], J.A.A.W. Elemans[2], Ingo Barke[1], and •Sylvia Speller[1] — [1]University of Rostock, Institute of Physics, 18051 Rostock, Germany — [2]Institute for Molecules and Materials, RU Nijmegen, NL

We study the influence of the local environment on the excitation and transport of Frenkel excitons in molecule crystals. Metallo-porphyrin aggregates [1] are prepared by dropcasting on graphite. We use AFM, STM, and Fluorescence Microscopy to study morphology and the spatial distribution of fluorescence. The mesoscopic structure shows molecular strands branching into finer structures. The fluorescence intensity is spatially varying along the strands and appears enhanced at junctions. We discuss possible origins for the observed variations.

[1] M.J.J. Coenen, et al., Phys. Chem. Chem. Phys. 15, 12451 (2013)

O 36.23 Tue 18:30 P1

**Photon emission from the tunneling contact of a low temperature STM for pristine and adsorbate covered metal sub-**

**strates** — •Ebru Özen, Maren C. Cottin, Tobias Roos, Detlef Utzat, Doris Steeger, Willy Platz, Rolf Möller, and Christian A. Bobisch — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

STM-induced light emission (STM-LE) has been a emerging field in scanning tunneling microscopy in the past years [1]. STM-LE experiments on organic molecules are of particular interest, since they can provide information about energy loss in certain organic molecules [2]. We find that Ag(111) terraces show a plasmonic excitation in the tunneling contact of a silver covered Pt-Ir tip for positive and negative sample bias. In addition experiments on Ag(111) surfaces partially covered by different organic molecules were performed. It is found that the organic molecules perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA), copper-phthalocyanine (CuPc) and the carbon-molecule $C_{60}$ reduce or completely suppress the emission of photons. Photon maps of molecularly resolved $C_{60}$ islands show a periodic modulation of the light intensity by the adsorbed $C_{60}$.

[1] R. Berndt and J. K. Gimzewski, Phys. Rev. B **48** 4746 (1993).

[2] C. Chen et al., Phys. Rev. Lett. **105**, 217402 (2010).

O 36.24 Tue 18:30 P1

**Decoupling in organic heterostructures of PTCDA and CuPc on single crystalline silver** — •Tino Kirchhuebel[1], Marco Gruenewald[1], Julia Peuker[1], Timothy Vajas[2], Roman Forker[1], and Torsten Fritz[1] — [1]Friedrich Schiller University, Institute of Solid State Physics, Max-Wien-Platz 1, Jena 07743, Germany — [2]The Ohio State University, Department of Physics, 191 West Woodruff Ave, Columbus, OH 43210

Here we report on organic heterostructures of highly-ordered ultrathin layers of the dye molecules 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) and copper-phthalocyanine (CuPc) grown on Ag(111) and characterized by LEED and LT-STM as well as optically by in-situ differential reflectance spectroscopy (DRS) [1].

The heterostructure consisting of CuPc on top of one monolayer PTCDA on Ag(111) is stable, and the DRS spectra show a clear monomeric behavior of CuPc as likewise observed on an inert mica substrate. In contrast, by LT-STM and DRS measurements we found that one monolayer of CuPc on Ag(111) is thermodynamically not stable when PTCDA is deposited on top. Besides of decoupling aromatic molecules from a metal by an organic interlayer the passivation is also possible by depositing thin films of alkali metal halides on top of the metallic surface [2]. Preliminary results for PTCDA on KCl/Ag(111) and CuPc on KCl/Ag(100) will also be discussed.

References: [1] R. Forker et al., Annu. Rep. Prog. Chem., Sect. C: Phys. Chem., 2012, 108, 34-68. [2] M. Müller et al., Surface Science, 2011, 605, 1090-1094.

O 36.25 Tue 18:30 P1

**Electronic "chirality" of transition metal phthalocyanine molecules adsorbed to noble metal surfaces** — •Jacob Senkpiel, Jens Kügel, Pin-Jui Hsu, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II,Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We have investigated the transition metal phthalocyanine (TM-Pc) molecules MnPc and CuPc on Cu(001) and Ag(001) by means of low-temperature scanning tunneling microscopy and spectroscopy measurements ($T \approx 5\,\mathrm{K}$). It is well-known that the symmetry axes of the adsorbed TM-Pc molecules are rotated with respect to the four-fold symmetry axis of noble metal (001)-surfaces. Symmetry considerations suggest that this should generally lead to chiral electronic distortion, which has been ascribed to charge transfer between the TM-Pc and the substrate. However, chirality was clearly observed only for some molecules, such as ZnPc on Cu(001) [1] and CuPc/NiPc on Ag(001) [2], while the topography of others appeared to be almost unaffected [2]. In this contribution we will present a detailed investigation of the molecular shape and the resulting electronic structure. Our results suggest that chirality is indeed a general phenomenon for TM-Pc's on four-fold symmetric substrates.

[1] Chen *et al.*,Appl. Phys. Lett. **100**, 081602 (2012)

[2] Mugarza *et al.*, Phys. Rev. B **85**, 155437 (2012)

O 36.26 Tue 18:30 P1

**Reversible conformational changes in manganese porphyrin molecules** — •Xianwen Chen[1], Christian Lotze[1], Paul Stoll[1], Nils Krane[1], José I. Pascual[1,2], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]CIC nanoGUNE San Sebastián, and Ikerbasque Foundation for Science, Bilbao, Spain

Using scanning tunneling microscopy and spectroscopy at 7 K, we investigate manganese tetra-pyridine-porphyrin (Mn-TPyP) molecules adsorbed on a Cu(111) surface. The molecules show notable structural flexibility, which leads to two adsorption states. The different adsorption configurations are characterized by two distinct orbital alignments. Noncontact Atomic Force Microscopy images indicate that the pyridine rings can lie in two meta-stable tilting angles on the surface. We can induce a reversible rotation of single legs or pairs of legs by the tip of the scanning tunneling microscope with a threshold voltage around 2V.

O 36.27 Tue 18:30 P1

**Biomolecules at metal interfaces: a novel force field approach including polarization** — •Isidro Lorenzo[1], Hadi Ramezani-Dakhel[2], Hendrik Heinz[2], and Marialore Sulpizi[1] — [1]Johannes Gutenberg University Mainz, Staudinger Weg 7 55099 Mainz — [2]Departament of Polymer Engineering, University of Akron, Ohio 44325

Increasing interest in bio-interfaces for medical and bio-technological applications calls for microscopic understanding and control of protein-surface interactions. In particular here we aim to provide a characterization of peptide / gold interactions at a molecular level in order to explain and interpret recent surface experimental results [1] and to fill the gap between fundamental science and real applications. Atomistic simulations have been performed with the GROMACS package using available force field parameters such as CHARMM27 using 12-6 Lennard-Jones potentials [2] force field. A novel scheme is devised to include the metal polarization (image charge effect) induced by the adsorbed molecules. Extensive tests have been performed for the force field validation and comparisons with quantum mechanics (QM) density functional theory (DFT) are also discussed. Results for the di- and tri-peptide of the insulin-like growth factor on gold are presented.

[1] Anne Vallee, Vincent Humblot, and Claire-Marie Pradier Acc. Chem. Res., 2010, 43 (10), pp 1297306

[2] Heinz H, Vaia RA, Farmer BL, Naik RR J. Phys. Chem. C 2008, 112, 17281 17290; Heinz H, Farmer BL, Pandey RB, Slocik JM, Patnaik SS, Pachter R, Naik RR. J. Am. Chem. Soc. 2009, 131, 9704-9714

O 36.28 Tue 18:30 P1

**Hybridization and Charge Transfer of Planar Pt(II) Triplet Emitters at the metal organic Interface** — •Alexander Timmer, Pascal Raphael Ewen, Jan Sanning, Chistian Alejandro Srassert, Daniel Wegner, Harry Mönig, and Harald Fuchs — Physikalisches Institut, Westfälische- Wilhelms Universität Münster, Deutschland

The physical and chemical properties of organic molecules on surfaces are strongly influenced by the coupling mechanisms involved. We examined the electronic structure and the adsorption behavior of the interfaces formed between electroluminescent Pt(II) complexes and various metal surfaces using photoelectron spectroscopy (PES) and scanning tunneling microscopy (STM). Furthermore we performed PES measurements on multilayer structures of these Pt(II) complexes to gain information about energy level alignment and possible charge transfer processes in stacks of such planar triplet emitters. In addition we methodically changed the substituent of the organo-metallic complexes, which in essence varied the adsorbate substrate distance, or in case of the multilayer structures alters the intermolecular stacking distance, respectively. Our results may provide further insight into the coupling and hybridization mechanisms of these molecular systems with electrodes, which are essential for the design of electroluminescent devices, such as organic light emitting diodes (OLEDs) or light emitting electrochemical cells (LEECs).

O 36.29 Tue 18:30 P1

**STM/STS investigation of ionic liquids adsorbed at metal surfaces** — •Thomas Gross, Matthias Stocker, and Berndt Koslowski — Institut für Festkörperphysik, Universität Ulm, D-89081 Ulm

In the last years, ionic liquids (ILs) gained more and more interest in the fields of, e.g., catalysis, electrolytes, liquid crystals, electro-elasticity etc. We employ scanning tunneling microscopy and spectroscopy (STM and STS) at low temperature to investigate the properties of such ILs being adsorbed at metal surfaces. We therefore deposited 1-butyl-1-methylpyrrolidiniumbis(trifluoromethylsulfonyl)-imide (BMP-TFSA) and 1-ethyl-3-methylimidazoliumtrifluoromethanesulfonate (EMIM-TFSA) on Ag(111) in the sub-monolayer range. Preliminary results are reported as follows: The ILs form stable islands frequently bound by steps in the substrate. The resolution within the islands depends strongly on the state of the tunneling tip. Enhanced resolution is achieved with an IL molecule adsorbed at the tip. The surface state of Ag(111) prevails underneath the IL monolayer and shifts by about +100 meV towards the unoccupied states. We derive the charge state of the adsorbed molecules by determining the differential barrier height thus discriminating the anions and kations at the surface.

O 36.30 Tue 18:30 P1

**Exploring coherent transport through $\pi$-stacked systems in molecular electronic devices** — •Qian Li[1], Gemma Solomon[1], Gediminas Kirsanskas[2], Karsten Flensberg[2], and Martin Leijnse[3] — [1]Nano Science Center and Department of Chemistry, University of Copenhagen, Denmark — [2]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Denmark — [3]The Division of Solid State Physics, Lund University, Sweden

Understanding electron transport across $\pi$-stacked systems will help to elucidate intermolecular tunneling in molecular junctions and in the design of effective molecular devices. Here we show how conjugation length and substituent groups influence the electron transport and thermoelectric response in the $\pi$-stacked structures by investigating five representative stacked molecular junctions. We found that a $\pi$-stacked system of two substituted anthracenes exhibit good thermopower and a high power factor, suggesting that increased conjugation can enhance thermoelectric response. The fully eclipsed structure of quinhydrone exhibits high power factor at the minimum energy structure and could be a better candidate in a thermoelectric device, compared with the other $\pi$-stacked systems considered.

O 36.31 Tue 18:30 P1

**Light-induced ring opening of a submonolayer nitrospiropyran electronically decoupled from a Cu(100) surface** — •Fabian Nickel[1], Matthias Bernien[1], Qingyu Xu[1,2], and Wolfgang Kuch[1] — [1]Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin — [2]Southeast University, Department of Physics, Nanjing 211189, P. R. China

The electronic properties of spiropyran (SP) molecules are known to change enormously after a ring opening to merocyanine (MC). Current research focuses on the isomerization of molecules in direct contact with a surface. These systems might have a great potential for applications to switch properties by external stimuli such as light. In this work the adsorption of SP on a Cu(100) surface covered by a double layer of 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) was studied by near-edge x-ray absorption fine structure (NEXAFS). PTCDA adsorbs planar on the Cu(100) surface and is supposed to reduce the interaction of the overlying molecular layer with the metal substrate. At a temperature of 200 K, the SP molecules are physisorbed in the closed-ring conformation. A ring opening by illumination with UV light could be achieved for this system. A change in the out-of-plane nitrogen x-ray absorption can clearly be assigned by density functional theory to the switching of SP to the zwitterionic MC mesomere. Polarization-dependent spectra of the nitrogen and oxygen K edge show a slight change of the angle dependence due to a possible tilting of the molecule.

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O 36.32 Tue 18:30 P1

**Honeycombenes: A novel class of hydrocarbon macrocycles made by surface-assisted synthesis** — •Min Chen[1], Jian Shang[2], Yongfeng Wang[2], Kai Wu[2], Qitang Fan[3], Cici Wang[3], Yong Han[3], Junfa Zhu[3], Julian Kuttner[1], Gerhard Hilt[1], and J.Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]College of Chemistry and Molecular Engineering, Peking University, China — [3]National Synchrotron Radiation Laboratory, University of Science and Technology of China, China

Surface-assisted synthesis provides an elegant route to molecules that cannot be synthesized in solution or that are too large for vapor-deposition. Both factors apply for [n]-honeycombenes, a novel class of planar hydrocarbon macrocycles of hexagonal geometry. [18]-Honeycombene or hyperbenzene ($C_{108}H_{72}$) consists of 18 phenyl rings and was made by surface-assisted Ullmann reaction from $4,4''$-dibromo-m-terphenyl (DBTP) on Cu(111). The molecules arrange in long-range ordered islands with hexagonal unit cell. [30]-Honeycombene ($C_{180}H_{120}$), a hexagon with 30 phenyl rings, was made on Ag(111) from $4,4''''$-dibromo-m-quinquephenyl (DBQP). DBQP gives also access to strained rings of heptagonal ($C_{210}H_{140}$), pentagonal ($C_{150}H_{100}$) and square ($C_{120}H_{80}$) shape. Using STS, the electronic structure along the ring perimeter and the confinement of surface state electrons trapped inside the macrocycles were studied. The large diameters of >2 nm and >3.5 nm make [18]- and [30]-honeycombene promising candidates for nanotroughs that can host other molecules or nanoparticles.

O 36.33 Tue 18:30 P1

**Electrospray deposition of $Mn_{12}$ and $Fe_4$ single molecule magnets** — •Philipp Erler[1], Eva-Sophie Wilhelm[1], Nicole Barth[1], Samuel Bouvron[1], Peter Schmitt[2], Stefan Ambrus[2], Ulrich Groth[2], Luca Gragnaniello[1], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Fachbereich Chemie, Universität Konstanz

Single molecule magnets (SMMs) have attracted significant interest during the past decades due to their unique magnetic properties like hysteresis of purely molecular origin and the possibility to observe quantum tunneling of magnetization. This material class allows for basic studies on quantum effects of magnetism at the molecular scale and is furthermore a promising candidate for preliminary studies aiming at ultrahigh density data storage devices or quantum computing applications. However, progress in this field is hindered by the difficulty of depositing intact SMMs on surfaces.

We have implemented electrospray ionization for the deposition of $Mn_{12}$-acetate SMMs on various substrates under ultra high vacuum conditions. The magnetic properties of thin films of $Mn_{12}$-acetate were investigated with SQUID magnetometry, whereas the structural and electronic properties of sub-monolayers and individual molecules were studied by means of low temperature scanning tunneling microscopy and spectroscopy (STM/STS) and X-ray photoelectron spectroscopy (XPS). Furthermore, first attempts have been made for the electrospray deposition of $Fe_4$ SMMs, which offer the advantage of an enhanced redox stability of the magnetic core.

O 36.34 Tue 18:30 P1

**Temperature induced dehydrogenation and substrate-mediated hydrogen transfer of tetra(*p*-hydroxyphenyl)-porphyrin - a photoelectron spectroscopy study** — •Lars Smykalla[1], Pavel Shukrynau[1], Michael Hietschold[1], Carola Mende[2], Heinrich Lang[2], and Dietrich R. T. Zahn[3] — [1]Technische Universität Chemnitz, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany — [2]Technische Universität Chemnitz, Institute of Chemistry, Inorganic Chemistry, D-09107 Chemnitz, Germany — [3]Technische Universität Chemnitz, Institute of Physics, Semiconductor Physics, D-09107 Chemnitz

We present photoelectron spectroscopy investigations of 5,10,15,20-tetra(*p*-hydroxyphenyl)porphyrin ($H_2$THPP) molecules adsorbed on Au(111) and Ag(110). Directly after deposition of the molecular layer, coexistence of $H_2$THPP molecules with the cationic form $H_4$THPP is found. Annealing leads to the dissociation of the central hydrogen atoms in the molecules. On Au(111) after annealing to high temperatures, subsequently, both $H_2$THPP and its doubly dehydrogenated form THPP are observed. On the other hand, on the more reactive Ag(110) surface after annealing to 300 °C, partial dissociation of the hydroxyl groups followed by diffusion and rebonding of hydrogen to the central nitrogen atoms and with this the formation of a zwitterionic species is found. Furthermore starting at this temperature, on both substrates partial C−H bond breaking at the pyrrole rings is observed, which affects the whole electronic structure of the molecule as shown in the valance band spectra.

O 36.35 Tue 18:30 P1

**Towards the formation of extended polycyclic aromatic hydrocarbons doped with nitrogen** — •Tim Sander[1], Maximilian Ammon[1], Philipp Hofmann[1], Natalie Hammer[2], Milan Kivala[2], and Sabine Maier[1] — [1]Department of Physics, University of Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Germany

The formation of extended polycyclic aromatic hydrocarbons (PAHs) by on-surface synthesis on metal surfaces has recently attracted increased interest owing to the current developments in the field of building new carbon allotropes in a bottom-up approach. We used planarized triarylamine molecules functionalized with diphenylmethylidene side groups and end groups of different types (e.g. alkylchains and trialkylsilyl moieties) as molecular building blocks. We investigated the potential of the functionalized triarylamine molecules to undergo a cyclodehydrogenation reaction on the Au(111) and Cu(111) surface to create novel extended PAHs doped with nitrogen heteroatoms. The thermal-stability of the different functional side and end groups as well as the adsorption configuration of the individual molecules will be discussed in detail by means of low temperature scanning tunneling microscopy under ultra-high vacuum condition.

O 36.36 Tue 18:30 P1

**Intramolecular Dipole of Merocyanine probed by Local Contact Potential Difference Measurements** — •Nils Krane[1], Christian Lotze[1], Xianwen Chen[1], José I. Pascual[1,2], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]CIC nanoGUNE, San Sebastián, and Ikerbasque, Basque Foundation for Science, Bilbao, Spain

The merocyanine form of the molecular switch 1,3,3-Trimethylindolino-6'-nitrobenzopyrylospiran exhibits an intramolecular dipole in gas phase and solution [1]. When adsorbed on a metal surface, charge redistribution and screening may considerably alter the expected dipole behaviour. Using a combined low-temperature scanning tunneling microscope/atomic force microscope, we investigate the adsorption and intramolecular charge distribution of merocyanine on Au(111). The lateral and vertical distribution of the local contact potential difference (LCPD) hint at the persistence of an intramolecular dipole.

[1] D. Lapienis-Grochowska *et al.* Journal of the Chemical Society, Faraday Transactions 2 75, 312 (1979)

O 36.37 Tue 18:30 P1

**STM Investigations of Spirobifluorene Tripodal Molecules on Au(111)** — •Kevin Edelmann[1], Lukas Gerhard[1], Marcin Lindner[1], Michal Valasek[1], Lei Zhang[1], Hilbert von Löhneysen[1,2,3], Elke Scheer[4], Marcel Mayor[1,3,5], Maya Lukas[1], and Wulf Wulfhekel[1,6] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), D-76021 Karlsruhe — [2]Physics Institute and Institute for Solid State Physics, Karlsruhe Institute of Technology (KIT), D-76049 Karlsruhe — [3]DFG Center for Functional Nanostructures (CFN), D-76049 Karlsruhe — [4]Physics Department, University of Konstanz, Universitätsstraße 10, D-78457 Konstanz — [5]Department of Chemistry, University of Basel, CH-4056 Basel — [6]Physikalisches Institut, Karlsruhe Institute of Technology (KIT), D-76131 Karlsruhe

Decoupling molecular functional electronic units from a metallic substrate in a controllable manner is a major challenge for the investigation of the electronic properties of single molecules by STM. A promising approach is to use a tripodal molecule as a platform that carries the actual molecular wires or functional unit. [1]. Before functionality is integrated into this tripodal stand, the positioning and coupling of the platform to the substrate needs to be characterized thoroughly. To this end, we investigated spirobifluorene tripodal molecules. Different deposition techniques were used to deposit the molecules onto a Au(111) surface (from solutions or sublimation in UHV). We report on the morphology and electronic properties of these molecules by STM measurements. [1] Lukas et. al., ACS Nano 2013 7 (7), 6170-6180

O 36.38 Tue 18:30 P1

**Investigation of the Hydrogenation of Graphene on Ni(111) via Temperature Programmed X-Ray Photoemission Spectroscopy and Temperature Programmed Desorption** — •Florian Späth, Wei Zhao, Karin Gotterbarm, Christoph Gleichweit, Hans-Peter Steinrück, and Christian Papp — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

The fundamental understanding of the reaction of hydrogen with graphene is of paramount importance for hydrogen-based energy storage and for tailoring the properties of graphene through chemical modification, and thus for future applications in hydrogen storage and semiconductor industries. Low defect graphene is prepared on Ni(111) by chemical vapor deposition; subsequent exposure to atomic hydrogen yields hydrogenated graphene. The hydrogenation process is thoroughly investigated with X-Ray Photoelectron Spectroscopy to gain insight in the chemical modification. The dehydrogenation process is investigated with Temperature Programmed X-Ray Photoemission Spectroscopy and Temperature Programmed Desorption. We gain detailed mechanistic insights and observe a two-step dehydrogenation independently with both methods. Furthermore, we determined the hydrogen saturation coverage, which corresponds to a full single-side hydrogenated layer. Additionally, we present a model for both the hydrogenation and dehydrogenation, and deduce a strong dependency of the hydrogen storage capacity on the substrate. A comparison to quasi free-standing graphene will be discussed.

O 36.39 Tue 18:30 P1

**Modeling catalytic reactions: graphene-supported Pd nanoclusters studied with high-resolution X-ray photoelectron spectroscopy** — •Karin Gotterbarm, Carina Bronnbauer, Udo Bauer, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

In our study, graphene was grown on a Rh(111) single crystal surface by chemical vapour deposition of propylene at elevated temperatures. The corrugated graphene layer serves as a template for the evaporation of Pd nanoclusters with a narrow size distribution. The growth of the clusters and their interaction with adsorbates was investigated by fast X-ray photoelectron spectroscopy (XPS) performed at the synchrotron facility BESSY II. We found a cluster-by-cluster growth mode. Upon annealing, we observe restructuring and agglomeration of the clusters. At temperatures above 850 K, intercalation of the palladium under the intact graphene sheet is observed. The interaction of the Pd particles with CO and $O_2$ was investigated in all relevant core levels in a temperature range from 150 up to 500 K. The adsorbate coverage varies with temperature and shows a strong dependency on the structure of the clusters.

O 36.40 Tue 18:30 P1

**Transport properties of epitaxially grown graphene nanoribbons** — •Jens Baringhaus[1], Frederik Edler[1], Christian Seidel[1], Claire Berger[2], Walter A. de Heer[2], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Georgia Institute of Technology, Atlanta, Georgia 30332-0430, USA

For graphene nanoribbons with zig-zag type edges the existence of topologically protected electronic edge states is theoretically predicted. Hence, exceptional transport phenomena such as ballistic transport with a mean free path in the $\mu$m range become accessible. The experimental realization of such nanoribbons requires a gentle patterning avoiding any damaging of the edges. For this purpose, we use a selective graphitization process on SiC mesa structures which allows the direct growth of graphene nanoribbons without post-processing. The electronic properties of the ribbons are investigated with scanning tunneling spectroscopy. A local density of states typical for a zig-zag type edge is observed, revealing features corresponding to the two topologically protected zeroth subbands. The transport properties of the ribbons are further analyzed by means of a 4-tip STM system. Extremely robust ballistic transport with a mean free path up to 10 $\mu$m is observed for temperatures up to room temperature. Transport in just one or both zeroth subbands can be detected depending on the probe spacing. Transport data of around 50 different ribbons are analyzed statistically, showing the reliability and reproducibility of the observed phenomena.

O 36.41 Tue 18:30 P1

**HRTEM characterization of epitaxially grown graphene nanoribbons** — Dennis Laube[1], •Jens Baringhaus[1], Atasi Chatterjee[1], Eberhard Bugiel[2], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Leibniz Universität Hannover, Institut für Materialien und Bauelemente der Elektronik, 30167 Hannover, Germany

The fabrication of well-ordered graphene nanostructures is essential for any kind of graphene based device. Since standard lithography methods typically induce a large amount of defects at the edges the so produced nanostructures do not exhibit the theoretically expected transport behavior such as a width dependent bandgap (armchair edges) or ballistic transport (zig-zag edges). We use a three-stepped selective graphitization process on SiC mesa structures to grow graphene nanostructures directly in the desired shape to avoid any damaging post-processing. First, the mesa structure is patterned into the SiC substrate. In the second step, the substrate is heated at temperatures slightly below the graphitization temperature to induce a refacetting process of the mesa edges. In the last step, the sample is heated to 1350 °C for the graphitization which starts at the facets due to the much weaker bonding of silicon atoms. The fabrication process is monitored by means of high resolution TEM. Parameters such as the angle of the SiC facets (which predetermines the width of the nanostructure) were deduced. Finally, the graphene grown on the facets is studied with respect to local bonding as well as interface properties.

O 36.42 Tue 18:30 P1

**Local transport properties of epitaxially grown graphene** — •Frederik Edler[1], Jens Baringhaus[1], Christoph Neumann[2], Christoph Stampfer[2], Stiven Forti[3], Ulrich Starke[3], and Christoph Tegenkamp[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany — [2]JARA-FIT and II. Institute of Physics A, RWTH Aachen University, 52074 Aachen, Germany — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

Transport properties of graphene are strongly affected by imperfections. A promising approach to large-scale graphene films which could be used in electronic circuits or new device structures is the epitaxial growth of graphene on SiC. For a better understanding of defect parameters, the epitaxial growth of graphene on a 6H-SiC(0001) substrate was stopped before the completion of large scale graphene areas which results in patches of different graphene perfection and transport regimes. By means of a four-tip STM/SEM system we were able to gently contact our sample on a nanometer scale without inducing strain to the graphene films. This allowed us to correlate the local morphology of monolayer graphene (as seen in SEM and STM images) with spatially resolved transport measurements. Further supporting spectroscopic characterizations were done by ARPES, Raman and STS measurements. Our detailed analysis of temperature dependency and variation of probe spacings clearly reveals two-dimensional transport regimes of Anderson localization as well as diffusive transport.

O 36.43 Tue 18:30 P1

**Thermolubricity of Xe monolayers on graphene** — Matteo Pierno[1], •Luca Bignardi[2,3], Maria Clelia Righi[4], Lorenzo Bruschi[1], Stefano Gottardi[2], Meike Stöhr[2], Pier Luigi Silvestrelli[1,5], Petra Rudolf[2], and Giampaolo Mistura[1] — [1]Dept. of Physics and Astronomy, University of Padova, Padova, Italy — [2]Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands — [3]Physikalisches Institut, University of Münster, Münster, Germany — [4]CNR and Dept. of Physics, University of Modena and Reggio, Modena, Italy — [5]IOM-CNR, Trieste, Italy

The nanofriction of Xe monolayers deposited on graphene was explored with a quartz crystal microbalance (QCM) at temperatures between 25 and 50 K. Graphene was grown by chemical vapour deposition and transferred to the QCM electrodes with a polymer stamp. At low temperatures, the Xe monolayers are fully pinned to the graphene surface. Above 30 K, the Xe film slides and the coverage beyond which the film starts sliding decreases with temperature. Similar measurements repeated on bare gold show an enhanced slippage of the Xe films and a decrease of the depinning temperature below 25 K. Nanofriction measurements of krypton and nitrogen confirm this scenario. This thermolubric behaviour is explained in terms of a recent theory of the size dependence of static friction between adsorbed islands and crystalline substrates.

O 36.44 Tue 18:30 P1

**AFM and Raman investigations of epitaxial graphene nanoribbons** — •Malte Halbauer[1], Jens Baringhaus[1], Christoph Neumann[2], André Müller[2], Christoph Stampfer[2], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]JARA-FIT and II. Institute of Physics A, RWTH Aachen University, 52074 Aachen, Germany

The synthesis of graphene nanoribbons (GNR) with well-oriented edges on a wafer-scale is a challenging task for the development of graphene based devices. Lithographic processing of graphene leads to a high amount of defects especially at the edges which destroy easily envisaged properties, e.g. ballistic edge channels. Hence, a self-organized growth of graphene nanoribbons is highly desirable. For this purpose we use the selective graphitization of refacetted SiC mesa structures. In order to reveal ideal growth parameters, the annealing processes have been studied and monitored by AFM as well as Raman spectroscopy. All heating steps have been performed in a face-to-face resistive heater. While AFM provides inside into the morphology of the mesa and facet structure, EFM has been used to record the local work function of the surface which is indicative for a selective growth of graphene nanostructues. The results correlate nicely with mappings of the 2D Raman signal indicating a successful growth of graphene nanoribbons. Best GNR structures have been obtained by annealing to 1200 °C for 20 min. For longer annealing times debunching of the initial MESA structure has been found as well as graphitization in between the ribbons.

O 36.45 Tue 18:30 P1

**Chemical and Electronic Modification of Graphene via Reactive Landing of Hyperthermal Molecular Ion Beams** — •Girjesh Dubey[1], Stephan Rauschenbach[1], Roberto Urcuyo[1], Marko Burghard[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, Stuttgart — [2]Institut de Physique de la Matiere Condensee, Ecole Polytechnique Federale de Lausanne, Switzerland

Tailoring the electronic properties of graphene by surface modification is of interest for switching devices and logic applications. However, chemical modification of graphene at stoichiometric densities is generally difficult, due to it's low reactivity. One unique solution to this challenge is to collide energetic molecular ion beams (10-200 eV) at the surface of the $sp^2$-hybridized basal plane. Upon impact, hyperthermal ion beams with energies considerably larger than that of a covalent bond (1-10 eV) are able to produce surface defects and create reactive fragments, leading to chemisorption. In this work, an electrospray ion beam deposition (ES-IBD) system is employed to carry out the modification in high vacuum. Singly charged cations of 4,4'-azobis(pyridine) are shown to reactively land on mechanically exfoliated and chemical vapor deposited graphene at moderate to high coverage. The resulting morphology, electronic transport properties, and vibrational spectra of the pyridine-functionalized surfaces are presented. These experiments highlight a facile approach for the controlled modification of graphene with a range of new molecules otherwise unreactive toward graphene by existing conventional methods.

O 36.46 Tue 18:30 P1

**All-carbon vertical van der Waals heterostructures: Non-destructive functionalization of graphene for electronic applications** — Miroslaw Woszczyna[1], •Andreas Winter[2], Miriam Grothe[1], Annika Willunat[2], Stefan Wundrack[1], Rainer Stosch[1], Thomas Weimann[1], Franz Ahlers[1], and Andrey Turchanin[2] — [1]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [2]Faculty of Physics, University of Bielefeld, 33615 Bielefeld, Germany

We present a route to non-destructive functionalization of graphene via assembly of vertical all-carbon van der Waals heterostructures. To this end, we employ single-layer graphene (SLG) sheets grown by low-pressure methane CVD on Cu foils and large-area dielectric ˜1 nm thick amino-terminated carbon nanomembranes (NH2-CNMs) generated by electron-beam-induced crosslinking of aromatic self-assembled monolayers. We encapsulate SLG sheets on oxidized silicon wafers with NH2-CNMs via mechanical stacking and characterize structural, chemical and electronic properties of the formed heterostructures by Raman spectroscopy and X-ray photoelectron spectroscopy as well as by electric and electromagnetic transport measurements. We unambiguously show that functional amino groups are brought in close vicinity of the SLG sheets and that their transport characteristics are not impaired by this functionalization; moreover, we demonstrate a functional response of the heterostructure devices to the protonation of the amino groups in water.

O 36.47 Tue 18:30 P1

**Plasmons in graphene bilayers** — •Phillipp Reck[1], Sam Shallcross[2], and Oleg Pankratov[2] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Lehrstuhl für Theoretische Festkörperphysik, FAU Erlangen

Plasmons are the fundamental collective excitations in the electron system which underlie various many-body phenomena. In two dimensions, plasmons have a square root dispersion. For a double layer system an additional linear branch arises which features a finite gap at q=0 which is due to the interlayer tunneling [1]. Multilayer graphene stacks offer an interesting possibility for realizing such systems. Moreover, stacks with mutually rotated layers present a novel 2D system which is periodically modulated due to the moiré pattern [2]. It was found [3] that the moiré potential alters the one particle spectrum and induces Anderson-type localization at certain energies.

Our work aims at exploring the many-particle effects in these moiré systems, where at first we investigate plasmons in the RPA, using the low energy, homogeneous Mele Hamiltonians [4]. We find qualitatively the same results as in 2DEG. To include the inhomogeneity effects of the moiré potential we shall accordingly adopt the RPA scheme by including the most important coupling reciprocal vectors of the moiré periodicity [3].

[1] S. Das Sarma and E. H. Hwang, Phys. Rev. Lett. 81, 4216 (1998)

[2] S. Shallcross et al, PRB 81, 165105 (2010)

[3] S. Shallcross et al, PRB 87, 245403 (2013)

[4] E. J. Mele, PRB 81, 161405(R) (2010)

O 36.48 Tue 18:30 P1

**"white graphene" on Ag(001)** — •Samuel Grandthyll, Karin Jacobs, and Frank Müller — Saarland University, Experimental Physics, D-66041 Saarbrücken

Monolayers of boron nitride (white graphene/h-BN) were grown via chemical vapor deposition of borazine on Ag(001) and characterized by X-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED). "The growth of h-BN on Ag(001) is the same as previously demonstrated for Ag(111), giving evidence that for weakly interacting transition metal surfaces the surface symmetry has no distinct impact on the h-BN growth." [1]

[1] F.Müller, S.Grandthyll, Surf. Sci. 617 (2013) 207.

O 36.49 Tue 18:30 P1

**Hybrid heterostructures of zero-dimensional and two-dimensional carbon** — Zhikun Zheng[1,2], Xianghui Zhang[1], •Christof Neumann[1], Andreas Winter[1], Henning Vieker[1], Wei Liu[3], Marga Lensen[2], Armin Gölzhäuser[1], and Andrey Turchanin[1] — [1]Faculty of Physics, University of Bielefeld, 33615 Bielefeld — [2]Department of Chemistry, Technical University of Berlin, 10623 Berlin — [3]Physical Chemistry and Electrochemistry, Technical University of Dresden, 01062 Dresden

Van der Waals heterostructures of free-standing two-dimensional (2D) materials open many avenues in the experimental physics and materials science of nanomaterials as they reveal unusual properties and phenomena. Here we present the fabrication of novel hybrid 0D/2D carbon-based heterostructures consisting of ~1 nm thick bifacial Janus Nanomembranes(JNMs) selectively functionalized with fullerenes (C60) or gold nanoparticles (AuNP) on one or both faces. We characterize the physical and chemical properties of the JNM/(C60-JNM)n stacks with n=1, 2, 3 and 4 and individual C60-JNM-AuNP sheets in their supported and free-standing states by optical microscopy, helium ion microscopy (HIM), X-ray photoelectron spectroscopy (XPS) as well as by bulge tests with an atomic force microscope (AFM). We discuss these results and the possible application areas of the engineered hybrid heterostructures in nanotechnology.

O 36.50 Tue 18:30 P1

**Ion Beam Characterisation with Graphene** — •Igor Zagoranskiy, Roland Kozubek, Oliver Ochedowski, and Marika Schleberger — Universität Duisburg-Essen, Duisburg, Deutschland

In ion irradiation experiments material modifications due to ion impacts are often studied as a function of fluence. A precise knowledge of the beam homogeneity and the spot size of the beam is therefore of utmost importance for the experiment. While the spot size analysis can be performed using a Faraday cup, the homgeneity has to be determined using a spatially resolving detector. These detectors are expensive and not applicable for every experimental setup. In our contribution we demonstrate that CVD graphene in combination with $\mu$-Raman spectroscopy mapping can be applied as an ion beam detector which can be used to determine the fluence and beam homogeneity on the micron scale.

As an example we present data from an experiment where we irradiated a CVD graphene sample with an ion beam of highly charged $Xe^{35+}$ particles (260 keV). By analysing the D-band originating from the ion induced defects, the beam homogeneity, spot size and the actual size of the ion-induced defects can be determined.

O 36.51 Tue 18:30 P1

**Damage in graphene and single layer hexagonal boron nitride due to electronic excitation induced by highly charged ions** — •Roland Kozubek, Johannes Hopster, Oliver Ochedowski, and Marika Schleberger — Universität Duisburg-Essen, Duisburg, Deutschland

In this work, we demonstrate that single layers of exfoliated graphene sustain significant damage from irradiation with slow highly charged ions of different charge states ($q$ = 28-42). By atomic force microscopy in lateral force mode we have observed nontopographical frictional defects induced by single ion impacts. To compare these results, we have repeated the experiment with single layers of hexagonal boron nitride (SL-hBN), which is an insulator with a bandgap of 5.5 eV. One can see, that the threshold potential energy for defect creation in graphene is much smaller than in SL-hBN, which can be explained by the classical over-the-barrier model. Here, the time of flight of the ion above the surface is the key parameter, which is varied in further studies by using different projectile velocities. From these experiments we expect to be able to create large defective areas at low kinetic energies. In order to achieve this, a novel deceleration system was installed and tested at our setup.

O 36.52 Tue 18:30 P1

**Two-photon photoemission study of gold-intercalated graphene on Ir(111)** — •David Nobis, Daniel Niesner, and Thomas Fauster — Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

We have investigated gold-intercalated graphene on Ir(111) as well as gold on clean Ir(111) using UV photoelectron spectroscopy (UPS) and two-photon photoemission (2PPE). Up to 5 monolayers (MLs) of gold were intercalated at several temperatures.

The measured work function of the Au/Ir system approaches the value of Au(111) after the deposition of 4 MLs of gold. In the graphene-covered case the work function (4.88 eV with 5 MLs gold) remains larger than expected [1]. The UPS spectra of Au/Ir(111) show a gold-related, upward-dispersing surface state around 0.47 eV below the Fermi level.

In the 2PPE spectra two image-potential states (IPS) are found. The second IPS shows a resonant transition from the Au surface state. The energetic positions of the IPS in combination with the large work function is evidence for incomplete intercalation of the gold. From the energetic spacing of the IPS the local work function of the intercalated areas is extrapolated to 4.69 eV which agrees with the calculated value of 4.74 eV [1]. With this local work function the binding energies of the first two IPS (0.85 eV and 0.21 eV) agree well with those measured on other graphene-covered noble-metal surfaces [2].

[1] Khomyakov, P. A. *et al.*, Phys. Rev. B **79** (2009) 195425

[2] Nobis, D. *et al.*, Phys. Rev. B **88** (2013) 195435

O 36.53 Tue 18:30 P1

**Doping on Epitaxial Graphen on SiC with Molecular Adsorbates** — •Martina Wanke[1], Anton Tadich[2], Mark Edmonds[3], Lothar Ley[4], Felix Fromm[1], Yaou Smets[3], Christian Raidel[1], Christian Heidrich[1], Zoran Mazej[5], John Riley[3], Chris Pakes[3], and Thomas Seyller[1] — [1]TU Chemnitz, Insitut für Physik, Germany — [2]Australian Synchrotron, Soft-X-ray-Beamline, Clayton, Victoria, Australia — [3]La Trobe University, School of Physics, Bundoora, Victoria, Australia — [4]FAU Erlangen-Nürnberg, Institut für Festkörperphysik, Erlangen, Germany — [5]Joseph Stefan Institute Ljubljana, Slovenia

Molecular doping of epitaxial graphene and quasi-freestanding graphene on SiC(0001) was used to tune the doping type character. Epitaxial graphene on SiC shows a strong intrinsical n-type character [1, 2]. It was possible not only to achieve charge neutrality as it was shown for F4-TCNQ [3,4], but to effectively p-type dope graphene by using of C60F48. While quasi-freestanding graphene is already p-type doped, it was possible to increase the amount of p-type doping. Angle-resolved photoemission was used to determine the amount of doping [3,4,5,6].

[1] T.Ohta,et al.,Science 313,951(2006). [2] J.Jobst,et al.,PRB 81,195434(2010). [3] W.Chen,et al.,JACS 129,10418(2007). [4] C.Coletti,et al.,PRB 81,235401(2010). [5] A.L.Walter,et al.,APL 98,184102(2011). [6] A. Tadich, et al., APL 102, 241601 (2013).

O 36.54 Tue 18:30 P1

**The Effects of Disorder and Defects on the Electronic Structure of Graphene** — •Jonathan Parnell[1], Sina Habibian[1], Klaus Kern[1,2], and Christian Ast[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne

A high electron mobility is one of the hallmarks of the two-dimensional graphene system. However, disorder and defects reduce the electron mobility, which places constraints on the different ways graphene can be modified. We simulate the effects of disorder and defects within graphene lattices on the electronic structure. For this we employ a simple real space tight-binding model. These simulations allow us to directly correlate theory and experiment by comparing the calculated results with angular resolved photo-emission data. In this way we can make a quantitative assessment of the density of the different types of defects with their signatures in the electronic structure.

O 36.55 Tue 18:30 P1

**many-body interactions in the sigma band of graphene** — •federico mazzola[1], justin wells[1], rositza yakimova[2], soren ulstrup[3], jill miwa[3], richard balog[3], marco bianchi[3], mats leandersson[4], johan adell[4], philip hofmann[3], and thiagarajan balasubramanian[4] — [1]Department of Physics, Norwegian University of Science and Technology (NTNU), N-7491 Trondheim, Norway — [2]Department of Physics, Chemistry, and Biology, Linkoping University, S-581 83 Linkoping, Sweden — [3]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark — [4]MAX IV Laboratory, Lund University, P.O. Box 118, 221 00 Lund, Sweden

Contrary to the case of Graphene's pi band structure, the deeper lying sigma bands have attracted little attention. Here we present a detailed study of the sigma band structure using angle resolved photoemission spectroscopy (ARPES). Graphene is prepared on different substrates and it is compared with graphite and quasi free standing graphene (graphene which is lifted up by oxygen intercalation after growth on Ir(111)). We find that such bands hide an unexpected large interaction close to the Gamma-bar point. A 'kink' deviates the band from the expected dispersion of a non-interacting band, and a corresponding broadening of the line width is seen. The experiment is supported by a numerical simulation of the many-body interaction, such that the nature of the kink can be probed. We conclude that electron phonon coupling plays a significant role and can satisfactorily account for the observed strong kink.

O 36.56 Tue 18:30 P1

**An STM-study on the Electronic Properties of epitaxial Graphene using Thermovoltage Effects** — •Philip Willke[1], Thomas Druga[1], Alexander Schneider[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Lehrstuhl für Festkörperphysik, FAU Erlangen, D-91058, Germany

We study the electronic properties of epitaxial-grown mono- and bilayer graphene on SiC by locally mapping the thermovoltage: This quantity is obtained by compensating a finite current present due to the temperature difference between sample and tunneling tip by adjusting the tip-sample voltage. According to theory, this property is sensitive to the change in LDOS at the Fermi level. [1] Recently, it was demonstrated that thermovoltage experiments on epitaxial-grown graphene can be used to distinguish between different domain structures induced by wrinkles. [2] By mapping the thermovoltage in a low-temperature STM operating at 6 K, we can comfirm the theoretical predictions given in [1] by comparing high-resolution spectroscopy and thermovoltage measurements. Moreover, we obtain information on the electron scattering behaviour on monolayer and bilayer graphene with the help of Fourier spectroscopy and we can also identify irregularities in the interface layer. This work was supported by SPP 1459 "Graphene".

[1] J. A. Stovneng and P. Lipavsky, Phys. Rev. B 42, 9214-9216 (1990)

[2] J. Park et al., Nanoletters 13(7) 3269-3273 (2013)

O 36.57 Tue 18:30 P1

**An influence of parallel electric field on the dispersion relation of graphene - a new route to Dirac logics** — Jakub Sołtys[1], Stanisław Krukowski[1,2], Jolanta Borysiuk[3,4], and •Jacek Piechota[1] — [1]ICM, University of Warsaw, ul. Pawińskiego 5a, 02-106 Warszawa, Poland — [2]Institute of High Pressure Physics, Polish Academy of Sciences, ul. Sokołowska 29/37, 01-142 Warsaw, Poland — [3]Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warsaw, Poland — [4]Faculty of Physics, University of Warsaw, ul. Hoza 69, 00-681 Warsaw, Poland

Ab initio density functional theory (DFT) simulations were used to investigate an influence of an electric field, parallel to single and multilayer graphene, on its electron dispersion relations close to the K point. It was shown that for both single layer and AAAA stacking multilayer graphene under an influence of a parallel field the dispersion relations transform to nonlinear ones. The effect, associated with the hexagonal symmetry breaking, opens a new route to high speed transistors and logical devices working in the Dirac regime. The implementation of such a device is presented.

O 36.58 Tue 18:30 P1

**Study of Spin-Polarized Behaviour in Cobalt Decorated Graphene** — •Eamon McDermott[1], Paul Bazylewski[2], Gap Soo Chang[2], and Peter Blaha[1] — [1]Institute of Materials Chemistry, Vienna University of Technology, Austria — [2]Department of Physics & Engineering Physics, University of Saskatchewan, Canada

Advances in sub-monolayer PVD deposition of metals on graphene have allowed us to consider the possibility of decorating graphene with magnetic species in the hope of controlling its electronic structure. Density Functional Theory calculations performed using WIEN2k, a scalar-relativistic, all-electron LAPW code, shows an opening of the band-gap of model Co-graphene systems, including those with oxidized Co and Co dimer decoration. When force-relaxed, the graphene layer remains unbuckled, even in the presence of a Co surface underneath the decorating atoms. Additionally, states near the Fermi level become spin polarized, suggesting the possibility of fabricating half-metallic Co-graphene devices.

O 36.59 Tue 18:30 P1

**Crystallographic Order and Decomposition of $[\mathbf{Mn}_6^{\mathbf{III}}\mathbf{Cr}^{\mathbf{III}}]^{3+}$ SMMs deposited on Various Substrates Analyzed by Means of KPFM and nc-AFM** — Aaron Gryzia[1], •Timm Volkmann[1], Armin Brechling[1], Ulrich Heinzmann[1], Veronika Hoeke[2], and Thorsten Glaser[2] — [1]Molecular and Surface Physics, Bielefeld University — [2]Anorganic Chemistry I, Bielefeld University

$[\mathbf{Mn}_6^{\mathbf{III}}\mathbf{Cr}^{\mathbf{III}}]^{3+}$ Single-Molecule Magnets (SMMs) consist of seven metal ions in its center and organic compounds and ligands in the periphery. On surfaces such as e.g. mica and HOPG, these organic parts and charge of 3+ play an important role regarding the adsorption of the molecule. For charge neutrality $[\mathbf{Mn}_6^{\mathbf{III}}\mathbf{Cr}^{\mathbf{III}}]^{3+}$ needs thus counterions. The resulting dipole moment of the SMM layer influences the local contact potential difference (LCPD). We are able to determine the LCPD of the sample by using frequency modulated Kelvin Probe Force Microscopy (FM-KPFM) at UHV conditions. By means of molecular resolved nc-AFM we found a two-fold symmetry close to a four-fold symmetry in the structure of the on HOPG absorbed SMM monolayer. The two lateral dimensions period matches the size of the molecule whereas these layers heights resemble the SMM's height. In addition we also observed layers with half the height of the molecules besides those of the full height. We interpret this observation as decomposition of $[\mathbf{Mn}_6^{\mathbf{III}}\mathbf{Cr}^{\mathbf{III}}]^{3+}$ into its molecular building blocks. These layers show a higher LCPD than the layers with full molecular height.

O 36.60 Tue 18:30 P1

**Bottom-up creation of metal-organic magnetic molecules based on cyclooctatetraene** — •Hasmik Harutyunyan[1] and Daniel Wegner[2] — [1]Westfälische Wilhelms-Universirät Münster — [2]Westfälische Wilhelms-Universirät Münster

Single molecule magnets (SMM) are metal-organic complexes where the spin is mostly carried by transition-metal atoms (3d or 4f), while the coupling is mediated by organic ligands. Due to their large size it is very difficult to deposit SMMs onto a surface under ultrahigh vacuum conditions. An alternative way is the creation of magnetic molecules in a bottom-up fashion. Here we show that single cyclooctatetraene (COT) molecules can be connected to isolated 3d-transition metal atoms (Fe, Co) by self-assembly or via atomic manipulation using a scanning tunneling microscope (STM at low temperature. Experiments have been performed on a Au(111) and a Ag(100) substrate. We compare the structural and electronic properties as gained from STM and tunneling spectroscopy (STS). The results will also be compared with theoretical predictions, and a strategic route toward COT-based SMMs will be shown.

O 36.61 Tue 18:30 P1

**Total Internal Reflection Ellipsometry to detect ultrathin adsorbed films** — •Lei Wang, Igor Siretanu, Michèl Duits, and Frieder Mugele — Physics of Complex Fluids, MESA+ Institute for Nanotechnology, University of Twente P.O. Box 217, 7500 AE Enschede, The Netherlands

To understand the adsorption/desorption of polar components of crude oil (model "asphaltene") onto polar (model "rock") substrates, is of great importance for optimizing the enhanced oil recovery (EOR) process via low salinity water flooding. However, much is still unknown from the molecular aspects about this process, and many components have to been screened. Total Internal Reflection Ellipsometry (TIRE) is capable of detecting ions or small molecules adsorbed at solid-liquid interfaces. In this work, the TIRE setup integrated with combinatorial microfluidics, enables parallel measurements on one substrate, making it a fast screening technique. Detection limit of this setup is 0.2 ng/cm2, and the sensitivity is demonstrated via the adsorption of Ca2+ at silica-water interfaces. Experimental evidences show that these adsorbed calcium ions enable the adsorption of Hexanoic Acid (HA), and the adsorbed HA film desorbs gradually when decreasing the salinity of flooding solutions, which is in consistent with the observations in EOR.

O 36.62 Tue 18:30 P1

**Computational screening of functionalized zinc porphyrins for dye sensitized solar cells** — •Kristian Baruël Ørnsø, Juan Maria Garcia-Lastra, and Kristian Sommer Thygesen — Center for Atomic-scale Materials Design, Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

The search for sustainable energy sources has been intensified during the past years and Dye Sensitized Solar Cells (DSSC) have since the emergence of the first efficient system in 1991[1] received extensive attention due to the promising nature of these in terms of cost efficiency and flexibility.[2] Commonly, either zinc porphyrins or ruthenium based dyes are used combined with the I-/I_3- redox pair as electrolyte in an acetonitrile solvent. The advantage of the porphyrin based dyes are the large absorption of visible light and the straightforward customizability by introducing side groups. We exploit this feature by presenting the calculated frontier energy levels, orbitals, and optical gaps for 1029 systematically functionalized zinc porphyrin dye candidates. Based on this we investigate trends in the selective tuning of energy levels and orbital shapes and estimate a (loss-less) DSSC level alignment quality of the candidate molecules.[3]

References: [1] B. O'Regan, and M. Grätzel. Nature, 1991, 353, 737-740. [2] A. Hagfeldt, G. Boschloo, L. Sun, L. Kloo, and H. Pettersson. Chem. Rev., 2010, 110, 6595-6663. [3] K. B. Ørnsø, J. M. Garcia-Lastra, and K. S. Thygesen. Phys. Chem. Chem. Phys., 2013, 15, 19478-19486.

O 36.63 Tue 18:30 P1

**Tuning the conductance of an unimolecular organic junction** — •Bogdana Borca[1], Verena Schendel[1], Ivan Pentegov[1], Ulrike Kraft[1], Hagen Klauk[1], Peter Wahl[1,2], Uta Schlickum[1], and Klaus Kern[1,3] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [2]School of Physics & Astronomy, University of St Andrews, St Andrews, KY16 9SS, UK — [3]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

To improve and realize future molecular based electronic devices, a good understanding of electronic properties at the individual molecular level and possible ways to tune the intrinsic properties of the charge transport through unimolecular junctions are needed. Scanning Tunneling Microscopy and Spectroscopy (STM/STS) represent an ideal tool to characterize and manipulate single atoms and molecules on surfaces. We investigate the behavior of the conductance of pentacene and one of its thioacenes derivatives, thiotetracen, with a low temperature (6.7K) STM. The organic molecules are thermally evaporated under UHV conditions on a clean Cu(111) surface. The submolecular resolution of the STM allows contacting individual molecules at the desired site and measure the flow of the electrical current through this metal-molecular-metal junction. In terms of conductance, a difference is observed between pentacene and the sulfur-containing structure. In addition, the functionalized side of the thiotetracene molecule may be bonded to a metallic adatom or to a molecule, varying the conductance in this way by a gating-like mechanism.

O 36.64 Tue 18:30 P1

**Functionalization of 6H-SiC(0001) and quartz surfaces with benzo[ghi]perylene-1,2-dicarboxylic anhydride dye through different organic linker molecules** — •Deb Kumar Bhowmick[1], Manfred Bartsch[1], Linda Stegemann[2], Cristian A. Strassert[2], and Helmut Zacharias[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Center for Nanotechnology (CeNTech), Westfälische Wilhelms-Universität, Münster, Germany

Due to different band gaps of semiconductors which control the electronic interactions between substrates and adsorbates, the hybrid semiconductor-organic interfacial systems have versatile applications like transistors, microelectronics, and biosensor. The covalent functionalization gives the stability to the hybrid system [1]. In this study we have chemically functionalized benzo[ghi]perylene-1,2-dicarboxylic anhydride dye on 6H-SiC and quartz surfaces through three different silane linker molecules, e.g., 11-aminoundecyl triethoxysilane (AUDTES), 3-aminopropyl triethoxysilane (APTES), para-aminophenyl trimethoxysilane (PAPTMS). These linkers have different electron conductivities [2]. These systems are characterized by ATR-IR and XPS, and are further studied by confocal fluorescence microscopy. These fluorescence measurements show a gradual decrease of the fluorescence lifetime from 7.6 ns to 1.3 ns from a non-conductive to a conductive linker.

[1] M. Auernhammer, et al., Applied Physics Letters 100, 101601 (2012) [2] D. K. Bhowmick, et al., Small 8, 592 (2012)

O 36.65 Tue 18:30 P1

**Surface melting of ice** — •M.Alejandra Sánchez[1], Marc-Jan van Zadel[1], Patrick Bisson[2], Mary J. Shultz[3], Mischa Bonn[1], and Ellen H.G. Backus[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Dartmouth College, Thayer School of Engineering at Dartmouth, Hanover, USA — [3]Laboratory for Water and Surface Studies, Chemistry Department, Tufts University, Medford, USA

Although ice is omnipresent on earth and in the atmosphere, its surface is poorly understood. It is well-known that a liquid-like layer is present on the surface of ice far below the bulk melting temperature of ice. However, there is intense debate on the microscopic nature of this interfacial melt. By using single crystal ice samples and Sum Frequency Generation (SFG) surface-specific vibrational spectroscopy, we aim to elucidate the nature of this layer. With SFG we obtain the vibrational spectrum of solely the interfacial molecules. Single Ih crystals rods of 2.5 cm diameter with a length of 20 cm are grown in a homebuilt ice machine based on the Bridgeman-Stockbarger method. By comparing SFG spectra at different temperatures varying from liquid water to ice, we obtain information about the hydrogen bond strength, and thus the nature, of the interfacial water molecules. Preliminary results show that at 258 K the water molecules are more strongly bonded than in liquid water at 293 K. In the future we will perform time resolved-SFG to elucidate the reorientational dynamics of the molecules at different temperatures, which gives additional information about the molecules' binding strength.

O 36.66 Tue 18:30 P1

**Experimental and theoretical studies of water orientation at the CaF2 interface at different pH.** — •Maria Jose Perez-Haro[1], Remi Khatib[2], Mischa Bonn[1], Marialore Sulpizi[2], and Ellen H.G. Backus[1] — [1]Max Planck Inst Polymer Res, D-55128 Mainz, Germany — [2]Johannes Gutenberg Univ Mainz, Dept Phys, D-55099 Mainz, Germany

The molecular arrangement of water molecules at solid-aqueous interfaces is important in numerous areas of science. It is very challenging to obtain molecular insights into this type of interfaces. We present here a combined experimental and theoretical approach to obtain those molecular insights into water at the interface between CaF2 and aqueous solutions at different pH.

The experimental results have been obtained with the surface-sensitive spectroscopy technique Vibrational Sum Frequency Generation (SFG), and the recently developed expansion of this technique: phase-sensitive SFG. The vibrational spectrum of the interfacial water molecules thus obtained with SFG reflects the organization and arrangement of interfacial water. We have unraveled the structure, including the absolute orientation of the water molecules at the interface. We clearly see an orientation inversion, 'flip-flop', of the water molecules as the pH of the aqueous phase is changed from acidic to alkaline. The experimental spectra are compared to calculated spectra obtained from first principles molecular dynamics simulations. This comparison provides new insight in the molecular species present at the interface.

O 36.67 Tue 18:30 P1

**Porous glass - epoxy interfaces investigated with an Atomic Force Microscopy** — •Aleksander Ostrowski, Marlena Filimon, Jörg Baller, and Roland Sanctuary — Laboratory for the Physics of Advanced Materials, University of Luxembourg

There has been a great interest in the field of interphases and interfaces in recent years. The understanding of phenomena occurring on the border of two materials is crucial in development of modern compounds. In this work we present the results of investigation performed for the porous glass * epoxy resin systems. The epoxy applied on porous glass penetrates its pores with an extent dependent on the pore size, temperature and epoxy components mixing ratio. Our study presents characterization of porous-glass/epoxy interfaces with the use of Atomic Force Microscopy.

O 36.68 Tue 18:30 P1

**Porous glass - epoxy interfaces investigated with an Atomic Force Microscopy** — •Aleksander Ostrowski, Marlena Filimon, Jörg Baller, and Roland Sanctuary — Laboratory for the Physics of Advanced Materials, University of Luxembourg

There has been a great interest in the field of interphases and interfaces in recent years. The understanding of phenomena occurring on the border of two materials is crucial in development of modern compounds. In this work we present the results of investigation performed for the porous glass - epoxy resin systems. The epoxy applied on porous glass penetrates its pores with an extent dependent on the pore size, temperature and epoxy components mixing ratio. Our study presents characterization of porous-glass/epoxy interfaces with the use of Atomic Force Microscopy.

O 36.69 Tue 18:30 P1

**STM and AFM investigations of [OMIm]Tf2N on Graphite** — •Rene Gustus[1,2], Timo Carstens[1], Oliver Höfft[1], and Frank Endres[1] — [1]Institut für Elektrochemie, TU Clausthal, D-38678 Clausthal-Zellerfeld, Germany — [2]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, D-38678 Clausthal-Zellerfeld, Germany

Electrochemical reactions can always be explained by the interaction of an electrochemically active solution with a solid surface. Besides aqueous solutions, Ionic Liquids (IL) have become an integral part of scientific research especially in electrochemistry but also in different fields of research like catalysis and solar cells, to name only a few. In this regard the physical and chemical properties of the liquid/solid interface like the adsorption mechanisms or the structure formation of the IL near the solid surface are of great interest. Here we investigated the interaction of [OMIm]Tf2N with a graphite surface (Highly Ordered Pyrolitic Graphite - HOPG) by means of scanning tunnelling (STM) and atomic force microscopy (AFM). In a first step in-situ STM measurements in an electrochemically controlled environment were performed. In addition we studied the adsorption of monolayers of [OMIm]Tf2N under UHV conditions. Therefore IL films with different thicknesses were prepared on clean HOPG by evaporation in UHV and were subsequently investigated by STM and AFM using especially force distance curves to study a potential layering of the IL at the interface.

O 36.70 Tue 18:30 P1

**Characterization of 1-octyl-3-methyl-imidazolium chloride interfaces with Photoelectron Spectroscopy and Metastable Induced Electron Spectroscopy** — •Marcel Marschewski[1], Wolfgang Maus-Friedrichs[1], Volker Kempter[1], Angela Ulbrich[2], Stefan Krischok[2], Frank Endres[3], and Oliver Höfft[3] — [1]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Physik und Institut für Mikro- und Nanotechnologien, TU Ilmenau, 98684 Ilmenau, Germany — [3]Institut für Elektrochemie, TU Clausthal, 38678 Clausthal-Zellerfeld, Germany

Room temperature Ionic Liquids are a class of materials, which has recently gained enormous interest. Due to the low vapour pressure ionic liquids interfaces can be investigated with photoelectron spectroscopy (UPS/XPS) and metastable induced electron spectroscopy (MIES). In this study we investigate the liquid solid and liquid vacuum interfaces of 1-octyl-3-methyl-imidazolium chloride ([OMIm]Cl). For the analysis of the solid/liquid interface we have prepared monolayers of [OMIm]Cl on Si(100) by vapour deposition at room temperature. The obtained data are compared with results for the multilayer films. The electron spectra of thick [OMIm]Cl films indicate, that the alkyl chain sticks out of the surface. The chlorine induced feature is not detected in the MIES spectra and the anion seems to be completely buried under the alkyl chain. In the monolayer case, due to the visibility of the chlorine feature in MIES, our results indicate a more flat adsorption of alkyl chains of the cation.

O 36.71 Tue 18:30 P1

**The evaporation of nanodroplet on a chemically heterogeneous substrate** — •Jianguo Zhang, Frédéric Leroy, and Florian Müller-Plathe — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie and Center of Smart Interfaces, Technische Universität Darmstadt, Alarich-Weiss-straße 4, D-64287 Darmstadt, Germany

The pinning phenomenon which causes a constant contact line model (CCL) was often experimentally observed in the evaporation of droplet on a substrate. It is usually believed that the pinning was originated from the substrate*s chemical [1] or/and topographical (rough)[2] heterogeneities. The effect of the topographically heterogeneous surface on the evaporation has been investigated recently by deposited a droplet on a pillared surface[3]. The pinning as well as the CCL model resulted from the roughness was confirmed. However, the chemical heterogeneity effect on the evaporation is still unknown. Here, the evaporation of nanodroplet on a chemically striped substrate has been studied by molecular dynamics simulations. Our results indicate that the chemical heterogeneity can indeed cause pinning and the CCL model when the strip width is larger than $2\sigma$ ($\sigma$ is the atom diameter). Moreover, a slip-jump-stick pattern was observed for the motion of the contact line. The mechanisms for each phase of the pattern have been explored.

[1] P. S. Swain and R. Lipowsky, Langmuir, 14(1998), 6772. [2] P. Lenz and R. Lipowsky, Eur. Phys. J. E 1(2000), 249. [3] X. Chen, R. Ma, et al, Phys. Rev. Lett. 109(2012), 116101.

O 36.72 Tue 18:30 P1

**Electrocatalytic activity of structurally well defined AgPt/Pt(111) monolayer surface alloys - correlation between structure and reactivity** — •Stephan Beckord, Albert K. Engstfeld, Sylvain Brimaud, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, 89069 Ulm

Bimetallic surface alloys often show an electrochemical and catalytic behavior very different from that of the respective metal components. This is evident, e.g., in the oxygen reduction reaction (ORR), where Pt is known to be the best single metal catalyst, but modification with transition or noble metals, such as Ni, Co, Cu has been found to result in an improved reactivity.[1]

In this work we report first results on the electrochemical and -catalytic properties of well defined $Ag_xPt_{1-x}$ surface alloys with different amounts of Ag (0% - 100% Ag) on Pt(111). The surface alloys were prepared under ultra high vacuum (UHV) conditions by evaporation of Ag on Pt(111), followed by annealing to 900 K to form a surface alloy. From scanning tunneling microscopy (STM) the atomic distribution in the topmost layer, as well as the abundance of catalytic relevant ensembles (e.g. $Pt_1Ag_2$, $Pt_2Ag_1$) can be determined. Subsequently the surfaces are characterized in an electrochemical flow cell on their ORR activity in sulfuric acid. Finally structural properties are discussed in comparison with electrochemical activity and theoretical predictions and will be compared to findings for $Au_xPt_{1-x}$/Pt(111).[2]

[1] J. Greeley et al., *J.Phys.Chem.* **113** (2009) 4932, [2] S, Brimaud et al., *J.Electroanal.Chem.*, 2013, in press.

O 36.73 Tue 18:30 P1

**Atomistic modeling of solid-liquid interface ordering and its effect on the growth kinetics of metallic alloys.** — •Mohammed Guerdane and Britta Nestler — Karlsruhe Institute of Technology (KIT) Institute of Applied Materials - Reliability of Components and Systems (IAM-ZBS)

The structure of solid-liquid interfaces remains an open question in condensed-matter science. Understanding this structure is of particular importance because its crucial influence on various physical phenomena such as freezing, wetting, and capillary osmosis. We illustrate here how local ordering in a metallic melt (NiZr) can transform into a massive in-plane ordering at the surface of a crystal (bcc Zr) when the solute-centered clusters of the melt match the periodic potential of the crystal surface. Linking molecular dynamics simulation to phase-field modeling allows to estimate quantitatively the influence of the surface effect on the growth kinetics. Furthermore, our study suggests a possibilty to give experimental evidence for the existence of the structural units of the melt by capturing them at suitable interfaces.

O 36.74 Tue 18:30 P1

**Low-temperature UHV-STM investigation of adsorbed $H_2O$ on metal surfaces** — •Martin Schilling, Albert K. Engstfeld, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

A better understanding of the elementary electrochemical/-catalytic processes on bimetallic electrode surfaces requires a detailed understanding of the solid-liquid interface, including the water-solid interaction. The latter has been studied in detail earlier, using model systems consisting of ice layers adsorbed on single crystal metal surfaces.[1]

Following these lines, we investigated the interaction of $H_2O$ with catalytically relevant mono- and bimetallic single crystal surfaces. Here we report *in situ* scanning tunnelling microscopy results obtained at variable temperatures (VT-STM, 95 K - RT). Submonolayers of $H_2O$ were deposited under well defined conditions under ultra high vacuum (UHV) at low temperature ($\sim$ 95 K) on single crystal surfaces such as Au(111) or Ru(0001). Depending on the dosing conditions ($H_2O$ pressure, dosing rate, sample temperature), the thermal treatment and the substrate, the deposited $H_2O$ was found to form monolayer and/or multilayer islands or three-dimensional clusters. Correlations between structure and deposition/post-treatment conditions are discussed.

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O 36.75 Tue 18:30 P1

**Electrocatalytic activity and stability of Pt nanoparticles on Ru(0001) supported graphene** — •Jens Klein, Albert K. Engstfeld, Sylvain Brimaud, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Pt-based catalysts consisting of carbon supported Pt nanoparticles are widely used, e.g. in fuel cell technology, and it is well known that the performance of these catalysts depends sensitively on the size, density, shape and stability of the Pt nanoparticles.

Here we present results of a model study on the activity and stability of small Pt nanoparticles with narrow size distributions and mean sizes between some 10 - 20 atoms and below 3nm, which were grown on Ru(0001)-supported graphene. The graphene monolayers were prepared under ultra high vacuum (UHV) by ethylene decomposition on Ru(0001) at 1050 K. Pt cluster/nanoparticle arrays with well known particle- and size-distributions were formed by physical vapor deposition of Pt and characterized by scanning tunneling microscopy (STM).[1] The electrodes were subsequently transferred to an electrochemical flow cell attached to the UHV system, to investigate their electrochemical properties and the electrocatalytic activity during CO oxidation. In a last step, the samples were transferred back to the UHV for STM characterization, to evaluate the stability of the particles and correlate the results from the electrochemical measurements with the change in particle sizes and distributions.

[1] Y.Han, A.K. Engstfeld, R.J. Behm, J.W. Evans, *J. Chem. Phys.* **138**, 134703 (2013).

O 36.76 Tue 18:30 P1

**Preparation of smooth and unreconstructed Pt(100)-(1x1)** — •Klaus Meinel[1], Florian Schumann[1], Benjamin Köhler[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck Institut für Mikrostrukturphysik, Halle, Germany

Pt(100) is known for its Pt(100)-hex reconstruction where a compressed quasihexagonal top layer is formed. For specific applications, the non-reconstructed quadratic (1×1) structure is desired. Surface reconstruction can be lifted by adsorbates. Using HREELS and LEED we show that upon exposure to Ar sputter gas in the presence of electrons an effective $C_2H_x$ adsorption takes place from the background which immediate lifts reconstruction. In STM, the resulting (1×1) surface appears extremely rough due to numerous two-dimensional islands (size 3 nm) formed by the surplus Pt atoms. Surface smoothing by intralayer diffusion at temperatures above 300 °C fails as the surface reconstruction recovers from small islands. Surface smoothing without reconstruction is attained by activating step edge diffusion at temperatures around 100 °C which promotes Smoluchowski ripening of the islands. When the island size increases to about 10 nm, islands no longer promote the surface reconstruction and allow pronounced Ostwald ripening even at temperatures around 450 °C. This yields a smooth surface which displays only large 2D islands. During annealing the surface remains covered by $C_2H_x$ showing after Ostwald ripening a $(\sqrt{2}\times2\sqrt{2})R45°$ structure. Final cleaning is attained by annealing in $O_2$ atmosphere at 150 °C at which adsorbates desorb as CO and $H_2O$.

O 36.77 Tue 18:30 P1

**Setup of a HHG-ARPES experiment with sub-femtosecond XUV pulses** — •Jürgen Schmidt[1], Sabbir Ahsan[2], Alexander Guggenmos[1], Soo Hoon Chew[1], and Ulf Kleineberg[1] — [1]LMU Physics Department, Munich, Germany — [2]KTH Royal Institute of Technology, Stockholm, Sweden

Attosecond electron streaking spectroscopy from solids using single attosecond XUV pump pulses and few-cycle IR streaking pulses has recently revealed first insight into the temporal dynamics of the photoemission process with unprecedented temporal resolution of 100 as [1]. Due to the inherent nature of the energy streaking of the liberated electrons in the IR polarization field, only electrons emitted perpendicular from the surface have been recorded. Our experimental setup however aims for both time- and angle-resolving photoelectron spectroscopy (TR-ARPES) revealing information about the sub-fs temporal band structure dynamics in energy and momentum space after transient excitation by few-cycle NIR laser pulses. Especially materials with high correlated electron systems (such as high Tc materials, exchange split materials or topological insulators) give indications for electron dynamics on a sub-fs time scale. As a proof of principle experiment we report about the setup and first measurements on a tungsten (110) surface.

[1] Cavalieri et al, Nature 449, 1029 (2007)

O 36.78 Tue 18:30 P1

**Iron surfaces in a sour gas environment** — •Mehmet Ali Ilhan, Mira Todorova, and Jörg Neugebauer — Department for Computational Material Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Low alloyed steels are particularly susceptible to sour gas corrosion, which leads to the formation of iron sulfides. The developing corrosion products typically do not form protective layers and have no passivating effect. Knowledge of the structure, stability and adhesion of such corrosion products is essential to the evaluation and improvement of their protective properties.

To address these questions we study the interactions of S, H and O with the (100) surfaces of bcc Fe by density-functional theory calculations. We find that the competition between adsorbates can cause H to be pushed below the surface, when S occupies the hollow surface adsorptions sites it prefers, while O/H co-adsorption leads to the formation of OH-groups. Increasing S coverage, on the other hand, leads to the formation of a layered structure, with loosely bound interatomic layers, which resembles Mackinawite (tetragonal FeS). The insight we gain from our calculations, regarding the protective behaviour of the forming corrosion products, will be discussed.

O 36.79 Tue 18:30 P1

**Adsorbate nanomesh causes lateral periodicity of segregation: Ab-initio study for *h*-BN on $Pt_{50}Rh_{50}(111)$** — •Wolfgang Heckel[1], Tobias C. Kerscher[1], Roland Stania[2], Irakli Kalichava[3], Juerg Osterwalder[2], Phil Willmott[3], Bernd Schönfeld[4], Thomas Greber[2], and Stefan Müller[1] — [1]Hamburg University of Technology, Institute of Advanced Ceramics — [2]Universität Zürich, Physik-Institut — [3]Paul Scherrer Institut Villigen, Swiss Light Source — [4]ETH Zürich, LMPT

The segregation profile of Pt–Rh surfaces strongly depends on the presence of adsorbates; e.g., at the top layer, the clean surface favors Pt enrichment, yet a small amount of C adsorbates leads to a significant depletion of Pt there [1]. Pt–Rh also serves as a substrate for self-assembled 2d adsorbate layers such as boron nitride (*h*-BN). The experiments on *h*-BN/$Pt_{50}Rh_{50}(111)$ show a corrugated, honeycombed $11 \times 11$ nanomesh adsorbate layer caused by the lattice constant mismatch of substrate and adsorbate. We present an ab-initio study combining DFT data and a cluster–expansion approach with UNCLE [2]. We elucidate the laterally periodic segregation profile of $Pt_{50}Rh_{50}(111)$ caused by *h*-BN. Our results perfectly confirm the experiment: Beneath the pores of the nanomesh the segregation profile shows a strong Rh enrichment, while beneath the wires the topmost layer favors platinum. By this, the *h*-BN layer induces a segregation profile with a lateral periodicity according to its honeycombed nanomesh.

[1] Kerscher et al., Phys. Rev. B **86**, 195420 (2012)

[2] Lerch et al., Modelling Simul. Mater. Sci. Eng. **17**, 055003 (2009)

O 36.80 Tue 18:30 P1

**Antiferromagnetic coupling in $Mn_2$ on Ag(111) induced by H attachment** — •Torsten Sachse[1,2], Nicolas Néel[1,3], Richard Berndt[3], Werner Hofer[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau —

[2]Stephenson Institute for Renewable Energy, University of Liverpool, Liverpool L69 3BX, Britain — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel

Manganese dimers on Ag(111) are investigated with scanning tunneling microscopy (STM) and density functional calculations. Two species of dimers coexist that differ in their apparent height and the absence or presence of submolecular structure. These species can be interconverted by electron and hole injection from the microscope tip. Calculations identify the two kinds of dimers as pristine Mn$_2$ and Mn$_2$H and show that hydrogen attachment to Mn$_2$ leads to marked changes in the dimer electronic and magnetic structure. Simulated constant-current STM images are in good agreement with the experimental data. The calculations further reveal an antiferromagnetic coupling of Mn magnetic moments in Mn$_2$H.

O 36.81 Tue 18:30 P1

**Image-Potential States on close-packed magnetic surfaces** — •Beatrice Andres, Marc Christ, Marko Wietstruk, and Martin Weinelt — Fachbereich Physik, Freie Universität Berlin, 14195 Berlin

The close-packed surfaces of ferromagnetic materials exhibit various surface states. One type are image-potential states (IPS). Located in front of the surface with a part of the probability density inside they overlap with the exchange-split bulk bands. This results in a small exchange splitting in the IPS. Due to spin conservation under laser excitation they act as excellent spin-filters in two-photon photoemission (2PPE) reflecting the spin-dependent properties of the bulk band structure.

We use spin- and time-resolved 2PPE to investigate the $n = 1$ IPS on Gd(0001), Ni(111) and Fe(110) thin films all grown *in situ* on a W(110) substrate. We find the exchange splitting of the IPS scales with a factor of 3 % to that of the valence bands.

The lifetimes of electrons excited to the initially unoccupied IPS show nearly no spin dependence on Ni(111) but differ by a factor of two on Fe(110) depending on the amount of majority and minority decay channels. The temporal evolution of the spin-dependent linewidths in 2PPE serves as an indicator for quasi-elastic scattering rates which were found to be mediated by magnon emission on Fe(001) while we find no influence of magnons on Ni(111).

O 36.82 Tue 18:30 P1

**magnetic properties of iron and cobalt nanostructures fabricated by focused electron induced processing** — •Fan Tu, Martin Drost, Florian Vollnhals, Esther Carrasco, Andreas Späth, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr.3, D-91058, Erlangen, Germany

Thin film nanostructures have wide-spread potential applications. With our specific approach to focused electron beam induced processing (FEBIP), we are able to fabricate clean nanostructures on surfaces with full lithographic control from adsorbed precursor molecules. With metal-organic precursors such as iron pentacarbonyl (Fe(CO)5) and cobalt tricarbonyl nitrosyl (Co(CO)3NO), we report the fabrication of clean metallic nanostructures with lateral dimensions as small as 15 nm[1]. In this contribution, we investigate Fe, Co and mixed Fe/Co nanostructures using laterally resolved X-ray absorption spectroscopy (XAS) to access the spatial chemical composition, and for the characterization of the magnetic properties X-ray magnetic circular dichroism (XMCD) was employed[2]. The bulk composition and the magnetic properties will be presented and discussed.

Supported by the DFG via grant MA 4246/2-1 and Excellence Cluster "Engineering of Advanced Materials (EAM)" at the FAU Erlangen-Nürnberg and two granted beamtimes at the PolLux instrument at the Swiss Light Source (SLS).

[1] M.M. Walz et al., Angw. Chem. Int. Ed., 49 (2010), 4669;

[2] G. Schütz et al., Phys. Rev. Lett., 58(1987), 737.

O 36.83 Tue 18:30 P1

**Magnetic interactions and spin dynamics in one-dimensional ordered alloys at step edges of vicinal Pt surfaces.** — •Oleg P. Polyakov[1,2], Oleg V. Stepanyuk[1,2], Dmitry I. Bazhanov[1,2], Alexander M. Saletsky[1], and Valeri S. Stepanyuk[2] — [1]Faculty of Physics, Moscow State University, GSP-1, Lenin Hills, 119991 Moscow, Russia — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Properties of low-dimensional atomic structures is a subject for intensive experimental and theoretical investigation in recent years. One of the most notable systems for further fundamental investigation are atomic chains and wires deposited on various surfaces [1]. In this work we present the first-principles study of the magnetic behavior in transition metals (TM=Mn, Fe, Co, Ni) based one-dimensional monatomic and alloyed wires on vicinal Pt(111) surfaces which could be deposited at their step edges. We demonstrate that atomic wires can exhibit ferromagnetic or anti-ferromagnetic orderings due to their atomic structure and interatomic exchange interactions between different atoms and atom types (TM-TM, TM-Pt) at step edges. We find that the value of exchange interaction between TM atoms in atomic wires can be drastically changed or switch a sign by Pt atoms incoming from the step edges. Also, we show that magnetic anisotropy energy is strongly affected in that case. The spin-dynamics is investigated by means of kinetic Monte Carlo method based on transition-state theory. This work was supported by the RFBR grant RFBR $N$13-02-01322.

[1] P. Gambardella et al. Nature (London) 416, 301 (2002).

O 36.84 Tue 18:30 P1

**FeNi nanoparticle deposition on a W(110) surface** — •Matthias Werner, Hendrik Bettermann, and Mathias Getzlaff — Institute of Applied Physics, University of Duesseldorf

By a continuously working arc cluster ion source (ACIS), nanoparticles consisting of Fe and Ni with equal amount are prepared and deposited under UHV and soft-landing conditions on a W(110) surface. The composition is defined by the alloy of the anode in the cluster source, in our case it is Fe$_{50}$Ni$_{50}$. Using this preparation procedure the nanoparticles are charged which allows a mass separation by an electrostatic field unit. Our experimental setup enables us to generate particles with diameters from 4 nm to about 15 nm. Size and shape of the deposited nanoparticles are determined by STM as these properties are expected to be mainly responsible for their electronic and magnetic behaviour.

O 36.85 Tue 18:30 P1

**Preparation of 3d nanoparticles by magnetron sputtering and deposition on a W(110) surface** — •Marek Wilhelm, Hendrik Bettermann, and Mathias Getzlaff — Institute of Applied Physics, University of Duesseldorf

The scientific research of nanoparticles is a broad interdisciplinary area of research, development and industrial activity. Our work is focused on the electronic and the magnetic behaviour which depends on the size and structure of particles. This contribution has an emphasis on FeNi alloy nanoparticles deposited on a W(110) surface. The particles are generated by a magnetron sputter source and subsequently mass selected in a quadrupole. Magnetron sputtering is possible due to thin sputter targets. Scanning Tunneling Microscopy (STM) is the main method to study these objects. The whole measurement system works in an ultra high vacuum environment in the order of $5 \cdot 10^{-10}$ mbar. We will report on our first results of this setup concerning size and structual properties of FeNi nanoparticles with diameters up to 5 nm.

O 36.86 Tue 18:30 P1

**Inelastic electron-phonon interaction: towards first principle calculations** — •Florian Rittweger[1], Nicki F. Hinsche[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, DE-06120 Halle — [2]Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, DE-06120 Halle

The many-body effect of the electron-phonon interaction is under investigation for a long time due to its basic influence on the phenomena of superconductivity.

While experimental access is given by ARPES measurements, the theoretical studies are related to the computation of the complex electron-phonon self-energy. Within this approach the renormalization of the electronic band structure and the finite lifetime $\tau$ of the states can be determined and the electron-phonon coupling strength $\lambda$ can be obtained. Usually the calculations of $\tau$, $\lambda$, etc. are done assuming a quasi-elastic scattering process, i.e. only states on the Fermi surface are considered. Within this conventional approach, phenomena like the phonon drag contribution to thermopower, can not be reproduced by first principle calculations.

Going beyond the quasi-elastic assumption we investigate the inelastic electron-phonon interaction using linear response density functional perturbation theory to study the impact on $\tau$, $\lambda$ and transport properties like the electrical conductivity, thermal conductivity and the thermopower. First results and discussions involving simple metals, i.e. Al and Cu, will be presented.

O 36.87 Tue 18:30 P1

**Electron-phonon self-energy in the KKR formalism** — •Carsten Eberhard Mahr, Marcel Giar, and Christian Heiliger — Justus-Liebig-Universität, Gießen, Germany

Electron-phonon coupling is one of the main incoherent inelastic scattering mechanisms in a wide variety of crystalline material systems at room temperature. Therefore, it is necessary to incorporate those effects in any realistic calculation of thermoelectric properties. We do so by extending our Korringa-Kohn-Rostocker (KKR) Green's function formalism code.

Instead of including the electron-phonon coupling in the Kohn-Sham Hamiltonian via an adjusted effective potential $V_{\text{eff}}$, we calculate the Green's function of the 'free' system (i.e., free of electron-phonon coupling) and employ Dyson's equation $G = G_{\text{free}} + G_{\text{free}}\Sigma_{\text{e-ph}}G$ to obtain the dressed Green's function.

The self-energy $\Sigma_{\text{e-ph}}$ is calculated using Keldysh NEGF formalism, which lends itself to a perturbative diagrammatic approach. Within this method it can be shown – ignoring any terms represented by disconnected Feynman diagrams – that at least so-called First Born Approximation is recovered.

O 36.88 Tue 18:30 P1

**Energy level alignment and quantum conductance of functionalized metal-molecule junctions: Density functional theory versus GW calculations** — •chengjun jin[1], mikkel strange[2], troels markussen[1], gemma solomon[2], and kristian thygesen[1] — [1]Center for Atomic-scale Materials Design, Department of Physics, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark — [2]Nano-Science Center and Department of Chemistry, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen Ø, Denmark

We study the effect of functional groups (CH3*4, OCH3, CH3, Cl, CN, F*4) on the electronic transport properties of 1,4-benzenediamine molecular junctions using the non-equilibrium Green function method. Exchange and correlation effects are included at various levels of theory, namely density functional theory (DFT), energy level-corrected DFT (DFT+$\Sigma$), Hartree-Fock and the many-body GW approximation. All methods reproduce the expected trends for the energy of the frontier orbitals according to the electron donating or withdrawing character of the substituent group. However, only the GW method predicts the correct ordering of the conductance amongst the molecules. The absolute GW (DFT) conductance is within a factor of two (three) of the experimental values. Correcting the DFT orbital energies by a simple physically motivated scissors operator, $\Sigma$, can bring the DFT conductances close to experiments, but does not improve on the relative ordering. We ascribe this to a too strong pinning of the molecular energy levels to the metal Fermi level by DFT which suppresses the variation in orbital energy with functional group.

O 36.89 Tue 18:30 P1

**Convergence of different gradient corrected functionals towards accurate prediction of formation energy of solids using experimental database** — •Mohnish Pandey and Karsten Wedel Jacobsen — Center for Atomic-scale Materials Design, Department of Physics, Technical University of Denmark, Denmark

In the work by Lany(Phys. Rev. B 78, 245207 (2008)), GGA(+U) has been used to accurately predict the formation energies of solids using experimental enthalpies by fitting the reference energies of elements. In this work we show that different functionals predict similar formation energies which is close to the experimental values as long as the reference energies are recalculated by fitting the DFT formation energies to the standard experimental enthalpies which shows the general applicability of the fitting scheme. We use PBE,RPBE and PBE+U gradient corrected methods for calculations. Different training and test sets have been used to validate the predictability of the method.

O 36.90 Tue 18:30 P1

**Forces in the FLAPW method revisited** — •Aaron Klüppelberg, Markus Betzinger, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Density functional theory (DFT) is nowadays the workhorse for simulating the electronic and geometric structure of real materials. Forces, i.e., the derivatives of the DFT total energy with respect to atomic positions, are indispensable for any structural optimization. Accurate forces, moreover, enable the calculation of phonon spectra using the finite displacement method and of subsequent quantities such as electron- and magnon-phonon interaction.

We analyze the accuracy of the force computed within the all-electron full-potential linearized augmented plane-wave (FLAPW) method as realized in the `FLEUR` code [1] according to the formalism of Yu *et al.* [2]. As one criterion for the accuracy we employ the drift-force, i.e., the sum of all atomic forces in the unit cell, which should strictly vanish. Another criterion is the quality of the symmetry of the force-constant matrix. We show that both criteria can be fulfilled to an accuracy of $1\mu$Htr/$a_0$ only if (a) the core-electron tails are properly taken into account and (b) a large angular momentum cut-off is applied. We propose a refined formulation of the force that cures the aforementioned demands on the LAPW setup to a great extent. As an example, we present results for MgO and $\mathrm{EuTiO_3}$.

[1] www.flapw.de

[2] R. Yu, D. Singh, and H. Krakauer, Phys. Rev. B **43**, 6411 (1991).

O 36.91 Tue 18:30 P1

**RPA correlation energy calculated within the FLAPW method** — •Markus Betzinger, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

According to the adiabatic-connection fluctuation dissipation theorem the exchange-correlation energy of Kohn-Sham density-functional theory (KS DFT) is expressed in terms of the many-electron density response function. Approximating the latter by the random-phase approximation (RPA) leads to the RPA correlation energy of KS DFT. It has been demonstrated that the RPA describes covalent, ionic, and vdW bonded systems equally well. The main obstacle in calculating the RPA correlation energy is the slow convergence of the KS response function in terms of the orbital basis set and the number of unoccupied states. We present an extension of the recently developed incomplete-basis-set correction (IBC) [1] to the frequency domain, which enables to compute the RPA response function accurately. The IBC, which is based on the FLAPW method, comprises a basis response term that lies in part outside the Hilbert space spanned by the original basis. The convergence of the RPA response function in terms of basis-set size and number of unoccupied states is considerably accelerated by the IBC. We show first results for RPA lattice constants and bulk moduli calculated for a set of prototype materials.

This work is supported by the Helmholtz Postdoc Programme.

[1] Phys. Rev. B **88**, 075130 (2013); *ibid.* **85**, 245124 (2012)

O 36.92 Tue 18:30 P1

**Efficient Path-Integral Molecular Dynamics with High-Order Decomposition of the Boltzmann Operator** — •Igor Poltavsky[1], Kim Kwang[2], and Alexandre Tkatchenko[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Center for Superfunctional Materials, Pohang University of Science and Technology, San 31, Hyojadong, Namgu, Pohang 790-784, Korea

Recently it has become possible to reach the so-called "chemical accuracy" of 1 kcal/mol for the binding energies of small molecules and supramolecular systems, which is an essential prerequisite for predictive first-principles modeling. However, at this level of accuracy another serious issue arises, namely the need to accurately account for the quantum nature of (light) nuclei that plays a vital role in the structure, stability, and dynamical properties of many systems, including water, ice, as well as most biological molecules.

The most widely used tool to study quantum nuclear effects is the imaginary-time path integral (PI) approach which can be easily incorporated into *ab initio* calculations. Here we propose efficient PI molecular dynamics (MD) methods based on third and fourth order decompositions of the Boltzmann operator. These methods decrease the required number of replicas by more than a factor of two comparing to the standard second-order PIMD simulations, while at the same time visibly increasing the accuracy for a wide range of temperatures. Results are shown for model systems and an accurate quantum-mechanical model of the water molecule.

O 36.93 Tue 18:30 P1

**Modified Mott-Wannier Model for Excitons in Atomically Thin Semiconductors** — •Simone Latini, Thomas Olsen, and Kristian S. Thygesen — Department of Physics Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

Despite the numerous extraordinary properties of pristine graphene, its application to (opto)-electronics is problematic due to the lack of a band gap. This issue inevitably requires the systematic research for new materials which combine a strong 2D nature and a semiconducting behaviour. As soon as a band gap is opened, excitonic effects start to play a fundamental role on the optical properties determining, for example, the onset of the optical transitions. The Bethe-Salpeter Equation (BSE) is nowadays the most refined method to quantitatively describe excitons but its applicability is limited to relatively simple systems because of its computational complexity. Here we propose a simple method to estimate the energy of the lowest bound exciton based on a modified Mott-Wannier model. For 2D semiconductors the dielectric function turns out to be strongly dependent on the wave vector and therefore the definition of the value for the dielectric constant to plug into the hydrogenic model has to be revised. This is done accounting for a quasi-2D picture of the exciton. The validity of the method is checked thoroughly benchmarking the binding energies and exciton radii for a large variety of 2D materials against the values obtained from the solution of the BSE. Our method has the merit to both keep the computational cost low and to provide a straightforward physical intuition on excitonic effects.

O 36.94 Tue 18:30 P1

**Effective interactions in the constrained random phase approximation** — •Merzuk Kaltak, Martijn Marsman, and Georg Kresse — University of Vienna, Computational Material Physics

We compare different approaches to the determination of the effective interaction parameters of Hubbard Hamiltonians within the constrained random phase approximation (CRPA) from ab-initio calculations. In addition, we investigate the dependence of the interaction parameters on the choice of the local bases, such as maximally localized Wannier functions (MLWF) and linear combination of atomic orbitals (LCAO).

O 36.95 Tue 18:30 P1

***Ab-initio* calculation of Hubbard *U* parameter for solids** — •Ersoy Sasioglu, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute forAdvanced Simulation, Forschungszentrum Jülich and JARA, 52425Jülich, Germany

The problem of calculating Hubbard $U$ parameter for solids from first-principles has been addressed by several authors and a number of different approaches have been proposed. Among them, the constrained random-phase approximation (cRPA) has recently become the most popular [1]. The basic idea of the cRPA is to define an effective Coulomb interaction $U$ between the localized $d$ ($f$) electrons by restricting the screening processes to those that are not explicitly treated in the effective model Hamiltonian. Using Wannier functions within the FLAPW method [2] we have developed a parameter-free realization of the cRPA method [3]. Employing the cRPA method we have calculated the Hubbard $U$ parameter for different classes of materials such as transition metals [3], half-metallic magnets [4], carbon-based systems [5], and surfaces of metals and insulators [6]. This work has been supported in part by DFG-FOR-1346.

[1] F. Aryasetiawan *et al.*, Phys. Rev. B **74**, 125106 (2006).
[2] www.flapw.de
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[5] T. O. Wehling *et al.*, Phys. Rev. Lett. **106**, 236805 (2011).
[6] E. Şaşıoğlu *et al.*, Phys. Rev. Lett. **109**, 146401 (2012).

O 36.96 Tue 18:30 P1

**Electronic communication through molecular bridges** — •Jonny Proppe and Carmen Herrmann — Institute of Inorganic and Applied Chemistry, University of Hamburg, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany

Various areas of scientific research focus on the concept of electronic communication through molecular bridges as it plays a major role in potentially innovative future devices and as an academic challenge due to its diverse manifestations, in particular exchange coupling between spin centers and macroscopic electrodes connected by single molecules. Recent results suggest a correlation between both mechanisms of communication in certain cases, which is supported by molecular orbital arguments [1,2]. While Ref. [1] provides a first overview, we systematically compare trends and aim at deriving rules to identify instances in which it is possible to transfer knowledge between the areas of molecular magnetism and molecular electronics. For this purpose, we study the influence of chemical modification on the electronic communication of organic diradicals and dithiols. We find that the energy gap between magnetic orbitals in diradicals correlates with the HOMO/LUMO energy gap in dithiols, both affecting the mechanisms of electronic communication. Thus, for certain bridges the kind of exchange spin coupling (either ferromagnetic or anti-ferromagnetic) may determine the conductance for a given molecular structure and *vice versa*.

[1] C. Herrmann, J. Elmisz, *Chem. Commun.* **2013**, *49*, 10456.
[2] M. L. Kirk, D. A. Shultz, D. E. Stasiw, D. Habel-Rodriguez, B. Stein, P. D. Boyle, *J. Am. Chem. Soc.* **2013**, *135*, 14713.

O 36.97 Tue 18:30 P1

**Bandgap engineering in two-dimensional heterostructures** — •Filip Anselm Rasmussen and Kristian Sommer Thygesen — Department of Physics, Technical University of Denmark, Kongens Lyngby, Denmark

Since the discovery of single layer graphene the search for other two-dimensional materials that might have equally interesting properties has begun. Contrary to graphene these materials may be anything from metals to large-gap insulators. Especially the possibility of combining materials with different band gaps may be useful for some applications like field-effect transistors and solar cells. Previously is has been shown that when a molecule comes in close proximity of a metal its energy levels shifts due to increased screening from the metal. To investigate if such an effect is also present in extended two-dimensional systems we have performed first principles calculations on heterostructures consisting of metal-2D insulator-2D semiconductor layers, to estimate the effect of screening from the metal on the semiconductor band gap. To include the effect of the long-range Coulomb interaction we have calculated the quasiparticle energies using the non-self-consistent $G_0W_0$ approximation and we find that the semiconductor band gap decreases from its vacuum value when brought in close proximity of a metal. This shows that it is possible to engineer the band gap of the 2D semiconductor by varying the number of insulating spacer layers.

O 36.98 Tue 18:30 P1

**Intrinsic LiNbO3 point defects from total-energy difference and Slater-Janak transition state calculations** — •Yanlu Li, Simone Sanna, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn, Paderborn, Germany

The formation energies and charge transition levels of the most relevant LiNbO3 point defects, i.e. Nb antisites and Li as well Nb vacancies are studied within density functional theory (DFT). In particular the effects of cell symmetry and the finite size error in calculations using periodic boundary conditions are examined. It is found that in particular the Nb vacancy causes a long-range strain field and requires large supercells for its adequate modeling. The extrapolation to infinitely large supercells decreases the relative stability of the Nb antisite and increases the relative stability of the Nb vacancy with respect to the Li vacancy, indicating the stability of VNb-5 in the wide range of Fermi level positions close to the conduction band minimum.

O 36.99 Tue 18:30 P1

**Semiclassics for matrix Hamiltonians and semiclassical perturbation theory and its use for graphene physics** — •Michael Vogl, Sam Shallcross, and Oleg Pankratov — Lehrstuhl für Theoretische Festkörperphysik Staudtstr. 7-B2 91058 Erlangen

Electrons in graphene based systems are for low energies often described very well by first quantized matrix Hamiltonians, such as the Dirac-Weyl Hamiltonian in the case of single layer graphene. Nevertheless, such Hamiltonians remain, especially for the more complex graphene multilayer systems such as the twist graphene bilayer, very difficult to solve. Semi-classical methods often give great insight into the underlying structure of such complex systems; in particular in terms of semi-classical orbits and 2-forms such as the Berry phase. Following Bolte and Keppeler [1] we derive a general semi-classical method for treating the matrix Hamiltonians that arise in graphene based systems. This is based on an ansatz for the time-dependent Greens function that allows one to effectively bypass the problems of solution matching that, in other approaches, severly curtails the efficiency of the semi-classical approach. This leads, for a $n \times n$ Hamiltonian, to $n$ Hamilton-Jacobi equations, and $n$ *transport equations*. From the latter arises a term that can be separated into a term resembling the Berry phase and a term arising from the coupling between the n classical systems. We implement this scheme for the Bernal bilayer modeled by the full $4 \times 4$ Hamiltonian, as well as exploring how the theory may be implemented for the more complex case of the graphene twist bilayer. [1]J. Bolte & S. Keppeler Phys. Rev. Lett. 81 (1998) 1987-1991

O 36.100 Tue 18:30 P1

**Structure formation on prepatterned surfaces** — •Oleg Buller and Andreas Heuer — Institut für Physikalische Chemie, WWU, Münster

The main focus of our investigations is the analysis of structure formation on prepatterned surfaces of deposited molecules. The resulting self-organisation strongly depends on the chosen conditions such as substrate temperature, flux, concentration or surface geometry. Here we study the structure formation on prepatterned stripes as well as on a prepatterned grid. We use discrete kinetic Monte Carlo simulations. It turns out that in particular the length of the aging period after the deposition process as well as the chosen particle concentration strongly influences the characteristics of the resulting structure. In contrast, the flux is much less relevant since the final structures mainly form during the aging period. We also characterize the stability of the structures. The simulation results are finally compared with corresponding experiments where organic molecules are deposited on prepatterned surfaces.

O 36.101 Tue 18:30 P1

**Catalytic oxidation of HCl over $CeO_2$ within kinetic Monte Carlo simulations** — •Stefano Mattiello[1], Stefan Kolling[1], Christian Heiliger[2] und Herbert Over[3] — [1]Institut für Mechanik und Materialforschung, Technische Hochschule Mittelhessen, Gießen, Germany — [2]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany — [3]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Germany

Understanding of catalytic oxidation of HCl over $CeO_2$ is a challenging task for theoretical as well as experimental solid state physics. In particular, the role of the elementary reaction steps in the entire process is not yet completely understood. Within kinetic Monte Carlo simulations the different reaction steps can be investigated. In order to achieve *ab initio* calculations the input for the simulations, i.e. energy barriers for the microscopic reactions, have to be determined by density functional theory (DFT). For the time being we focus on the oxygen sub-lattice. We investigated the possibility of ad- and desorption of oxygen on the ceria (111)-surface as well as the diffusion of the oxygen vacancies on the surface and in the bulk. In particular the agglomeration of vacancies on the surface has been considered. The competition between the different elementary reactions was also investigated in detail.

O 36.102 Tue 18:30 P1

**CPMD simulations of liquid Sn anodes for solid oxide fuel cells** — •Sebastian Gsänger, Jakub Goclon, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Liquid Sn is a very promising material for anodes in solid oxide fuel cells due to its high robustness toward sulfur contaminations in the gas feed. Very little is known about the bulk and surface chemistry of liquid Sn. Using Car-Parrinello Molecular Dynamics (CPMD) simulations we studied first the structural and dynamic properties of the liquid Sn itself and of dissolved oxygen, sulfur and hydrogen atoms. Subsequently, slabs of liquid Sn were used and the influence of the surfaces on the distribution and diffusion of the impurity atoms was studied. Finally, first molecular dynamics simulations on the interaction of hydrogen and methane gas phase molecules with the liquid Sn surfaces were performed.

O 36.103 Tue 18:30 P1

**Electron-hole pair–vibrational coupling during scattering of HCl/Al(111): TDDFT-MD and model study** — Michael Grotemeyer and •Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, 24098 Kiel, Germany

*Ab initio* simulations using time-dependent density functional theory together with Ehrenfest dynamics for the nuclei have revealed a very efficient energy transfer into substrate electron-hole pair excitations in case of highly vibrationally excited HCl-molecules that scatter at an Al(111) surface. The mechanism of vibrational–electron-hole pair coupling has been traced back to the periodic shift of the LUMO eigenenergy as the HCl bond length oscillates. We present an overview over our results for the energy transfer per vibrational period of the molecule as a function of its initial vibrational excitation energy and molecule-surface separation. The results can be qualitatively recovered by a simple tight-binding model. Notably, the energy dissipation rate goes through a maximum at a certain distance above the surface, *i.e.* not at very close molecule–surface separations. This is different from the steering mechanism suggested by Shenvi *et al.* for NO/Au(111) [1]. The coupling mechanism becomes less efficient for low vibrational excitation energy. We suggest this to explain the in comparison to NO small electronic contribution to the $v = 0 \rightarrow v = 1$ vibrational excitation observed experimentally for HCl-surface scattering [2].

[1] N. Shenvi, S. Roy, J.C. Tully, Science **326**, 829 (2009).

[2] Q. Ran, D. Matsiev, D.J. Auerbach, A.M. Wodtke, Phys. Rev. Lett. **98**, 237601 (2007).

O 36.104 Tue 18:30 P1

**CPMD simulations of oxidized Si clusters** — •Paul Schwarz[1], Carola Kryschi[2], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Physical Chemistry, FAU Erlangen-Nürnberg

The oxidation of small Si clusters was studied by Car-Parrinello Molecular Dynamics (CPMD) simulations in order to obtain reasonable structures for oxygen-passivated clusters with a crystalline Si core with size of about 1 nm. The method of simulated annealing was applied to allow for atomic rearrangements and to find favorable low-energy configurations. The clusters were equilibrated at different temperatures, quenched to room temperature and finally relaxed. By increasing stepwise the amount of oxygen, four types of oxidized $Si_{63}$ clusters with composition of $Si_{63}O_{24}$, $Si_{63}O_{32}$, $Si_{63}O_{48}$, and $Si_{63}O_{68}$ were obtained.

It is found that at low oxidation clusters with crystalline and amorphous Si core are rather similar in energy. The energy of the clusters is lowered by formation of free-standing $SiO_2$ groups at the surface, under the condition that the crystalline core is retained during the simulation. These free-standing $SiO_2$ groups could be precursors for the formation of surface silanone groups. The crystalline core is furthermore stabilized by increasing oxidation. Finally, hydrogen and methyl groups were added at the surface of pure and oxidized Si clusters, with the aim of finding vibrations that could explain the vibronic structure in the photoluminescence spectra of synthesized Si clusters.

O 36.105 Tue 18:30 P1

**Border Search Method - potential energy surface mapping technique alternative to Metadynamics** — •Prokop Hapala and Pavel Jelinek — Institute of Physics , Academy of Sciences of the Czech Republic, Cukrovarnická 10, Prague, 16253, Czech Republic

Mapping of Potential Energy Surface (PES), searching for local and global minima of atomistic systems or paths with minimal energy barrier between these local minima is a long term goal of computational chemistry and material science. We propose novel robust method inspired by Meta-Dynamics [1] providing advantages in several aspects: (a) No force evaluation is needed. (b) Positions in configuration space are sampled systematically and homogeneously. (c) Method setup has less parameters and is easier to control (d) Lowest energy barrier is always found (e) Number of PES evaluations required to reliable exploration of lowest energy path to neighboring local minimum is reduced by prohibiting re-examination of the same area.

[1] B. Ensing, et. al. Metadynamics as a tool for exploring free energy landscapes of chemical reactions. Acc. Chem. Res., 39, 73-81 (2006).

# O 37: Posters: Plasmonics, Electronic Structure and Spin-Orbit Interaction, Semiconductor and Insulator Surfaces, Nanostructures

Time: Tuesday 18:30–22:00 Location: P2

O 37.1 Tue 18:30 P2

**Free-standing gold nanoantennas for enhanced infrared spectroscopy** — •Christian Huck[1], Andrea Toma[2], Frank Neubrech[1,3], and Annemarie Pucci[1] — [1]Kirchhoff-Institute for Physics, Heidelberg, Germany — [2]Istituto Italiano di Tecnologia (IIT), Genova, Italy — [3]4th Physics Institute and Research Center SCoPE, Stuttgart, Germany

Plasmon-polariton excitations of metal nanoparticles can couple to other excitations of similar energy, which gives rise to strong vibrational signal enhancement in the infrared. For a optimization with respect to the enhancement it is necessary to carefully design the optical properties of the antenna, e.g. by the geometry of the structure but also by the supporting substrate. Plasmonic nanostructures prepared on substrates with high refractive indices, such as silicon and zinc sulphide, feature lower quality factors, a lower extinction cross-section and a red-shifted resonance position compared to the low refractive index substrates glass and calcium fluoride. This behavior can be explained by induced screening charges in the substrate, leading to a more damped electron oscillation in the nanorods and thus to lower vibrational signal enhancements in SEIRS. In this contribution we present one way to reduce the undesirable influences of the substrate by fabricating elevated gold nanowires which are only partly in contact with the substrate. We show a comparison of the plasmonic response as well as the SEIRS activity between rods prepared by standard EBL and rods which were additionally treated with reactive ion etching to remove the silicon substrate around the hot-spots of the rods.

O 37.2 Tue 18:30 P2

**Thermal annealing of gold infrared nanoantennas** — •Jochen Vogt[1], Frank Neubrech[1,2], Andrea Toma[3], and Annemarie Pucci[1] — [1]Kirchhoff-Institute for Physics, University of Heidelberg, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [3]Italian Institute of Technology (IIT), Genoa, Italy

For the successful fabrication and application of plasmonic nanostructures, such as nanoantennas, proper material quality is indispensable. Often the material quality strongly affects the plasmonic properties of nanoantennas, which are essential for their application, e.g. for surface-enhanced infrared spectroscopy (SEIRS). In this work we demonstrate that thermal annealing can significantly improve the plasmonic properties of low quality polycrystalline nanowires, fabricated with standard electron beam lithography. Up to a certain temperature, thermal annealing leads to clear blue-shifts in resonance frequency accompanied by strong increases in extinction cross section. Beyond this limit, the annealing turns into a destruction of the nanowires due to the Rayleigh instability. In order to monitor the impact of thermal treatment on the morphology and the plasmonic properties, atomic force microscopy and microscopic infrared spectroscopy, respectively, were performed.

O 37.3 Tue 18:30 P2

**Mechanical control of plasmonic resonances** — •Anja Löhle, Audrey Berrier, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

The control of light-matter interactions in real time deepens our understanding of materials, in particular in the attractive field of plasmonics. The optical properties of plasmonic structures are influenced by geometrical parameters such as shape, size or ordering of the particles, as well as by the material properties of both the environment and of the resonant particle itself. This project proposes the investigation of the active control on plasmonic structures using mechanical stretching. We report on the mechanical tuning of the optical properties of different plasmonic systems, consisting of thin metallic layers or colloidal ensembles on top of a flexible substrate. The samples are uniaxially stretched to modify the inter-particle spacing or to induce changes in the geometry of the thin films. It is shown that it is possible to go from a conductive layer to an insulating regime and back to a conductive state by stretching the substrate and subsequent release of the strain. This is monitored by reflectance measurements associated to spectroscopic ellipsometry where models are applied to extract the complex permittivity of the layers. Understanding of the behaviour of these novel, active materials is crucial to the development of novel technologies and emerging applications.

O 37.4 Tue 18:30 P2

**Magneto-optic surface plasmon resonance of Au/IrMn/Co/Au exchange biased layer systems** — •Sebastian Kübler, Nicolas Müglich, and Arno Ehresmann — Department of Physics, CINSaT, University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

The magneto-optic surface plasmon resonance (MOSPR) in transverse geometry of glass/Au/IrMn/Co/Au/dielectric exchange biased (EB) thin film systems has been studied as a function of the Au-cap layer thickness for the dielectric air and water. The results show that it is possible to achieve either an optimal steepness of the reflectivity as compared to a glass/Au(48 nm)/dielectric layer system or to maximize the magneto-optic activity. As the Au-cap layer thickness is increased the magneto-optic activity is reduced whereas the steepness of the reflectivity in the range of the resonance is raised. The width of the reflectivity curves and the magneto-optic signals are broadened for thin Au capping layers. The presented results demonstrate that the EB system under investigation can be optimized by adjustment of the Au-cap layer thickness for SPR and MOSPR based biosensing applications.

O 37.5 Tue 18:30 P2

**Advantages of a quantum cascade laser for surface enhanced infrared spectroscopy** — •Anton Hasenkampf, Niels Kröger, Annemarie Pucci, and Wolfgang Petrich — Universität Heidelberg, Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg

The main tool for surface-enhanced infrared spectroscopy (SEIRS) is the Fourier transform infrared (FTIR) spectrometer with a globar source. It allows spectroscopy of a sample over a broad spectral range, which in our case covers 1 $\mu m$ to 20 $\mu m$. The disadvantage of this system is very low spectral power density of the globar. This usually is compensated by long measurement times. In this work, we present measurements with an external cavity quantum cascade laser (QCL) with grating in Littrow configuration which is integrated into a scanning microscopy setup. The QCL enables spectral measurements in the range of 1140 to 1430 $cm^{-1}$. The $10^8$ times higher spectral power density as compared to a globar reduces measurement time drastically. Also the detection with a deuterated triglycine sulfate (DTGS) instead of a nitrogen cooled mercury cadmium telluride (MCT) is possible. The tuning range of the QCL of 290 $cm^{-1}$ nicely matches the requirements of SEIRS since, for nanoantennas, the enhancement occurs over a limited spectral range of the same order.

O 37.6 Tue 18:30 P2

**Mueller matrix characterization of three-dimensional gold spiral nanostructures** — •Elvira Mbekwe Pafong, Audrey Berrier, Bruno Gompf, Bettina Frank, Harald Giessen, and Martin Dressel — Physikalisches Institut and Research Center SCoPE, Pfaffenwaldring 57, 70550 Stuttgart

Mueller matrix (MM) spectroscopy is a powerful tool to characterize nanostructures as it provides both amplitude and phase information. The decomposition of the measured MM grants the extraction of all the optical parameters such as linear birefringence/dichroism and circular birefringence/dichroism. However, it is difficult to attribute effective parameters to artificial nanostructures, especially when they are three-dimensional (3D). A full characterization in a large frequency range and broad reciprocal space is therefore necessary. Along with angle-resolved transmission measurements to determine the spectral position and the dispersion of the resonant modes, we perform MM spectroscopy to obtain phase information and compare the optical behaviour to that of conventional crystals. The measured MM elements are compared with simulations based on general oscillator models taking into account the azimuthal and spectral positions of the resonances. We find that the 3D nanospirals exhibit a complex optical response that cannot be reproduced by basic optical properties such as birefringence or optical activity only. Spirals with different geometries are compared in order to extract the optical response intrinsic to their 3D nature. This study sheds light on the complex response of plasmonic nanostructures and is useful for future designs of novel optical devices.

O 37.7 Tue 18:30 P2

**Superlensing in n-doped GaAs investigated by near-field microscopy** — •Markus Fehrenbacher[1], Stephan Winnerl[1], Harald Schneider[1], Jonathan Döring[2], Susanne Kehr[2], Lukas M. Eng[2], Yongheng Huo[3], Oliver G. Schmidt[3], Kan Yao[4], Yongmin Liu[4], and Manfred Helm[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [4]Northeastern University, Boston, USA

It has been shown that materials with negative refractive index n, so-called metamaterials, can be exploited as perfect lenses characterized by a point-to-point projection. In the near-field regime where the distance between object and image is much smaller than the applied wavelength, negative permittivity is sufficient to create such super-resolution images. Those superlenses are based on heterostructures of different chemical composition, where the negative permittivity is induced by phonons. In contrast, in our sample this dielectric behavior is due to the electronic response of a doped GaAs layer sandwiched between two intrinsic layers. This is a simple and elegant way of producing a superlens as its resonant frequency can be controlled simply by varying the dopant level. In our experiments we investigate a sample with a charge carrier concentration tuned for superlensing at a $20\mu$m IR wavelength as explored using a free-electron laser.

O 37.8 Tue 18:30 P2

**Spectral properties of ordered nano-particle assemblies** — •Simon Dickreuter, Emre Gürdal, Dieter Kern, and Monika Fleischer — Institute for Applied Physics, Eberhard Karls University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Plasmonic nano-particles have proven to be useful for many applications like bio-sensing or near-field imaging. But due to their complex nature they are not yet fully understood. In this recently started project, the coupling between colloidal nano-particles is investigated. The plasmonic properties of single gold-colloids are well known, thus we chose gold-colloids as the building blocks for the fabrication of nano-particle assemblies. The techniques of e-beam lithography and diblock copolymer self-assembly are employed to fabricate ordered hole arrays, which can be filled with colloidal nano-particles by using capillary or convective self-assembly. This way controlled assembly of nano-particles inside the holes is possible. By choosing different geometries for the templates, one can fabricate oligomers consisting of a defined number of nano-particles. The assemblies are analyzed by dark-field spectroscopy to see how the coupling of several nano-particles affects the plasmonic resonances they exhibit. The methods of fabrication of the assemblies and first dark-field spectra will be presented.

O 37.9 Tue 18:30 P2

**Near-field optics of conductive ferroelectric domain walls** — •Denny Lang, Susanne C. Kehr, Mathias Schröder, Alexander Haussmann, and Lukas M. Eng — IAPP, George-Bähr-Straße 1, 01069 Dresden

Ferroelectric domain walls (DWs) are planar interfaces of a few nm thickness that separate areas with different spontaneous polarizations. DWs show electric conductivity under certain conditions [1], e.g. when being illuminated by UV light, and thus are interesting as nanometer-scale optoelectronic devices [2]. We investigate the optical response of these topologically novel systems on the nm length scale by means of scattering-type scanning near-field optical microscopy (s-SNOM).

We inspect the domain wall conductivity in z-cut lithium niobate using different scanning probe methods. Firstly, we characterize the general domain structure by conventional piezoresponse force microscopy (PFM) in order to both allocate the exact DW position and quantify the magnitude of polarization in adjacent domains. Secondly, we measure the conductivity of a single DW rendered conductive by UV illumination with conductive atomic force microscopy (c-AFM). Thirdly, we study the optical response of the DW applying s-SNOM at visible and at infrared wavelengths. Here, we expect a near-field contrast since the DW constitutes a conductive singularity within a wide-bandgap insulator.

[1] M. Schröder et al., Adv. Funct. Mater. 22 (18), 3936-3944 (2012)

[2] A. Haussmann et al., Nano Lett. 9 (2), 763-768 (2009)

O 37.10 Tue 18:30 P2

**Self-assembly of gold nanoparticle structures** — •Emre Gürdal, Simon Dickreuter, Dieter Kern, and Monika Fleischer — Institute for Applied Physics, Eberhard Karls University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

In the last decade plasmonic nanoparticle assemblies took an important role in emerging nanotechnologies. Gold particles show resonances in the visible and infrared spectral range and exhibit a very strong near field in their close vicinity. This can be used e.g. for biosensing or optical antennas. Ordered arrays of such particles can be fabricated by using substrates with hole templates. There are several possibilities to fabricate such templates. E-beam lithography on the one hand which provides good control but is time consuming and costly, and the self-assembly of block-copolymers on the other, which is a larger area parallel process. We investigate the accumulation of gold nanospheres into the voids of either e-beam resist or diblock-copolymer layers. For the formation of cylindrical structures on top of a silicon substrate by diblock-copolymers selecting the optimum layer thickness is important. Furthermore it is a challenge to achieve a gold nanosphere monolayer in such cylindrical holes. An overview over different methods for fabricating gold nanosphere oligomers will be presented.

O 37.11 Tue 18:30 P2

**Optical Properties of Self-assembled Fluorescent and Metal Nanoparticle Arrays** — •Franziska Barho, Mario Fey, and Peter J. Klar — Justus-Liebig-Universität Giessen, Germany

Localized plasmons in metal nanoparticles may influence the photoluminescence of adjacent fluorescent nanoparticles. Depending on the distance between the different nanoparticles, an enhancement of the photoluminescence signal as well as its quenching is possible. The influence caused by different arrangements of nanoparticles is going to be investigated.

The samples were prepared by electron beam lithography defining cavities in PMMA resist. Both types of nanoparticles, in our case gold particles, whose plasmon resonance frequency is located in the visible part of the spectrum, and fluorescent polystyrene spheres, were then placed into these structures by a horizontal dip coating process. With this self-assembling process, different arrangements of particles can occur which allow us to study their optical properties like the transmission and photoluminescence characteristics.

O 37.12 Tue 18:30 P2

**Optical Properties of Self-assembled Metal Nanoparticle Arrays** — •Mario Fey[1], Jan Kuhnert[2], Sangam Chatterjee[2], and Peter J. Klar[1] — [1]Justus-Liebig-Universität Giessen, Germany — [2]Philipps-Universität Marburg, Germany

The investigation of the optical properties of metal nanoparticles has long been of interest in physics. Since these particles have particular properties as their size approaches the nanoscale, like tunable surface plasmon resonances, they can be employed in different research fields e.g. surface-enhanced Raman spectroscopy. To gain more insight into surface plasmons, self-assembled gold and silver nanoparticle arrays as well as single arrangements consisting of a few nanoparticles were investigated by optical transmission spectroscopy. The samples were fabricated by electron beam lithography and a horizontal dip-coating process. The former step enabled us to define cavities of different sizes and shapes in the PMMA resist deposited on glass substrates. Size and shape of the cavities allow one to control the number and arrangement of the nanoparticles assembled by the horizontal dip-coating process in the cavities. Thus different arrays or rather formations of metal nanoparticles (single particles, pairs of particles etc.) on glass were obtained. Optical transmission spectroscopy allowed us to investigate the surface plasmon resonances of arrays of metal nanoparticles depending on the formation of the metal particles.

O 37.13 Tue 18:30 P2

**GRIN lenses with plasmonic structures as compact elements for biosensing** — •Andreas Horrer[1], Michael Metzger[2], Sabrina Rau[2], Dominik A. Gollmer[1], Julia Fulmes[1], Dai Zhang[2], Alfred J. Meixner[2], Günther Gauglitz[2], Marc Brecht[2], Dieter P. Kern[1], and Monika Fleischer[1] — [1]Institute for Applied Physics, University of Tuebingen, Auf der Morgenstelle 10, 72076 Tuebingen, Germany — [2]Institute of Physical and Theoretical Chemistry, University of Tuebingen, Auf der Morgenstelle 10, 72076 Tuebingen, Germany

Light scattering by metallic nanostructures shows resonances at certain wavelengths which are due to the plasmonic properties of the structures. These resonances show a characteristic wavelength shift when the medium and thereby the refractive index in the range of the near field of the structures is changed. This can be used for the detection of molecules with high sensitivity. Nanostructures can be fabricated in defined shapes and sizes by standard electron beam lithography. It is however difficult to use this method on small or non-planar surfaces.

GRIN lenses are small glass cylinders with a diameter of only a few millimeters and a built-in radial gradient of the refractive index, which enables focusing of incident parallel light onto one of their plane surfaces. For structuring of GRIN lens surfaces we use a process in which gold nanostructures fabricated on silicon can be transferred directly onto the lenses. These structures are automatically in the focus when excited through the lens and therefore allow for compact sensing setups. The fabricated structures on GRIN lenses as well as their optical properties will be presented.

O 37.14 Tue 18:30 P2

**Plasmonic nanostructures for organic photovoltaic cells** — •Yagmur Ipek, Dominik A.Gollmer, Christopher Lorch, Frank Schreiber, Dieter P. Kern, and Monika Fleischer — Institute for Applied Physics, Eberhard Karls University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

The topic of our research are OVP cells prepared by organic molecular beam deposition (OMBD). Diindenoperylen (DIP) [1] is used as the electron donor and Buckminster-Fullerene (C60) as the electron acceptor. The goal is to increase the efficiency of OPV cells by fabricating the transparent electrodes of OVP cells with plasmonic nanostructures, in particular gratings, such that the light harvesting properties of these cells may be improved. The plasmonic nanostructures are fabricated by electron-beam lithography or nanoimprint lithography. The OVP cells are measured via their current-voltage characteristics (I-V curve). Optical characterization of the structures by extinction measurements are compared with numerical simulations. An overview over the composition, different methods of nano fabrication and measurement methods of OVP cells will be presented.

[1] (J. Wagner et al., Adv. Funct. Mater.20 (2010) 4295)

O 37.15 Tue 18:30 P2

**Characterisation and Control of SPPs in silver waveguides using PEEM** — •Kellie Pearce[1,2], Christian Späth[1], Soo Hoon Chew[1,2], Sebastian Nobis[1], Jürgen Schmidt[1], and Ulf Kleineberg[1] — [1]Department of Physics, Ludwig Maximilian University of Munich, Garching, Germany — [2]Max Planck Institute of Quantum Optics, Garching, Germany

Surface plasmon polaritons (SPPs) have garnered much interest because of their unique properties. They are able to travel at speeds comparable to that of light, whilst capable of being confined to dimensions much smaller than the diffraction limit. Potential applications rely on being able to fabricate, characterise and optimise SPP guiding structures.

To investigate potential waveguides, a technique is needed to observe plasmons with high spatial and temporal resolution. Photoemission microscopy (PEEM) is one such technique. Combining time-of-flight PEEM with two-photon photoemission enables plasmons and plasmon-induced hotspots to be mapped. We fabricate and examine various SPP-waveguides to determine the effect of waveguide geometry, composition, and laser polarisation on the generation, steering and focusing of SPPs in metal nano- and microstructures. Additionally we initiate first steps towards using the the carrier envelope phase of ultrashort pulses for plasmonic control.

O 37.16 Tue 18:30 P2

**Extraordinary optical transmission and cathodoluminescence in thin layers with subwavelength holes** — •Dan-Nha Huynh[1], Christian Matyssek[1], and Kurt Busch[1,2] — [1]Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik und Photonik, Newtonstr. 15, 12489 Berlin, Germany — [2]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany

We examine properties of nano-plasmonic thin layers utilizing a self-implemented Discontinuous Galerkin Time-Domain (DGTD) program package. Specifically, metal films including subwavelength and wavelength-scale holes lead to interesting optical properties due to the excitation of surface plasmons such as extraordinary optical transmission.

We quantitatively explore the complex plasmon dynamics in these systems via optical transmission, electron energy loss and cathodoluminescence computations.

O 37.17 Tue 18:30 P2

**Nonlinear optics with hybrid metal/dielectric nanostructures** — •Heiko Linnenbank and Stefan Linden — Physikalisches Institut, Universität Bonn, Germany

Particle plasmons, i.e, coherent excitations of the conduction band electrons, govern the optical properties of metallic nanostructures in the visible and in the near-infrared spectral region. Excitation of particle plasmons with ultrashort light pulses can give rise to a spatiotemporal concentration of the electromagnetic field in the vicinity of the metallic nanostructure. The intensity in these hot spots can exceed the incident intensity by orders of magnitude. Conversely, localized fields within these hot spots can be efficiently transferred to the far field. By carefully varying the geometry of the metallic nanostructures it is possibly to tune their resonance and also to build structures with multiple resonances. In several studies it has been shown that gold nanostructures show a huge nonlinear response in terms of second and third harmonic generation to ultrashort light pulses. Here, we demonstrate that it is possible to influence the nonlinear emission of metallic nanoparticles by placing a dielectric material with a high second and third order nonlinear coefficient in the above mentioned hot spots. Furthermore, we show that the nonlinear processes can be tuned by building a metallic nanostructure which is not only resonant for the incoming light field but also for the generated field.

O 37.18 Tue 18:30 P2

**Optimizing arrangements of a few Au-nanoparticles for SERS applications** — •Kathrin Kroth, Thomas Sander, Sabrina Darmawi, Limei Chen, and Peter J. Klar — JLU Gießen

Surface-enhanced Raman spectroscopy (SERS) allows one to detect analytes on single-molecule level. The electric field of the impinging excitation light as well as the locally scattered light can be enhanced by several orders of magnitude in the gaps between metal-nanoparticles. SERS-substrates out of Au-nanoparticles have been prepared by combining top down nanofabrication with self-assembly of nanoparticles. At first a periodical array of cavities with different size and shape was fabricated by electron beam lithography (EBL) on a silicon substrate out of PMMA. The Au-nanoparticles from colloidal suspensions were arranged inside the cavities by a horizontal dip-coating process. The number and the orientation of the Au-nanoparticles in the cluster can be controlled by the size and shape of the PMMA-cavity. For the characterization of the different nanoparticle arrangements by Raman-imaging, a Raman-active molecule was deposited on top of the SERS-substrates allowing to study enhancement effects with respect to the nanoparticle arrangements and the polarization of the excitation light.

O 37.19 Tue 18:30 P2

**Few-cycle laser photoelectron microscopy and spectroscopy using single-shot phase tagging technique** — •Soo Hoon Chew[1], Alexander Gliserin[1], Sebastian Nobis[1], Florian Schertz[2], Yingying Yang[3], Kellie Pearce[1], Peter Geisler[4], Jürgen Schmidt[1], Peter Hommelhoff[5], Bert Hecht[4], Matthias Kling[1], and Ulf Kleineberg[1] — [1]Faculty of Physics, Ludwig Maximilian University of Munich, 85748 Garching, Germany — [2]Institute of Physics, University of Johannes Gutenberg, 55128 Mainz, Germany — [3]Institute of Semiconductors, Haidian District, Beijing 100083, P. R. China — [4]Institute of Physics, University of Würzburg, 97074 Würzburg, Germany — [5]Department of Physics, University of Erlangen-Nürnberg, 91058 Erlangen, Germany

A single-shot phase-tagged time-of-flight-photoelectron emission microscope has recently been developed to investigate and control carrier-envelope phase (CEP) effects on tailored plasmonic nanostructures. First experiments measuring the CEP dependence on single gold nanoparticles on gold plane (NPOP) have been performed with 10 kHz few-cycle laser pulses via a multiphoton photoemission process. We report the results from calculations and observation of a CEP feature from the NPOP sample as well as the challenges of the experiments. We also address the possible solutions to improve the plasmonic sample quality and design for probing and control the plasmonic dynamics via the CEP effect. The experimental setup provides a versatile tool for both spatial-resolved and energy-resolved studies of the attosecond control of electrons in plasmonic nanostructures.

O 37.20 Tue 18:30 P2

**Transmission of surface plasmon polariton through nanometric constriction** — •Golaleh Ghafoori[1], Daniel Benner[2], Johannes Boneberg[3], Paul Leiderer[4], and Elke scheer[5] — [1]golaleh.ghafoori@uni.konstanz.de — [2]daniel.benner@uni.konstanz.de — [3]University of Konstanz — [4]University of Konstanz — [5]University of Konstanz

We study the excitation and propagation of surface plasmons polariton (SPPs) on a 4 micrometer wide gold stripe of thickness about 100nm.

For the excitation we use an optimized grating in the stripe. The surface plasmons propagate towards and across a constriction. We show that SPPs are transmitted with high probability across a constriction, with smallest lateral dimensions of atomic. For comparison we performed FDTD(Finite Difference Time Domain) simulations with Lumerical. We model a supported gold stripe in the same geometrical arrangement as the sample. These studies allow the determination of local intensities in experiments with mechanically controllable break-junctions under light irradiation [1].

O 37.21 Tue 18:30 P2

**Transmission of surface plasmon polariton through nanometric constriction** — •Golaleh Ghafoori[1], Daniel Benner[2], Johannes Boneberg[3], Paul Leiderer[4], and Elke scheer[5] — [1]golaleh.ghafoori@uni.konstanz.de — [2]daniel.benner@uni.konstanz.de — [3]University of Konstanz — [4]University of Konstanz — [5]University of Konstanz

We study the excitation and propagation of surface plasmons polariton (SPPs) on a 4 micrometer wide gold stripe of thickness about 100nm. For the excitation we use an optimized grating in the stripe. The surface plasmons propagate towards and across a constriction. We show that SPPs are transmitted with high probability across a constriction, with smallest lateral dimensions of atomic. For comparison we performed FDTD(Finite Difference Time Domain) simulations with Lumerical. We model a supported gold stripe in the same geometrical arrangement as the sample. These studies allow the determination of local intensities in experiments with mechanically controllable break-junctions under light irradiation [1].

O 37.22 Tue 18:30 P2

**Third Harmonic Spectroscopy of Polymer-Nanoantenna Hybrid Systems** — •Gelon Albrecht[1,2], Bernd Metzger[1], Sybille Allard[3], Ullrich Scherf[3], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, Stuttgart 70569, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstraße 1, Stuttgart 70569, Germany — [3]Bergische Universität Wuppertal, Gaußstraße 20, Wuppertal 42119, Germany

Nonlinear plasmonics [1] has gained a lot of interest lately due to its potential to tailor novel nonlinear optical materials. Plasmonics is a promising approach as it allows for nanofocusing electromagnetic energy into small spatial regions [2].

We perform third-harmonic (TH) spectroscopy using an 8 fs TiSa laser oscillator on polymer-covered gap-nanoantenna arrays made from gold. We use this hybrid system mainly for two reasons. First, antennas are an ideal system to transfer energy from the far-field of an electromagnetic wave to the near-field around the antenna, especially into the antenna gap region. Second, nonlinear polymers show a very large third-harmonic susceptibility. The combination of this two systems leads to a hybrid system which exhibits a strong wavelength-dependent resonant third-harmonic response function. Furthermore this response is sensitive to the gap size and to the plasmonic resonance of the antennas. [1] M. Kauranen and A.V. Zayats, Nat. Photonics 6, 737*748 (2012) [2] M. Hentschel , T. Utikal, H. Giessen, and M. Lippitz, Nano Lett. 12, 3778-3782 (2012)

O 37.23 Tue 18:30 P2

**Impact of rotational symmetry on the nonlinear optical response of gold nanoantennas** — •Franziska Zeuner[1], Shumei Chen[2], Guixin Li[3], Shuang Zhang[2], and Thomas Zentgraf[1] — [1]Department of Physics, University of Paderborn — [2]School of Physics & Astronomy, University of Birmingham, UK — [3]Department of Physics, Hong Kong Baptist University

The strength of a nonlinear optical response of natural materials is highly sensitive to their crystallographical symmetry. Because of the high interest in metamaterials and their potential in photonics, we want to investigate the impact of rotational symmetry on the nonlinear optical signal strength of plasmonic structures. By fabricating gold nanoantennas with four different rotational symmetries but the same plasmon resonance frequency, we are able to compare the symmerty induced change in the nonlinear optical response.

O 37.24 Tue 18:30 P2

**Surface plasmon enhanced chemiluminescence at metal surfaces using internal photodetection** — Ulrich Hagemann, Felix Becker, and •Hermann Nienhaus — Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, D-47048 Duisburg, Germany

Light emission during reactions on metal surfaces is generally quenched. If detectable at all the photon yield is low. The study presents data from two model reactions at low temperatures, i.e., the oxidation of Mg and the chlorination of K surfaces [1]. The metals are prepared as thin layers on a rough 5 - 200 nm Ag film grown on $p$-Si(111) surfaces. The Ag/Si(111) contact is used as a Schottky photodiode allowing an internal $2\pi$ detection of the chemiluminescence photons. The photoyield can be enhanced up to an order of magnitude by varying the Ag film thickness. For Ag films in the thickness range between 30 and 50 nm, the yield shows characteristic maxima. The results can be explained by surface plasmon polaritons (SPP) in the Ag layer which are excited by the non-adiabatic chemical reaction on the Mg or K surface. The SPP decays radiatively into Si inducing the photocurrent. Model calculations are able to reproduce the observed yield maxima at certain Ag film thicknesses.

[1] F. Becker et al., JCP 138 (2013) 034710.

O 37.25 Tue 18:30 P2

**Sphere-based cantilever for SNOM** — •Critian Gonzalez Mora, Daniela Bayer, Elena A. Ilin, Egbert Oesteschulze, and Martin Aeschlimann — University of Kaiserslautern Erwin Schroedinger Str. 46 D-67663, Kaiserslautern

We present the development and first measurements with a new kind of cantilever sensors, which allow an enhanced transmission of light keeping the possibility to perform SNOM (Scanning Near-field Microscope) measurements in contact to the sample.

The characterization performed my measuring Au Nano-rings show a clear polarization dependence for the excited plasmons. These new cantilevers are a modification of the traditional aperture cantilevers for aperture based SNOM and consist, basically, of a glass micro-sphere at the apex of the tip of the sensor.

O 37.26 Tue 18:30 P2

**Photoluminescence study of SPP-supporting hybrid semiconductor-metal structures** — •Sören Kreinberg[1], Matthias Salewski[1], Lars E. Kreilkamp[1], Ilya A. Akimov[1], Christian Schneider[2], Sven Höfling[2], Martin Kamp[2], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany — [2]Lehrstuhl für Technische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

We study the optical properties of hybrid nanostructures comprising self-assembled InGaAs quantum dots (QDs) located in the direct vicinity from the surface which is covered with Au grating. The Au period is optimized in oder to support the excitation of surface plasmon polaritons (SPP) by excitons in QDs emission and vice versa. Angle dependent transmission and reflection spectra show clear signatures of SPP resonances. We investigate SPP influence on exciton dynamics measured by means of time-resolved photoluminescence.

O 37.27 Tue 18:30 P2

**Towards superlens-based infrared near-field nanospectroscopy: imaging dielectric contrasts with $\lambda/30$-resolution** — •Peining Li[1], Tao Wang[1], Benedikt Hauer[1], Gennady Shvets[2], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen University, Aachen 52056, Germany — [2]Department of Physics and Center for Nano and Molecular Science and Technology, The University of Texas at Austin, Austin, Texas 78712, USA

Near-field superlenses present great capabilities for overcoming the diffraction limit [1], bringing new applications in optical lithography [2] and near-field imaging [3]. Here, using the combination of a silicon carbide superlens and scattering-scanning near-field optical microscopy (SL-SNOM), the infrared imaging of dielectric contrasts with a resolution of down to $\lambda/30$ (about 350 nanometers) has been verified. This achieved resolution is an almost 2-fold improvement compared to state-of-the-art superlens results [3]. From quantifications of the superlens dispersion via near-field mapping of surface phonon polaritons (SPhPs), the physical mechanism behind the obtained ultra-high resolution is directly visualized to be the field enhancement by short-$\lambda$ SPhPs at the superlensing condition. Our results pave the way to superlens-based infrared spectroscopic applications for revealing vibration information of dielectric samples.

[1] J. B. Pendry, Phys. Rev. Lett. 85, 3966 (2000).

[2] N. Fang, et al., Science 308, 534 (2005).

[3] T. Taubner, et al., Science 313, 1595 (2006).

O 37.28 Tue 18:30 P2

**Plasmon Enhanced Fluorescence from Nanocrystals doped with Rare-earth Ions** — •Tobia Mancabelli[1], Dawid Piatkowski[2], Nikolai Hartmann[1], Nina Mauser[1], Sebastian Mackowski[2], and Achim Hartschuh[1] — [1]Department Chemie & CENS, Ludwig-Maximilians-University, Munich, Germany — [2]Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Torun, Poland

We investigated the plasmonic enhancement of two-photon upconverted fluorescence of NaYF4:Er3+/Yb3+ nanocrystals (NCs) for two different metallic structures. First we used NCs-decorated silver nanowires (NWs): a strong enhancement of the NC emission is observed for laser polarization parallel to the orientation of the NW, indicating that the silver NW is able to locally enhance absorption. Using Fluorescence Lifetime Imaging Microscopy we then observed a faster decay dynamics for NCs close to the NW, proving that the NC-plasmon interaction can increase the radiative decay rate of the rare-earth ions. This is further supported by angular-resolved emission patterns recorded in the Fourier plane [1] showing that the NCs can relax via coupling to the NW. Second we recorded fluorescence images of NCs at sub-diffraction spatial resolution using a sharp gold antenna tip [2]. The decay dynamics in presence of the tip was found to be faster consistent with what we observe in presence of silver NWs. This shows that plasmonic metal structures can be used to enhance absorption and emission in rare-earth doped NCs. [1] N. Hartmann, et al.; ACS Nano, 11, 2013. [2] N. Mauser, et al.; Chem. Soc. Rev., 2013.

O 37.29 Tue 18:30 P2

**Active stabilization of a vector field synthesizer applied for spatiotemporal optical near-field control** — •Stanislaw Nickel, Michael Birlo, Dominik Differt, and Walter Pfeiffer — Department of Physics, University Bielefeld, 33615 Bielefeld, Germany

Ultrafast spatiotemporal optical near-field control in nanostructures and random scattering media requires full control of spectral amplitude and phase for both polarizations components. Conventional polarization pulse shapers that rely on a common optical path for both polarization components are limited and thus also allow only limited optical near-field control. Vector field synthesizers use independent pathways and thus are no longer restricted in their pulse shaping capabilities. However, because of the independent pathways interferometric stability of the whole setup is required. Here we demonstrate stable and reliable generation of polarization shaped pulses using a vector field synthesizer with active stabilization mechanism to correct the inherent mechanical instabilities of the setup because of vibrations and thermal drift. The phase between both pathways in the setup is detected by adding light from a cw laser diode operating at a wavelength just outside the fs-laser spectrum and measuring the output polarization. Using a piezo-driven wedge (pair) and an analog PID controller, the relative phase between both pathways is stabilized. With active stabilization the standard deviation is smaller than $2\pi/50$, i.e. 10 times improved compared to unstabilized operation, and no drift occurs over one hour.

O 37.30 Tue 18:30 P2

**Strong-field gas excitation and EUV light generation in plasmonic nanostructures** — •Frederik Busse, Murat Sivis, and Claus Ropers — IV. Physical Institute - University of Göttingen, Göttingen, Germany

Spatial confinement of electromagnetic fields in tailored plasmonic nanostructures allows for the enhancement of a variety of high-order nonlinear optical phenomena using low-energy laser pulses at MHz repetition rates. Here, we present a detailed study of extreme-ultraviolet (EUV) light generation in noble gases employing bowtie-antennas and tapered hollow waveguides for field-enhancement. In contrast to former expectations [1], we do not observe any signature of coherent high harmonic generation. Instead, we identify atomic and ionic fluorescence induced by multiphoton or strong-field gas excitation and ionization as the predominant mechanisms of EUV light generation in such plasmon-assisted scenarios [2, 3]. Furthermore, we discuss novel nonlinear effects such as the formation of a waveguide nanoplasma exhibiting a strong bistability, manifest as a pronounced intensity- and pressure-dependent hysteresis in the fluorescence signal. These observations lead to a deeper understanding of nanostructure-enhanced gas excitations and EUV light generation, representing an intriguing link between strong-field physics, plasma dynamics and ultrafast nanooptics.

[1] S. Kim *et al.*, Nature **453**, 757 (2008).
[2] M. Sivis *et al.*, Nature **485**, E1 (2012).
[3] M. Sivis and C. Ropers, Phys. Rev. Lett. **111**, 085001 (2013).

O 37.31 Tue 18:30 P2

**Hydrogen-sensing with complex arrow-headed Au/Pd nanorods** — •Domenico Paone[1], Xingchen Ye[2], Nikolai Strohfeldt[1], Andreas Tittl[1], Chris Murray[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCOPE, University of Stuttgart — [2]Department of Materials Science and Engineering, and Department of Chemistry, University of Pennsylvania

Sensitive and reliable hydrogen detection is a key safety requirement for industrial process monitoring and catalysis. Hybrid plasmonic nanoparticles combine highly-resonant noble metal nanoparticles with chemically sensitive materials to detect a variety of gases. Furthermore, chemically synthesized nanoparticles can be grown with high yield and thus at low cost. Here, we demonstrate hydrogen-sensing with arrow-headed Au nanorods that are covered with a small amount of palladium (Pd). The arrow-headed shape was chosen to maximize the plasmonic field enhancement at the tips of the gold nanorods, allowing them to detect very small hydrogen-induced changes in the adjacent Pd. We perform dark-field scattering measurements on single nanorods while exposing the sample to different concentrations of hydrogen in nitrogen carrier gas and find pronounced spectral shifts. In addition, we investigate nanorods with a variety of geometrical parameters and correlate them with the sensing performance. In future, our nanosensor platform will enable single particle sensing and spectroscopy of a variety of gases down to very low concentrations.

O 37.32 Tue 18:30 P2

**Hybrid Plasmonic Nanostructures: Characterization of Coupled Quantum Dot - Nanoantenna Systems** — •Cody Friesen, Manuel Peter, and Stefan Linden — Physikalisches Institut, Universität Bonn, Nußallee 12, 53115 Bonn, Germany

This poster will provide an overview of the fabrication and characterization methods we use to investigate hybrid plasmonic nanostructures. Specifically, our structures consist of a quantum dot strongly coupled to a nanoscale gold dipole antenna.

The fabrication utilizes electron beam lithography, with a PMMA resist. First a PMMA mask defining the antennas is created, and gold evaporation is used to deposit the actual material. Following the structure fabrication a second PMMA mask is created that describes the areas for quantum dot deposition. A chemical linking process binds the quantum dots to the exposed substrate.

The antennas have resonances tuned to the excitation wavelength of the quantum dots ($\lambda$=780 nm), which are pumped via a green laser. The red-shifted emission light of the dots is collected using a confocal microscope and fiber coupled either into a spectrometer or into a lifetime measurement device which uses a photodiode. The diode is used for dot lifetime and emission intensity measurements, while the spectrometer allows for the measurement of spectral shifts and changes in the spectral structure.

O 37.33 Tue 18:30 P2

**k-space polarimetry on an adiabatic nanofocusing near-field probe** — •Martin Esmann, Simon F. Becker, Jens H. Brauer, Petra Gross, Ralf Vogelgesang, and Christoph Lienau — Carl von Ossietzky Universität, 26111 Oldenburg, Germany

Adiabatic nanofocusing of surface plasmon polaritons (SPPs) propagating on tapered metallic waveguides bears great potential as a novel method for apertureless near-field scanning optical microscopy (SNOM) [1,2]. SPP wavepackets are excited on a grating-coupler and for an ideal cone-shaped waveguide come to a complete halt at the taper apex. Hence, a single point-dipole like light source is formed there. This, however, is only true for the lowest rotationally symmetric taper eigenmode [3]. Higher eigenmodes of the waveguide disturb the imaging process in SNOM as they radiate into the far field before reaching the taper end leading to unwanted background signals.

We have therefore developed and implemented a k-space imaging technique to analyse and separate contributions from the different eigenmodes [3]. Using Stokes polarimetry, we show that the symmetry of the lowest taper eigenmode gives rise to a radially polarized mode in k-space, which is clearly identified. Furthermore, we performed approach curve scans across metallic nanostructures to investigate the influence of the near-field coupling between probe and sample on the polarization dependent intensity distribution in k-space.

[1] M. I. Stockman, PRL 93, 137404 (2004) [2] S. Schmidt et al., ACS Nano 6, 6040 (2012) [3] M. Esmann et al., BJ Nano 4, 603 (2013)

O 37.34 Tue 18:30 P2

**Pump-probe infrared near-field nanospectroscopy on germanium and silicon** — •Frederik Kuschewski[1], S.C. Kehr[1], B. Green[2], Ch. Bauer[2,3], M. Gensch[2], and L.M. Eng[1] — [1]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [3]Freie Universität Berlin, 14195 Dahlem, Germany

Scattering-type scanning near-field optical microscopy (s-SNOM) was applied to investigate the local infrared-optical properties of germanium, silicon and SiGe thin film in a pump-probe experiment below the diffraction limit. The novel combination of s-SNOM with pump-probe techniques allows us to study electron excitation processes at an ultimate temporal resolution and to investigate their decay behavior.

Our s-SNOM is based on a non-contact atomic force microscope. The optical near-field is demodulated at higher-harmonics, which is extended to a novel side-band demodulation technique that allows for the direct measurement of pump-induced effects. Pump excitation is exhibited with a Nd:YAG ps laser while near-field probing was carried out either by a cw $CO_2$ laser or by the tuneable FELBE free-electron-laser at the Helmholtz-Zentrum Dresden-Rossendorf (HZDR).

All three samples show a clear time-variable pump-effect in the near-field when being probed at $\sim 10\ \mu$m wavelenght. Image scans clearly proof the resolution far beyond the diffraction limit. The experiment provides a definite proof of the applicability of our approach for investigating ultrafast phenomena in the near-field.

O 37.35 Tue 18:30 P2

**Time-domain characterization of scattered fields from nanotextured thin film absorbers** — •Dominik Differt, Stanislaw Nickel, and Walter Pfeiffer — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

Recent investigations revealed that light trapping in localized photonic modes enhances absorption in thin film silicon solar cells with nanotextured interfaces. These localized modes can be detected and characterized by spectral interferometry of backscattered radiation if a sufficiently small illumination spot is chosen. Here we use dual channel spectral interferometry to fully characterize the temporal evolution of the backscattered light from fs laser materials processed amorphous silicon layers and nanotextured thin film silicon solar cells illuminated by ultra short laser pulses. Performing a 2D point to point surface scan of the backscattered light over the sample with a high resolution reveals localized photonic modes in both samples. Finally, the prospect to coherently control absorption in these modes by use time-reversed or adaptively optimized light pulses generated using a vector field pulse shaper is discussed.

O 37.36 Tue 18:30 P2

**Circular Plasmons in cross shaped nanoantennas** — •Martin Lehr[1], Peter Klaer[1], Xiaofei Wu[2], Bert Hecht[2], Florian Schertz[1], Gerd Schönhense[1], and Hans Joachim Elmers[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, D-55099 Maiz, Germany — [2]Institut für Physik, Julius-Maximilians- Universität, Am Hubland, 97074 Würzburg, Germany

Optical near-fields generated by coupled plasmonic modes can have defined polarization states. In analogy to cross dipole antennas for radio waves, the cross-shaped arrangement of dipole nanoantennas investigated here concentrates not only intensity, but also the angular momentum of circularly polarized infrared light. The field enhancement of individual nanoantennas has been measured by the relative photoemission intensity using a photoemission electron microscope with front side illumination at grazing incidence and backside illumination at normal incidence. The analysis of the polarization dependence reveals the excitation of a unique circular plasmon mode. The strong confinement of angular momentum promises a strong coupling of the photon angular momentum to magnetic moments and to the spin of photo-emitted electrons.

Funded by DFG (EL172-16)

O 37.37 Tue 18:30 P2

**Implementation of Pulse Shaping in an Ultrafast confocal microscope** — •Kevin Donkers, Alberto Comin, Richard Ciesielski, and Achim Hartschuh — Ludwig Maximilians Universität München & CeNS

The area of ultrafast spectroscopy has been of interest for many years yet its application to microscopy has been hindered by the difficulty of focusing femtosecond laser pulses. The use of high numerical aperture objectives with such short, broadband pulses leads to the introduction of very large values of Group Delay Dispersion (GDD), as well as higher order derivatives of the phase, which can elongate a laser pulse from less than ten femtoseconds to several picoseconds.

We implemented a pulse shaping scheme using a Liquid Crystal Modulator (LCM) and Prism Compressor in a microscopy setup with NA=1.3 allowing us to control the phase and amplitude of a strongly focused ultrafast pulse. We first used Multiphoton Intrapulse Interference Phase Scans (MIIPS) to recover laser pulses close to their original pulse length. We then have developed an advanced scheme to improve this further and demonstrate the compensation of linear chirp introduced by glass, the effect on non-linear photoluminescence of graphene and the increase of second-harmonic generation on beta-barium borate.

O 37.38 Tue 18:30 P2

**Spatial and spectral near-field distributions of strongly coupled plasmons** — •Florian Schertz, Martin Lehr, Hans-Joachim Elmers, and Gerd Schönhense — Johannes Gutenberg Universität Mainz, Institut für Physik, Staudinger Weg 7, 55128 Mainz

The mutual interaction of plasmons results in a strongly enhanced and confined near-field in the interspace between the plasmon supporting structures. The spectral near-field distribution is known to deviate from the corresponding far-field characteristics for strongly coupled plasmons with interspace (gap) sizes in the sub-nm range [1]. To understand the origin of this difference, we calculated the phase distribution of the electric near-field of strongly coupled plasmons at specific excitation frequencies numerically. From the phase distribution the charge distribution at specific instants of time can be derived. The obtained multipole-like distribution of the near-field gives rise to a spatial-dependence of the near-field enhancement in the gap of the plasmon-supporting structures. The results are discussed for various systems of strongly coupled plasmons in dependence of characteristic parameters such as e.g. gap size, particle size and particle aspect ratio. [1] F. Schertz et al., Nano Lett. 12 (4), 1885, (2012).

O 37.39 Tue 18:30 P2

**Plasmonically enhanced Grätzel cells for photovoltaics** — •Jonas Schwenzer and Harald Giessen — 4th Physics Institute and Research Center SCOPE, University of Stuttgart, Germany

Dye sensitized solar cells are one of the most promising alternatives to silicon-based solar cells. Improvements on these cells were achieved by changing the different components e.g. the titania layer, the dye, or the electrolyte. The rather low stability of these cells was improved by solid state hole transport materials instead of liquid electrolytes. Another promising step to improve the output power are plasmonic Grätzel-cells with incorporated silica coated gold-nanoparticles. We blendend Au-$SiO_2$ nanoparticles with diameters of 150 nm and different shell sizes into the titania paste. The energy conversion efficiency was enhanced by 42% compared to cells with bare titania. Current voltage measurements showed that this enhancement is caused by an increase of the current while the open circuit voltage and the fill factor did not change significantly. Furthermore the study shows that the efficiency of the cell is higher if the silica shell is thinner. Another result of our work is the dependence of power conversion efficiency on the concentration of the nanoparticles.

O 37.40 Tue 18:30 P2

**Diffraction-limited few-cycle shaped laser pulses for plasmon microscopy** — •Sebastian Goetz[1], Monika Pawlowska[1], Christian Dreher[1], Christian Rewitz[1], Enno Krauss[2], Peter Geisler[2], Gary Razinskas[2], Bert Hecht[2,3], and Tobias Brixner[1,3] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Nano-Optics and Biophotonics Group, Experimentelle Physik 5, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Röntgen Center for Complex Material Systems (RCCM), Am Hubland, 97074 Würzburg, Germany

For the investigation of ultrafast processes on the nanoscale by far-field radiation, the temporal resolution of femtosecond laser pulses has to be combined with the spatial resolution of a high-NA microscope. Both resolutions need to be conserved when the incoming light field is manipulated, which is a prerequisite for the demanding concept of coherent control. These functionalities are implemented in our group by pairing confocal microscopy with phase and amplitude pulse shaping of few-cycle NIR pulses using an LCD pulse shaper in $4f$ single-pass geometry. The capability of the setup is demonstrated by investigating the influence on the diffraction-limited focus of LCD imperfections and spatio-temporal coupling. We examine the laser focus on plain gold surfaces and nanostructures by spectrally and spatially resolved analysis of reflections from the sample plane.

O 37.41 Tue 18:30 P2

**Infrared conductivity measurement of nanostructures** — •Annemarie Pucci[1,2,3], Christian Huck[1], Jochen Vogt[1], Fabian Hötzel[1], Akemi Tamanai[1,2], Jens Trollmann[1,2], and Tobias Glaser[1,2] — [1]Kirchhoff Institute for Physics (KIP), Heidelberg University, Heidelberg, GERMANY — [2]InnovationLab GmbH, Heidelberg, GERMANY — [3]Centre for Advanced Materials (CAM), Heidelberg University, Heidelberg, GERMANY

Nanostructures from materials with free charge carriers, as for example gold, ITO, and doped semiconductors, may show plasmonic absorption in the infrared, which allows conductivity measurement without electrical contacts. The electronic relaxation rate as a measure of crystalline quality can be separately derived from the spectra, even for nanowires.

O 37.42 Tue 18:30 P2

**Tuning the Localized Surface Plasmon Resonance in Silver Nanostructures prepared by Nanosphere Lithography** — •Stefan Moras, Ovidiu D. Gordan, and Dietrich R. T. Zahn — Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz

Metallic nanoparticles and regular nanostructures attract great interest because of their unusual properties. The outstanding optical response of such structures stems from the Localized Surface Plasmon Resonance (LSPR) produced by oscillations of the electronic charge density under electromagnetic radiation. Recent advancements in producing ordered metallic objects at nanoscales enabled the use of LSPRs for light manipulation and made them a valuable tool for chemical and biological sensing experiments. Optical properties associated with LSPRs are determined by shape, size, structure, and local dielectric environment. In the present work we study the possibility to tune the LSPRs by changing the size and shape of ordered silver nanostructures. These structures were produced by nanosphere lithography. A close-packed monolayer of polystyrene nanospheres self-assembled at the air-water interface is transferred to arbitrary substrates like glass or silicon. After silver deposition and nanosphere removal only regular silver nanotriangles remain on the substrate. UV-Vis spectroscopy was used to determine the LSPR of these nanostructures on glass substrates. While nanostructures with a high aspect ratio lead to a blue shift with respect to the LSPR of lower aspect ratio structures such a blue shift can also be obtained by annealing.

O 37.43 Tue 18:30 P2

**Scanning near-field optical microscopy and nano-FTIR spectroscopy on sub-nanometer MoS2 structures by using synchrotron radiation** — •Georg Ulrich[1], Piotr Patoka[1], Peter Hermann[2], Ariana Nguyen[3], John Mann[3], Arne Hoehl[2], Burkhard Beckhoff[2], Ludwig Bartels[3], Peter Dowben[4], Gerhard Ulm[2], and Eckart Rühl[1] — [1]Physikalische und Theoretische Chemie, Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, Berlin, 10587, Berlin, Germany — [3]Department of Chemistry, University of California Riverside, 0124 Pierce Hall, Riverside, California, U.S.A. 92521 — [4]Department of Physics and Astronomy, University of Nebraska, Lincoln, T. Jorgensen Hall, Lincoln, Nebraska, U.S.A. 68588-0299

We report on IR-spectromicroscopy on MoS2 demonstrating the successful coupling of scattering type scanning near-field optical microscopy (s-SNOM) with a synchrotron radiation infrared source, provided by the electron storage ring Metrology Light Source (MLS). The technique provides high spatial resolution (<50 nm) spectromicroscopy in the infrared regime with chemical selectivity from nano-Fourier-transform-infrared (nano-FTIR) spectroscopy. The used synchrotron radiation has the advantage compared to lasers, that it covers the entire infrared regime, ranging from the near- to the far-infrared. The correlation of topographically well defined islands grown by chemical vapor deposition, as determined by atomic force microscopy, with the IR signature of MoS2 is illustrated by s-SNOM the approach.

We will present the results on optical mapping of MoS2 monolayers on SiO2 gained with a tunable CO2-laser and the influence of such MoS2 islands on SiO2-phonon resonance by means of nano-FTIR measurements with broadband synchrotron-radiation. The results suggest either a significant carrier concentration in MoS2, likely as a result of substrate interactions, or strong MoS2-SiO2 substrate dipole interactions.

O 37.44 Tue 18:30 P2

**Enhancement of nonlinear optical effects by plasmonic nanoantennas** — •Nils Weber, Thomas Zentgraf, and Cedrik Meier — University of Paderborn, Experimental Physics & CeOPP, Warburger Str. 100, 33098 Paderborn

The light-matter interaction for nonlinear processes is known to be rather weak. Consequently, high excitation powers are required for efficient light-light-interaction. Plasmonic nanostructures are a promising approach to achieve strong near-field enhancement.

In this work, silver split rings are used as plasmonic nanoantennas for the local enhancement of the electric field in a $SiO_2$/ZnO/$SiO_2$-microdisc, hence increasing the nonlinear optical response. The microdiscs are realized on a $SiO_2$-Si(111) substrate by electron beam lithography, utilizing molecular beam epitaxy (MBE)-grown ZnO-layer as an optical emitter. With diameters ranging from $7\mu m$ to $8\mu m$, the discs show whispering gallery modes with high quality factors of up to 5000. Furthermore, the electron beam lithography enables the patterning of nanostructures with high precision on top of the microdisc, allowing the deposition of silver split rings with outer diameters of 600nm in a concentric geometry. Finite-differences time-domain (FDTD) simulations show a strong enhancement of the electric field within the gap of the split rings in the near infrared. The optimization of the fabrication process as well as different sizes and geometries of nanoantennas are studied.

O 37.45 Tue 18:30 P2

**Scanning tunneling microscopy investigation of the phase change material $Ge_2Sb_2Te_5$** — •Jens Kellner[1], Christian Pauly[1], Marcus Liebmann[1], Alessandro Giussani[2], Volker Deringer[3], Raffaella Calarco[2], Richard Dronskowski[3], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen University and JARA-FIT, Germany — [2]Paul Drude Institut für Festkörpelektronik, Berlin, Germany — [3]Institute of Inorganic Chemistry, RWTH Aachen University, Germany

We investigated the phase change material GST-225. Despite the fact that GST is already commercially used, there is still no complete theory which can explain the ultra fast switching speed, the strong contrast and the high endurance of the Ge-Sb-Te alloys. One ingredient of such a theory is an atomic scale understanding of the electronic properties of GST.
Scanning tunneling microscopy (STM) measurements are used to achieve atomic resolution on metastable cubic GST. The STM data show the regular hexagonal Te lattice, which exhibits an additional irregular contrast. Comparison with DFT calculations reveals that subsurface defects create such contrast. For different subsurface arrangements of Ge, Sb and vacancies, simulated STM images show good agreement with experimental data. Scanning tunneling spectroscopy (STS) data revealed p-type doping and a band gap of 0.4 eV.

O 37.46 Tue 18:30 P2

**Solution of the *GW*-based quasiparticle-equation beyond the diagonal approximation: improvements in energies and wavefunctions** — •Ferdinand Kaplan[1], Michiel van Setten[2], and Ferdinand Evers[1] — [1]Karlsruhe Institute of Technology — [2]Université catholique de Louvain

One of the most used approaches for the computational study of solids, nanoscale systems and molecules is the density functional theory (DFT). However, as is well known, DFT calculations of single particle excitation spectra, e.g. ionization potentials, often suffer from approximations in exchange correlations potentials. To systematically improve the estimation of quasi-particle energies for molecular system, we have implemented the so called GW method into a standard quantum chemistry package ($G_0W_0$-level). The approach represents a perturbative expansion of the many-body Green's function with respect to the screened interaction, $W$.

A central mathematical step in GW is the solution of the quasiparticle (qp-) equation. It finds the poles of the (approximate) many-body Greens function, that define the qp-energies. A common simplification in this procedure is to neglect all off-diagonal elements of the self-energy matrix, that enters the qp-equation. We investigate the quantitative error associated with this approximation for a typical set of molecules and find significant effects. Including the off-diagonal terms the ionization potential experiences shifts (usually towards less binding) reaching 100mV or more.

O 37.47 Tue 18:30 P2

**Photoemission spectroscopy using high-order harmonics driven by a MHz fiber laser** — •Cheng-Tien Chiang[1,2], Michael Huth[1], Andreas Trützschler[1,2], Jürgen Kirschner[1,2], and Wolf Widdra[2,1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120, Halle(Saale), Germany — [2]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120, Halle(Saale), Germany

We report a laboratory photoemission setup using high-order harmonic generation (HHG) as a light source driven by a fiber amplifier laser system at MHz repetition rate. The HHG light source consists of a compact generation chamber and a monochromator. Output of the fiber laser is expanded and focused in a tight focusing geometry into an argon or a xenon gas jet, producing vacuum ultraviolet light with photon energy from 16 to 40 eV. With this light source in combination with a time-of-flight electron spectrometer we demonstrate photon energy dependent photoemission experiments on a Ag(001) surface. Technical details of the setup will be presented.

O 37.48 Tue 18:30 P2

**Temperature-dependent scanning tunneling microscopy of Se-doped IrTe$_2$** — •Matthias Vogt[1], Tobias Mauerer[1], Pin-Jui Hsu[1], Weida Wu[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

We present variable-temperature scanning tunneling microscopy (STM) measurements of cleaved IrTe$_{2-x}$Se$_x$ ($x = 0.5$). A charge modulation period $q = 1/6$ is observed at room temperature, 50 K, and 4 K. This observation is in accordance with the previously reported transition from a polymerized state above [1] to periodic dimer stripes below $T_\mathrm{C} \approx 400\,\mathrm{K}$ [2]. The data are compared to undoped IrTe$_2$, for which STM measurements revealed a 1/5 charge modulation below a much lower transition temperature ($T_\mathrm{C} = 275\,\mathrm{K}$) and convergence to the 1/6 ground state below a second transition at $T_\mathrm{S} = 180\,\mathrm{K}$ [2]. The 1/5 modulation was interpreted as a soliton lattice and its alteration to 1/6 upon Se-doping can consistently be explained by a weakening of the Te-Te bonds by the more electronegative Se atoms, which also increases the transition temperature.

[1] Y. S. Oh *et al.*, Phys. Rev. Lett. **110**, 127209 (2013)

[2] P. J. Hsu *et al.*, arXiv:1311.3015v1 (2013)

O 37.49 Tue 18:30 P2

**Density functional study of GaN(0001)/AlN(0001) high electron mobility transistor structures** — Jakub Sołtys[1], Maria Ptasińska[1], •Jacek Piechota[1], and Stanisław Krukowski[1,2] — [1]ICM, University of Warsaw, Pawińskiego 5a, 02-106 Warsaw, Poland — [2]Institute of High Pressure Physics, Polish Academy of Sciences, Sokołowska 29/37, 01-142 Warsaw, Poland

AlN/GaN high electron mobility transistor (HEMT) structures were theoretically investigated using the density functional theory (DFT). An existence of two-dimensional electron gas (2DEG), generated by strong polarization fields at the AlN/GaN interface, was confirmed by abinitio calculations. The potential profiles were analyzed for the HEMTs with different number of AlN layers, indicating that very thin AlN barrier could not provide a high density of carriers and good confinement of 2DEG. It was shown that for six AlN layers (thickness about 13Å), no electron gas is present as shown by the potential profile. In the investigated electronic structure, the band states associated with the two-dimensional electron gas were identified. It was shown that for a thicker AlN barrier, the occupancy of this states is higher, that is consistent with the available experimental data.

O 37.50 Tue 18:30 P2

***ab-initio* investigation of topological states in $\alpha$-Sn surfaces** — •Sebastian Kuefner, Juergen Furthmueller, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

The properties of topological insulators recently have been discussed with rising attention in solid state physics. Topological insulators are insulating as a bulk material but exhibit metallic surface or edge states that are topologically protected and, therefore, are independent of orientation and passivation of interfaces or surfaces. Usually, the edge states show a Dirac-cone like dispersion. Mercury telluride has been proven to be a two dimensional topological insulator because of its inverted band structure. However, although $\alpha$-tin shows a very similar electronic structure, it is still under debate whether $\alpha$-tin is a topological insulator as well. We use density-functional theory based on a hybrid functional to investigate the electronic structure $\alpha$-Sn(001) surfaces and show the existence of a topological edge state close to the Fermi level.

O 37.51 Tue 18:30 P2

**Growth of epitaxial Bismuth films on vicinal Si(111)** — •Monika Jäger[1], Christian Brand[1], Daniel Lükermann[1], Saddam Banyoudeh[1], Sergeii Sologub[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Institute of Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine

Vicinal semi-metallic Bi-films are expected to reveal topologically protected edge states. In this study the growth of Bi-multilayer structures on Si(557) substrates has been investigated by LEED and STM. Thereby, wetting layer structures formed prior to the film deposition on Si(557) surfaces turned out to be crucial for epitaxial growth. Only in the presence of Bi-wetting layers well-ordered films can be grown. Depending on coverage of the Bi-wetting layers either stepped Bi(111) or Bi(110) have been found. In addition, Bi(221) surfaces have been obtained only on Bi-wetting layers formed by less than a monolayer. The formation of Si(335)-facets during formation of the wetting layers turns out to be essential for the growth of the these structures.

O 37.52 Tue 18:30 P2

**Multichannel-Spin-Polarimetry for the Analysis of Spin-Transport in Metal-Organic Interfaces** — •Erik Schaefer[1,2], Dima Kutnyakhov[1], Gerd Schönhense[1,2], and Hans-Joachim Elmers[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, D-55128 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudinger Weg 9, D-55128 Mainz, Germany

The spin-resolved analysis of electronic properties of hybrid metal-organic interfaces is of great interest. Metal-organic materials are promising candidates for spintronic applications because of their advantageous properties and chemical flexibility.

Over the past decades, the various forms of photoemission experiments have become one of the standard measurement techniques in surface physics. In contrast to conventional photon optics, an effective spin polarisation analysis of a given electron beam is difficult. Since organic materials also tend to degrade within a short period, a massive reduction of spin-resolved data acquisition time is crucial.

The recently developed multichannel spin- and angle-resolved photoemission spectroscopy[1] solves this issue by enhancing the figure of merit by several orders of magnitudes, making the analysis of spin-transport (e.g. spin diffusion lenght) in metal-organic interfaces possible. Both, the analysis of the novel measurement technique and metal-organic interfaces will lead to new insights and prospects.

Funded by Stiftung Rheinland Pfalz für Innovation (project 1038)

[1] M. Kolbe et al., Phys. Rev. Lett. 107, 207601 (2011)

O 37.53 Tue 18:30 P2

**Electronic and magnetic properties of the MnO(001), FeO(001), CoO(001), and NiO(001) surfaces** — •Andreas Schrön and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Due to their antiferromagnetic ordering, the 3*d* transition metal monoxides (TMOs) MnO, FeO, CoO, and NiO provide important benchmark materials for novel methods to investigate magnetic structures with atomic resolution. However, only little is known about the orientation of the local magnetic moments of the TM ions with respect to the bulk. The effect on the broken symmetry at surfaces, e.g. on the size and orientation of the local magentic moments, has not been investigated yet.

We present *ab-initio* calculations of the TMO(001) surfaces in order to approach the open questions related to the reduced symmetry at their surfaces. The calculations have been performed in the framework of spin-polarized density functional theory (DFT). Exchange and correlation (XC) are treated within the local density approximation (LDA) and an additional on-site Coulomb interaction $U$ acting on the transition-metal 3*d* shells is included (LDA+$U$). Spin-orbit interaction is included self-consistently during all calculations and non-collinear arrangements are allowed.

We focus especially on the influence of the broken symmetry at the surface on the magnitude and orientation of the local magnetic moments of the 3*d* TM ions.

O 37.54 Tue 18:30 P2

**Photoemission calculations for surface states in 2DEGs within the models of $\vec{k}\cdot\vec{p}$ theory** — •Markus Flieger, Jürgen Henk, and Ingrid Mertig — Martin-Luther-Universität Halle-Wittenberg, Germany

Surface states in two-dimensional electron gases like Rasbha-split and topological surface states attracted recently a lot of attention due to their unique electronic structure and spin texture. An appropriate method for investigating them is spin- and angle-resolved photoelectron spectroscopy (SPARPES).

These kinds of surface states are well described by model Hamiltonians which are derived within $\vec{k}\cdot\vec{p}$ perturbation theory. We report on analyses for model Hamiltonians of systems with different symmetries in the process of photoemission. In addition, we compare theoretical intensities and spin polarizations of the photoelectrons with results from experiments and *ab initio* calculations.

O 37.55 Tue 18:30 P2

**Multi probe transport measurements on $\mathrm{Bi_2Se_3}$ thin films** — •Sebastian Bauer, Paul Graf, Rolf Möller, and Christian A. Bobisch — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

Since their prediction, topological insulators (TIs) like $\mathrm{Bi_2Se_3}$ are very popular in condensed matter physics due to their peculiar electronic properties. At the surface of 3D TIs a conducting and spin polarized surface state evolves, which does not allow the direct backscattering of electrons [1]. We studied the transport field of a 4.5 QL thin $\mathrm{Bi_2Se_3}$ film by scanning tunneling potentiometry, an extended scanning tunneling microscopy (STM) technique which allows us to analyze the microscopic topography and the correlated microscopic electrochemical potential of the surface simultaneously [2]. The $\mathrm{Bi_2Se_3}$ film was prepared in-situ on a reconstructed Si(111)-($\sqrt{3}$x$\sqrt{3}$)-Bi according to Zhang et al. [3]. On large scale measurements of the electrochemical potential we observe a lateral gradient of the electrochemical potential of the $\mathrm{Bi_2Se_3}$ surface. Both, the microscopic sheet conductance and the macroscopic sheet conductance of the 4.5 QL film agree well to other data from literature [4]. A thermovoltage signal at surface step edges indicates the local variation of the density of states [5].

[1] M. Z. Hasan, C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010). [2] A. Bannani, C. A. Bobisch, R. Möller, Rev. Sci. Instrum. 79, 083704 (2008). [3] G. Zhang, et al., Appl. Phys. Lett. 95, 053114 (2009). [4] A. A. Taskin et al., Phys. Rev. Lett. 109, 066803 (2012). [5] T. Zhang et al., Phys. Rev. B. 87, 115410 (2013).

O 37.56 Tue 18:30 P2

**Specular reflection of spin-polarized electrons from W(001) spin-filter crystal in a larger range of scattering energies and angles** — •D. Kutnyakhov[1], H.J. Elmers[1], G. Schönhense[1], C. Tusche[2], J. Kirschner[2], S. Borek[3], J. Braun[3], J. Minàr[3], and H. Ebert[3] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz — [2]MPI für Mikrostrukturphysik, Halle — [3]Department Chemie, Physikalische Chemie, Universität München

Extending our previous work on the novel imaging spin-filter technique based on electron diffraction from W(001) in the specular (00)-LEED spot [1,2], we studied the scattering energy (E) and angle of incidence (theta)-landscape of the spin sensitivity S, and reflectivity I/I$_0$. The setup includes a spin-polarized GaAs electron source and a rotatable delayline detector for spatially-resolving detection. We measured the intensity and spin asymmetry of the specularly reflected beam for a large range of energies and angles of incidence of spin-polarized primary electrons. Resulting energy-angular landscape show rather good agreement with theory (relativistic layer KKR SPLEED code [3,4]). The results identify several regions of high asymmetry and figure of merit. These regions open a path for the development of the multichannel spin-filter for electron spectroscopy and momentum microscopy with higher performance. Funded by BMBF (05K13UM1).

[1] C. Tusche et al., APL 99 (2011) 032505; [2] M. Kolbe et al., PRL 107 (2011) 207601; [3] R. Feder in Polarized Electrons in Surface Physics (World Scientific, Singapore, 1985); [4] H. Ebert et al., Rep. Prog. Phys. 74, 096501 (2011)

O 37.57 Tue 18:30 P2

**Growth morphology of thin films on the metallic and oxide surfaces** — •Aleksander Krupski — Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom.

In this work we briefly review recent investigations concerning growth morphology of thin metallic films on the $Mo(110)$ and the $Ni_3Al(111)$ surfaces, and $Fe$ and $CopperPhthalocyanine(C_{32}H_{16}N_8Cu)$ on the $Al_2O_3/Ni_3Al(111)$ surface. Comparison of $Ag$, $Au$, $Sn$, and $Pb$ growth on the $Mo(110)$ surface has shown a number of similarities between these adsorption systems except surface alloy formation that has only observed in the case of $Sn$ and $Au$. In the $Pb/Mo(110)$ and $Pb/Ni_3Al(111)$ adsorption systems selective formation of uniform $Pb$ island heights during metal thin film growth has been observed and interpreted in terms of quantum size effects. Furthermore, our studies showed that $Al_2O_3$ on $Ni_3Al(111)$ exhibits a large superstructure in which the unit cell has a commensurate relation to the substrate lattice. In addition, $CopperPhthalocyanine$ chemisorbed weakly onto an ultrathin $Al_2O_3$ film on $Ni_3Al(111)$ and showed a poor template effect of the $Al_2O_3/Ni_3Al(111)$ system. In the case of iron cluster growth on $Al_2O_3/Ni_3Al(111)$ the nucleation sites were independent of deposition temperature, yet cluster shape showed a dependence. In this system, $Fe$ clusters formed a regular hexagonal lattice on the $Al_2O_3/Ni_3Al(111)$.

O 37.58 Tue 18:30 P2

**Structure and manipulation of h-BN on Ir(111)** — •Domenik M. Zimmermann, Ulrike A. Schröder, and Thomas Michely — II. Physikalisches Institut, Zülpicher Str. 77, Universität zu Köln

The formation of high quality hexagonal, 2D boron nitride (h-BN) through thermal decomposition of borazine($B_3N_3H_6$) on Ir(111) is investigated by scanning tunneling microscopy (STM).

As growth methods chemical vapor deposition (CVD) and temperature programmed growth (TPG, room temperature adsorption followed by annealing) are applied in the temperature range from 1000 K to 1400 K. In contrast to graphene, the morphology depends strikingly on the growth method applied, resulting in nearly perfect, large h-BN flakes (CVD) or percolation networks with nanoscale holes (TPG).

Unlike graphene, h-BN consists of two distinct sublattices, made up of B and N atoms, respectivly. Exchanging B and N atoms results in two different domains, that are observed with STM. We investigate the preferred domain orientation depending on growth temperature and growth method.

The monolayer is further treated in the electric field of the STM tip. Periodic, 2-dimensional defect structures are achieved by tip-induced manipulation. A threshold bias voltage for this nanomesh creation is obtained and the manipulation probability is investigated as a function of tunneling parameters.

O 37.59 Tue 18:30 P2

**Properties of ultrathin Pb layers on the Ni3Al(111) studied by AES/LEED/STM/DFT** — •Katarzyna Miśków and Aleksander Krupski — Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom.

The morphology, atomic and electronic structure of ultrathin Pb layers deposited on the $Ni_3Al(111)$ face in ultrahigh vacuum at the substrate temperature, ranging from 200 K to 950 K, were investigated with the use of Auger electron spectroscopy (AES), low-energy electron diffraction (LEED), directional elastic peak electron spectroscopy (DEPES), scanning tunnelling microscopy (STM). Density functional theory calculations (DFT) with the use of CASTEP code were used to describe atomic and electronic structure of the $Pb/Ni_3Al(111)$ system. The analysis of AES and STM measurements indicate that two-dimensional growth of the first Pb monolayer wetting layer takes place. For T = 200 K, lead on the $Ni_3Al(111)$ grows layer-by-layer, while for T = 300 K flat three atomic-layer-high islands seem to grow after the completion of the first lead monolayer. Above 350 K, the Stranski-Krastanov growth mode is observed. The ordered LEED paterns are observed. Above $\theta > 1.0$ ML, a three-dimensional growth of the Pb islands was observed with a strongly preferred atomic-scale magic height (N), hexagonal shape and flat-tops. At coverage $\theta = 3.5$ ML, only islands containing N = 3, 5, 7 and 11 atomic layers of Pb are observed. At the higher coverage $\theta = 5.5$ ML, three types of regular hexagonal islands with side lengths of 25, 30 and 45 nm are observed. Furthermore, three different island adsorption configurations were observed.

O 37.60 Tue 18:30 P2

**Growth study of nickel nanoislands on Ir(111)** — •Stefan Wilfert, Lydia El-Kareh, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We have investigated the growth of Ni nanoislands on Ir(111) by means of low-temperature scanning tunneling microscopy (STM) and spectroscopy (STS). Both, iridium and nickel, exhibit a fcc crystal structure in the bulk with a lattice mismatch of about 8%. Ni deposition at room temperature initially leads to equally spread islands with a diameter of about 10 nm. The early onset of 3D islands nucleation is observed. After a post-annealing process we observe coalescence into larger hexagonally shaped islands up to 40 nm in diameter while maintaining the 3D island character.

O 37.61 Tue 18:30 P2

**XPD structure determination of $HfSi_2$ islands grown on Si(110) surfaces** — •Frank Schönbohm[1,2], Tobias Lühr[1], Dominique Handschak[1,2], Philipp Espeter[1,2], Christoph Keutner[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

Perspective replacement candidates of the $SiO_2$ gate dielectrics in MOSFETs are the so-called *high-k* materials like $HfO_2$. The thermal stability of thin $HfO_2$ films on Si(110) surfaces plays an important role during the production process and was studied by means of x-ray photoelectron spectroscopy (XPS) and photoelectron diffraction (XPD). The sample was stepwise annealed within the temperature range from 500°C up to 770°C. XPS spectra of the Si 2p, Hf 4f, and O 2s signal were recorded as a function of the annealing temperature. The measurements indicate a stable $HfO_2$-film for temperatures up to 730°C. Further annealing at temperatures up to 770°C removed the oxygen completely from the sample and the remaining Hf was bound to the substrate forming $HfSi_2$. SEM investigations of the surface showed that the $HfSi_2$ is arranged in islands at the surface. An XPD pattern of the Hf 4f signal was recorded in order to investigate the internal atomic structure of the $HfSi_2$ islands. The experimental diffraction pattern was compared to simulated pattern resulting in a structure model for the $HfSi_2$ islands.

O 37.62 Tue 18:30 P2

**Structural and optical investigations of organic-organic heterosystems** — •Julia Peuker, Falko Sojka, Matthias Meissner, Marco Gruenewald, Roman Forker, and Torsten Fritz — University of Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany

Here, we report on the epitaxial growth of quaterrylene (QT) on one monolayer of hexabenzocoronene (HBC) on graphene, epitaxially grown on silicon carbide (SiC(0001)). During the deposition the change of the optical properties is observed with Differential Reflectance Spectroscopy (DRS). This *in-situ* method provides information on the interaction of the molecular transition dipoles and a possible charges transfer. It is also used for the control of the layer thickness to get a well-defined structure. The resulting structure is characterized by Low Energy Electron Diffraction (LEED). Finally, other heterostructures serve as comparison.

It is already known that an organic interlayer can change the interaction between the substrate, here epitaxial graphene, and the subsequently deposited molecules drastically. This effect can be used for electronic decoupling. [R. Forker, D. Kasemann, T. Dienel, C.Wagner, R.Franke, K. Müllen, and T. Fritz, *Adv. Mater.* **2008**, 20, 4450 - 4454.]

O 37.63 Tue 18:30 P2

**Growth of coronene-layers on reactive and inert substrates** — •Tobias Huempfner, Falko Sojka, Marco Gruenewald, Roman Forker, and Torsten Fritz — Friedrich-Schiller-University Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany

Here we report on the growth of ultrathin coronene-layers on different substrates deposited via Organic Molecular Beam Epitaxy (OMBE) under ultra-high vacuum conditions. On the one hand we used reactive substrates like Ag(111) and Au(111), on the other hand inert substrates like mica. The differences in the optical properties due to the molecule-substrate interactions were observed in situ during the deposition using Differential Reflectance Spectroscopy (DRS) [1]. The resulting molecular structures of the coronene-films are characterized with Low Energy Electron Diffraction (LEED) as well as Scanning Tunneling Microscopy (STM) for metallic and Atomic Force Microscopy (AFM) for inert substrates, respectively, at about 1 K.

A layer system consisting of potassium-chloride (KCl) on a Ag(100) surface gains special interest as a substrate for this molecule, because KCl-layers seem to be easy to prepare on this surface [2]. Moreover, STM investigations are still possible due to the metal-crystal below the KCl-layer, although the coronene still grows electronically decoupled from the Ag(100) surface.

[1] R. Forker *et al.*, Annu. Rep. Prog. Chem., Sect. C: Phys. Chem., **2012**, 108, 34-68.

[2] M. Müller *et al.*, Surface Science, **2011**, 605, 1090-1094.

O 37.64 Tue 18:30 P2

**Growth of epitaxial $Bi_{1-x}Sb_x$ films** — •Julian Koch, Philipp Kröger, Herbert Pfnür, and Christoph Tegenkamp — Leibniz Universität Hannover, Inst. für Festkörperphysik, Appelstr. 2, 30167 Hannover

The alloy $Bi_{1-x}Sb_x$ was the first 3D topological insulator to be discovered. Depending on the relative concentrations of Bi and Sb the surface states can be tuned between topologically trivial and nontrivial (e.g. see PRB 83, 201104(R)). The fundamental difference of these states can be probed in principle by surface transport. However, in order to identify these different regimes, control of the film quality as well as the atomic defect structure is mandatory. In-situ epitaxy is a well established concept to grow such high-quality films.

In this study this material class was epitaxially grown by co-deposition on Si(111) substrates and investigated by means of low energy electron diffraction. Films of different stoichiometry ranging from $x = 0.07 - 0.3$ have been grown by co-deposition at various temperatures and correlated with their lattice constants. In order to achieve epitaxial growth of (111)-oriented $Bi_{1-x}Sb_x$-films a buffer layer is necessary which has been realized by growth of 10 bilayer Bi. Growth of contiguous $Bi_{1-x}Sb_x$-films with single domain structures succeeds for deposition temperatures below 400 K. At higher temperatures the film is ruptured accompanied by segregation of Sb as confirmed by XPS.

O 37.65 Tue 18:30 P2

**Surface investigation of ceria films on Si(111) after post deposition annealing** — •Robert Oelke[1], Wanja Spiess[1], Henrik Wilkens[1], Marvin H. Zoellner[2], Gang Niu[2], Thomas Schroeder[2,3], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — [2]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [3]BTU Cottbus, Institute of Physics, Konrad-Zuse-Str.1, 03046 Cottbus, Germany

$CeO_2(111)$ films are a promising candidates in the field of microelectronics due to their high dielectric constant and the very small lattice mismatch in respect to Si(111). Furthermore, $CeO_2$ films can be used as model systems to study its catalytic properties. The generation of oxygen vacancies is of particular interest since they have a strong influence on the catalytic, as well as, the electronic properties.

Therefore, we present a post deposition annealing study of several $CeO_2(111)$ films grown on hex-$Pr_2O_3$/Si(111) system. Films with thicknesses in the range of 8 to 250 nm are annealed under UHV conditions. After each annealing step low energy electron diffraction measurements combined with spot profile analysis (SPA-LEED) are performed.

Several superstructures are formed at elevated temperatures indicating a periodic order of oxygen vacancies during reduction. Spot profile analysis show that the crystalline quality increases with higher film thickness.

O 37.66 Tue 18:30 P2

**Constructive electromigration of indium on silicon(111)** — •Paul Graf, Alexander M. Bernhart, Mark R. Kaspers, Christan A. Bobisch, and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

Electromigration (EM) is the material transport driven by an electron current or by an electric field [1]. This process is technically very important for thin/small conductors in electronic devices (e.g. CPUs) since the dimension of such structures reach the range of 10 nm or less. Here, we investigate in situ the EM of Indium on a Si(111) surface using a four probe scanning tunneling microscope (STM) and a scanning electron microscope (SEM). We study the indium induced surface reconstruction on Si(111) [2] with $\mu m$-scaled indium islands. To apply an electric field in parallel to the surface two tips make contact to islands. Using the SEM we observe the formation of additional In islands in between the contacted islands, which results from the material transport from the indium reconstruction. In contrast to the usual destructive EM, we use this transport to form Indium wires; the method may become a starting point for the directed growth of small electronic networks.

[1] R. Landauer and W. Woo, Phys. Rev. B 10, p. 1266 (1974).
[2] Eli Rotenberg et al., Phys. Rev. Lett. 91, 246404 (2003).

O 37.67 Tue 18:30 P2

**In situ control of step formation on Si(100) in process gas ambient** — •Sebastian Brückner[1,2], Oliver Supplie[1,2], Peter Kleinschmidt[2,3], Henning Döscher[2], Anja Dobrich[2], and Thomas Hannappel[1,2,3] — [1]Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — [2]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98693 Ilmenau — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

Double-layer step formation on Si(100) substrates is a crucial prerequisite for antiphase-domain free III-V heteroeptitaxy. Si(100) preparation in hydrogen process gas ambient, which is commonly employed for Si and III-V device preparation, differs strongly from preparation in ultra-high vacuum due to strong interaction between $H_2$ and the Si surface. In situ surface characterization by reflection anisotropy spectroscopy allowed us to study and control the domain formation of Si(100) surfaces directly in dependence on process parameters during MOVPE preparation. Here, we show that energetically and kinetically driven step formation on Si(100) compete depending on MOVPE process conditions. While preparation of vicinal substrates at low $H_2$ pressure leads to predominant (2×1) surface reconstruction with $D_B$ steps (i.e. dimer rows perpendicular to step edges), preparation at high $H_2$ pressure resulted in a predominant (1×2) reconstructed surface with $D_A$ steps (dimer rows parallel to step edges). On nearly exact Si(100), Si monolayer removal in $H_2$ ambient results in an oscillating A- and B-type majority domain formation.

O 37.68 Tue 18:30 P2

**SPA-LEED studies on structure and morphology of $Ce_xPr_{1-x}O_2$ films** — •Wanja Spiess[1], Henrik Wilkens[1], Marvin H. Zoellner[2], Gang Niu[2], Thomas Schroeder[2,3], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — [2]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [3]BTU Cottbus, Institute of Physics, Konrad-Zuse-Str.1, 03046 Cottbus, Germany

Rare earth oxides (REOs) are in the focus of research for several catalytic applications, e.g. the three-way automotive exhaust catalysis. Lattice oxygen directly participates in these surface redox reactions based on the Mars-van-Krevelen mechanism. Therefore, the structural properties of the REOs and especially oxygen vacancies have a strong impact on the catalytic reactivity and selectivity. In addition, the intermixing of different REOs gives further opportunity of tuning the catalytic properties. We present a post deposition annealing study of mixed $Ce_xPr_{1-x}O_2$ films grown on Si(111) using SPA-LEED (spot profile analysis at low energy electron diffraction) to control structural properties. Several crystalline structures are stabilized at moderate temperatures while at high temperatures silicide is formed. Spot profile analysis of the fundamental diffraction spot reveals a strong correlation between surface morphology (atomic steps) and the stoichiometry of the films.

O 37.69 Tue 18:30 P2

**Two-Photon Photoemission from magnesium oxide** — •Rebecca Pöschel, Andrej Classen, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Staudtstr. 7, D-91058 Erlangen

We prepared MgO by evaporating magnesium on a well-defined Ag(100) single-crystal surface kept at 473 K in $10^{-7}$ mbar oxygen. Thin films of different thicknesses between 0.25 and 10 monolayers (ML) were deposited on the crystal. The samples were studied by two-photon photoelectron spectroscopy (2PPE) (1.55 eV and 4.65 eV) and by vacuum ultra-violet (VUV) photoelectron spectroscopy (21.2 eV). The work function decreases with increasing thickness and reaches a value of 3.14 eV for 10 ML. The image potential states of Ag(100) are seen for MgO coverages up to 1 monolayer. Between 1 and 2.5 ML the 2PPE spectra are rather structureless and make MgO an ideal substrate for the study of unoccupied electronic states of adsorbed molecules.

O 37.70 Tue 18:30 P2

**Growth and magnetic properties of ultrathin iron oxide films on MgO(001) and STO(001)** — •Nico Pathé, Olga Schuckmann, Tobias Schemme, Matthäus Witziok, Karsten Küpper, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück

In this work, ultrathin iron oxide films were reactively grown on MgO(001) and STO(001) at 250 °C depositing Fe in $5 \cdot 10^{-6}$ mbar oxygen. Previous to this, NiO interlayers were reactively grown on both materials at 250 °C and an oxygen partial pressure of $10^{-5}$ mbar. All samples were investigated via X-Ray Photoelectron Spectroscopy (XPS) and X-Ray Absorption Spectroscopy (XAS). The surface structures were determined by Low Energy Electron Diffraction (LEED) and the magnetic properties of the films were analyzed with Magneto-Optic Kerr Effect (MOKE) and X-Ray Magnetic Circular Dichroism (XMCD). XPS data show that stoichiometric magnetite was grown on all surfaces. This result was confirmed by the expected $(\sqrt{2} \times \sqrt{2})R45^\circ$ superstructure obtained in LEED measurements. XMCD results indicate that the substrate has a strong influence on the critical film thickness, where stoichiometric magnetite occurs. All ironoxide films were found to be ferrimagnetic and most of them show a fourfold magnetic in-plane anisotropy in MOKE studies.

O 37.71 Tue 18:30 P2

**Electronic structure of the polar ZnO(0001) surface with Ga and N substitution: A density functional theory study** — •Jacek Piechota[1], Jakub Sołtys[1], and Stanisław Krukowski[1,2] — [1]ICM, University of Warsaw, ul. Pawińskiego 5a, 02-106 Warszawa, Poland — [2]Institute of High Pressure Physics, Polish Academy of Sciences, ul. Sokołowska 29/37, 01-142 Warsaw, Poland

An extensive theoretical investigation of the polar ZnO(0001) surface, with Ga and N substitution for Zn and O, respectively, was performed. It was shown that some extra bands, located near the valence-band maximum, emerge due to dangling bonds existing at nonsaturated O or Zn layers. These dangling bonds were subsequently saturated by the hydrogen atoms. The surface related electron bands were than calculated for slabs where the Zn atom was substituted by the Ga atom, or the O atom by the N atom. In all cases, for different distances between the surface atoms and hydrogen saturation atoms the electric field within the ZnO slab was computed. It was demonstrated that the slab polarization depends on the distance between the slab surfaces and the hydrogen atoms. The Fermi level is pinned at both faces of the slab, and this fact determines the electric field within the slab. Also, the properties of the ZnO(0001) surface, as a function of the Fermi energy of the system, were examined. The obtained results were compared with experimental and other theoretical data.

O 37.72 Tue 18:30 P2

**Electronic properties and optical response of nonpolar GaN surfaces** — •Marc Landmann, Eva Rauls, and Wolf Gero Schmidt — University of Paderborn, Germany

In nonpolar or semipolar GaN, the hexagonal c axis is orthogonal or inclined to the growth direction, in order to eliminate or limit the internal piezoelectric and spontaneous polarization fields that inherently limit the performance of optoelectronic devices. [1] We have calculated the electronic structure of the semipolar m-plane GaN(1-100) and a-plane GaN(11-20) surfaces within density functional theory (DFT). The band gap underestimation of (semi)local density functionals is corrected by a non-local Heyd-Scuseria-Ernzerhof (HSE) type hybrid-functional with an adjusted fraction of exact exchange. Surface characteristic states and their microscopic origin are identified in the calculated surface band structure and density of states. While the complex dielectric functions of GaN bulk and surface slabs, calculated within the independent particle approximation (IPA) on the HSE hybrid functional DFT level of theory, fail to reproduce prominent near band-edge features of the optical response, the inclusion of excitonic effects via solution of the Bethe-Salpeter equation for Coulomb correlated electron-hole pairs reproduces the experimentally observed spectral features. The optical anisotropies of the semipolar surfaces are investigated by calculation of the reflection anisotropy spectroscopy (RAS) [2] spectra and discussed alongside experimental data.

[1] J. Schörmann et al., Appl. Phys. Lett. 89 (2006) 131910.
[2] W. G. Schmidt, phys. Stat. sol. (b) 242 (2005) 2751.

O 37.73 Tue 18:30 P2

**Adsorption of PTCDA on KCl and NaCl surfaces** — •Hazem Aldahhak, Wolf Gero Schmidt, and Eva Rauls — Theoretische Physik, Universität Paderborn

In recent years, various highly regular supramolecular architectures of self-organized molecules on crystals have been designed and used in the bottom-up device technology. In the past, metal surfaces have frequently been used as substrate. However, metal substrates induce screening and quenching effects and thus hamper the detailed spectroscopy of the adsorbed overlayer. In contrast, molecular adsorption on ionic crystals like sodium or potassium chloride opens the possibility to study electronically decoupled molecules. Here we present density-functional theory calculations on the adsorption of single PTCDA molecules on KCl and NaCl (100) surfaces. Thereby, the adsorption on flat surfaces as well as on stepped substrates has been investigated. In order to unterstand and rationalize the adsorption mechanisms leading to the formation of these structures, a large variety of interface geometries was studied and analyzed with respect to the contribution of ionic, covalent and van-der-Waals interactions between adsorbates and substrates. The influence of the substrate and bonding mechanism on the molecular electronic structure has been investigated in detail and compared with the experimental data available. The calculation of the potential energy surface (PES) allows us to determine the activation energy for the mobile molecules on the surface.

O 37.74 Tue 18:30 P2

**Liquid Crystal Adsorption on Lithium Niobate (0001) Surfaces** — •Christian Braun, Simone Sanna, Eva Rauls, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn, Paderborn, Germany

$LiNbO_3$ (LN) is a man-made ferroelectric with a extraordinary high spontaneous polarization of 0.7 $C/m^2$. The polarization creates a net electric field outside of the LN crystal, which can be locally patterned by switching ferroelectric domains. This opens the possibility for selective molecular adsorption, in particular of polarizable molecules, at the LN surface. Liquid crystals are highly interesting adsorbates, as their optical properties are easily manipulated by electrical or magnetic fields. Indeed, they are currently employed for the realization of modern displays, as well as in other optic and opto-electronic devices. Therefore, the detailed knowledge of the adsorption mechanisms of liquid crystal on LN, as well as the understanding of the influence of the ferroelectric substrate on the molecular ordering, would be highly desirable. In order to model the interaction of liquid crystals with ferroelectric surfaces, we have investigated the adsorption of 4-*n*-octyl-4′-cyanobiphenyl (8CB) molecules at the LN(0001) surfaces from *first-principles*. The adsorption energy and configuration are found to be both strongly polarization and coverage dependent. Van der Waals interactions, accounted for by Grimme-type corrections to the total energy, are found to yield a major contribution to the bond strength and influence the adsorbate orientation.

O 37.75 Tue 18:30 P2

**Heat induced passivation of $CuInSe_2$ surfaces: A strategy to optimize the efficiency of chalcopyrite thin film solar cells?** — Harry Mönig[1,2], •David Lockhorn[1,2], Nabi Aghdassi[1], Alexander Timmer[1,2], Christian A. Kaufmann[3], Raquel Caballero[4], Helmut Zacharias[1,2], and Harald Fuchs[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, Germany — [2]CeNTech, Center for Nanotechnology, Münster, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [4]Departamento de Física Aplicada, Universidad Autónoma de Madrid, Madrid, Spain

Despite the success of chalcopyrite thin film solar cells, many open questions concern the complex defect physics at the interface between the n-type window layer and the p-type absorber, which crucially determines the device efficiency. Therefore, our study addresses this issue by scanning tunneling spectroscopy, photoelectron, and inverse photoelectron spectroscopy. After removing oxides by a KCN treatment and subsequent UHV annealing at 280°C, a complete passivation of defect levels is observed, which goes along with a type inversion and an enlarged band gap at the surface. Therefore, this sample state consolidates three exclusively beneficial properties, which potentially minimize interface recombination losses and increase the open circuit voltage in completed devices. In contrast, oxidation of the surface by annealing in air reduces the surface band bending and creates a high density of charge compensated defect levels.

O 37.76 Tue 18:30 P2

**A density functional theory study of the structural and electronic properties of the GaN(000-1) surface** — •Jacek Piechota[1], Maria Ptasińska[1], Jakub Sołtys[1], and Stanisław Krukowski[1,2] — [1]ICM, University of Warsaw, Pawińskiego 5a, 02-106 Warsaw, Poland — [2]Institute of High Pressure Physics, Polish Academy of Sciences ul. Sokołowska 29/37, 01-142 Warsaw, Poland

Nitrogen terminated GaN(000-1) surface was studied using the density functional theory (DFT). It was shown that some extra bands, located near the valence-band maximum, emerge due to dangling bonds existing at nonsaturated N or Ga surfaces, respectively. These dangling bonds were subsequently saturated by the hydrogen atoms. The surface related electron bands were calculated for different distances between the surface atoms and hydrogen saturation atoms. The electric field within the GaN slab was computed, showing that the slab polarization depends on the distance between the slab surfaces and the hydrogen atoms. The Fermi level is pinned at both faces of the slab, and this fact determines the electric field within the slab. Also, the properties of the GaN(000-1) surface, as a function of the Fermi energy of the system, were examined. The obtained results were compared with experimental and earlier theoretical investigations data.

O 37.77 Tue 18:30 P2

**The interaction of benzaldehyde with water-saturated Si(001)** — •Sebastian Frey, Daniel Laumann und Ulrich Köhler — Ruhr-Universität , Bochum, NRW

In the last years the interaction between organic compounds and silicon got importance regarding the connection of organic and inorganic conductors in semiconductor technology. Particular interest lies on molecules containing conjugated $\pi$-electrons, since they often act as organic (semi-)conductors. The adsorption of Benzaldehyde (BAH) on Si(100)-2x1 surfaces can be used as a model system to understand the interaction of aromatic species with semiconductor surfaces. In technology the Si dimers are mostly saturated with O adatoms or OH-groups due to contact with water molecules. We investigated the bonding between BAH and such dimers with HR-EELS to further understand the adsorption mechanism and to clarify the role of H- and OH-terminated Si. Water, deuterium, hydrogen and hydroxil saturated and unsaturated Si was exposed to normal and deuterium labeled BAH to check whether the H adatom or the OH group is involved in the adsorption process.

O 37.78 Tue 18:30 P2

**Poly(phenylene-ethynylene)s and related bichromophoric molecules on HOPG: An STM study** — •Stefan-S. Jester, Klaas Remmerssen, Daniela Schmitz, and Sigurd Höger — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Conjugated polymers have attracted increased attention in the last decades due to their interesting optical and electronic properties. We have recently synthesized and investigated model dimers of conjugated oligomers, linked in a macrocyclic scaffold. Two monodisperse conjugated oligomers of distinct chain length, based on phenylene-ethynylene-butadiynylene entities, are intramolecularly connected by two rigid clamp units, providing a defined distance and alignment in parallel. The lengths and distances of the chromophores are synthetically defined and adjustable with atomic-scale precision. Self-assembled monolayers (SAMs) of the compounds at the solid/liquid interface of highly oriented pyrolytic graphite (HOPG) and 1,2,4-trichlorobenzene (TCB) are studied by scanning tunneling microscopy (STM) with submolecular resolution. The results provide understanding about the shape and structure of the compounds. [1] S.-S. Jester, A. Idelson, D. Schmitz, F. Eberhagen, S. Höger *Langmuir* **2011**, *27*, 8205; [2] S. Liu, D. Schmitz, S.-S. Jester, N. J. Borys, S. Höger, J. M. Lupton *J. Phys. Chem. B* **2013**, *117*, 4197; [3] S.-S. Jester, D. Schmitz, F. Eberhagen, S. Höger, *Chem. Commun.* **2011**, *47*, 8838.

O 37.79 Tue 18:30 P2

**Imaging and controlling organic molecule adsorption on metal plated silicon surfaces: formation and structure of organic-silicide monolayers** — •Pavel Shukrynau, Marius Toader, Lars Smykalla, and Michael Hietschold — 1 Institute of Physics Technische Universität Chemnitz, Reichenhainer Straße 70, D-09107 Chemnitz, Germany.

We have employed variable temperature scanning tunneling microscopy (STM) to follow the adsorption of fluorinated cobalt-phthalocyanine (F16CoPc) on Fe plated silicon 7*7 reconstructed surface. The coverage of F16CoPc varied from 0.05 up to 3 monolayers (ML). At coverage more than a monolayer the surface is completely covered with roundly shaped 3D clusters of typical size of ˜1 nm. Each cluster has lobe-like pattern that may suggest that they consist of several perpendicular standing phthalocyanine molecules. Tunneling spectra taken over each individual lobe within a cluster reveal small energy gap, showing semiconductor-like behavior of constituent parts. The general structure of the surface, i.e., shape of the step edges, remains unchanged, however, the cluster coverage/cluster size is substrate dependent. The interplay between the electronic and structural properties of molecular layers and transition metal silicide is the key to tune the functionalities of hybrid organic-semiconductor interfaces.

O 37.80 Tue 18:30 P2

**Barium titanate: A promising candidate for the use of oxide-based electronics.** — •Peter Lutz[1,2], Sebastian Fiedler[1,2], Chul-Hee Min[1,2], Hendrik Bentmann[1,2], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, 97074 Würzburg, Germany — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institute für Technologie KIT, 76021 Karlsruhe, Germany

Barium titanate (BTO) belongs to the material class of transition metal oxides which recently arouse a great deal of attention because of their multifunctional character and the rich physics occurring especially at oxide interfaces [1,2]. BTO is a particularly interesting oxide material showing ferroelectric properties and several structural phase transitions as a function of temperature [3,4]. One idea is to use this material as a substrate for thin films and to modify the film properties through the electric polarization direction. This requires detailed knowledge of the surface electronic and structural properties. To this end we investigate the influence of different preparation processes on the surface properties of BTO using tunneling spectroscopy (STM/STS), electron spectroscopy (XPS/UPS) and electron diffraction (SPALEED). We focus in particular on the processes for the evolution of oxygen vacancies at the surface in regard of their influence on the electronic structure and of their function in the formation of thin layers on the substrate.

[1] H. Y. Hwang et al., Nature Mat., 11, 103 (2012) [2] C. H. Ahn et al., Nature, 424, 1015 (2003) [3] R. E. Cohen, Nature, 358, 136 (1992) [4] W. Zhong et al, PRL, 73, 1861 (1994)

O 37.81 Tue 18:30 P2

**Structure determination of CdO(100): A combined quantitative LEED and DFT study** — •James Mudd[1], Katarzyna Miśków[1], Jacopo Ardini[2], Georg Held[2], Aleksander Krupski[1], and Chris McConville[1] — [1]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom. — [2]Department of Chemistry, University of Reading, Reading, RG6 6AD, United Kingdom

Cadmium oxide (CdO) is a transparent conducting oxide, with potential applications in solar cells and gas sensing. In addition it exhibits interesting surface electronic properties including electron accumulation resulting in a quantized 2D electron gas (Q2DEG), despite this there have so far been no studies of the surface structure of CdO. The surface structure of CdO(100) has been determined by quantitative low-energy electron diffraction LEED I(V) analysis and density functional theory (DFT) calculations. An analysis of LEED I(V) spectra from the CdO(100) surface has been performed by comparing measured intensities with data calculated using an automated CLEED program package. All DFT calculations have been performed with the CASTEP code (Cambridge Sequential Total Energy Package) using a plane-wave pseudopotential formalism.

O 37.82 Tue 18:30 P2

**Structure determination of $TiO_2(001) - (4 \times 1)$ surface using quantitative low-energy electron diffraction** — •Katarzyna Miśków[1], James Mudd[1], Jacopo Ardini[2], Sean McMitchell[1], Georg Held[2], Chris McConville[1], and Aleksander Krupski[1] — [1]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom. — [2]Department of Chemistry, University of Reading, Reading, RG6 6AD, United Kingdom

Titania ($TiO_2$) is a non-toxic, wide band-gap semiconductor with three different crystal polymorphs (brookite, rutile and anatase). Systems based on $TiO_2$ have a large variety of possible applications including photocatalysis, heterogeneous catalysis, electrochloric devices and solar cells for hydrogen and electric energy production. Here we report a quantitative structural determination of the anatase $TiO_2(001)$-$(4\times1)$ surface with the use of low energy electron diffraction. An analysis of LEED I(V) spectra from the $(4\times1)$ surface has been performed by comparing measured intensities with data calculated using the automated CLEED program.

O 37.83 Tue 18:30 P2

**CO on NiO(001)** — •Josef Grenz, Alexander Schwarz, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany

Tips functionalized with CO molecules have recently been used in AFM studies to enhance the resolution to the submolecular level [1]. While investigating single CO molecules with metallic tips on different substrates various studies observed a ring-like structure (e.g. [2]). Since metallic tips should always exhibit a dipole moment [3] and CO, at least in the gas phase, also possesses a dipole moment, we attribute the observed contrast pattern to an interplay between attractive van-der-Waals and repulsive electrostatic dipole-dipole interactions. The latter should become relevant before the Pauli repulsion, which can be probed at even smaller distances.

In this contribution a detailed analyses of CO adsorbed on the bulk insulator NiO(001) will be shown. Adsorption sites, diffusion and the possibility to quantify the magnitude of the dipole moment via imaging and spectroscopy will be discussed.

[1] L. Gross, *et al.*, Science **325**, (2009) 1110.

[2] Z. Sun, *et al.*, Phys. Rev. Lett. **106**, (2011) 046104.

[3] G. Teobaldi, *et al.*, Phys. Rev. Lett. **106**, (2011) 216102.

O 37.84 Tue 18:30 P2

**Characterization of the adlayer formation of CO on the NaCl(100) surface based on diffuse LEED intensities** — •Jochen Vogt and Birgit Vogt — Chemisches Institut der Uni Magdeburg, Magdeburg, Germany

Changes of the diffuse background in low-energy electron diffraction patterns can be used to characterize the stages of adlayer formation on well-ordered surfaces. Using the MCP-LEED technique, such experiments are also possible with bulk insulators without extensive surface charging. Although a helium atom diffraction study reported a $p(1\times1)$ symmetry of the system CO/NaCl(100) at temperatures above 35 K [1], superstructure features of the low-temperature $p(2\times1)$ phase are visible in LEED diffraction patterns well above this temperature. At 40 K, the subtraction of subsequently recorded LEED patterns reveals the formation of a diffuse background in the initial stages of the adlayer growth, consistent with an earlier proposed adsorption of CO at isolated sites [2]. The superstructure peels off from the background at a coverage of about half a monolayer. With the intention to develop a structure model of the disordered adsorbate, we present calculated diffraction patterns based on energy optimized local geometries. [1] D. Schmicker, J. P. Toennies, R. Vollmer, H. Weiss, J. Chem. Phys. 95 (1991), 9412 [2] C. Noda, G. E. Ewing, Surf. Sci. 240 (1990), 181

O 37.85 Tue 18:30 P2

**Pentacene adsorption and oxidation on a cobalt oxide bilayer film** — •Marina Schuler, Pascal Ferstl, Lutz Hammer, and M.Alexander Schneider — Lehrstuhl f. Festkörperphysik, FAU Erlangen-Nürnberg, 91058 Erlangen

As a prototypical example of the adsorption of functional organic molecules on an oxide surface we investigate pentacene on a bilayer of CoO epitaxially grown on Ir(100) [1] by STM and TDS in UHV. At 300 K the molecules adsorb flat-lying and a maximum areal density of 0.66 molecules per $nm^2$ is obtainable before multi-layer growth sets in. For single-layer coverage we observe a well-defined rotational alignment of the molecules with respect to the crystallographic axes of the CoO layer. The lateral binding configuration, in contrast, is variable on the atomic scale, since the molecules always bridge many inequivalent sites of CoO. From the absence of any lateral long-range order of the molecular film even after annealing to 400 K we conclude that the molecule-substrate interaction is dominating.

Pentacene starts to get oxidized by the CoO film already at 420 K, the molecules decompose into $CO_2$, $H_2O$, CO and $H_2$. In the beginning of the reaction the oxide layer gradually transforms into ordered sub-oxide structures. At higher temperatures and lower oxygen content of the cobalt oxide layer the dominant reaction products shift from $CO_2$ and $H_2O$ to CO and $H_2$. We note that the sub-oxides can be reoxidised in the same temperature regime, hence a full catalytic cycle of molecule oxidation is achievable.

[1] C. Tröppner, et al., PRB **86**, 235407 (2012)

O 37.86 Tue 18:30 P2

**Preparation and characterization of phenylphosphonic acid self-assembled monolayers on ZnO substrates** — •Alexandra Ostapenko and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7,35032 Marburg, Germany

Metal oxides are promising materials for fabrication of organic/inorganic hybrid structures. Surface functionalization by means of self-assembled monolayers (SAMs) is a promising approach to tailor their electronic interface properties or to fixate molecular chromophores. However, in contrast to widely used SAMs on gold surfaces, the molecular interaction and stability of such films on metal oxides have been much less studied. Here we report on the formation, thermal stability and molecular orientation of phenylphosphonic acid (PPA) SAMs on the Zn- and O-terminated basal planes of ZnO crystals that were studied by combining x-ray photoelectron spectroscopy (XPS), near edge x-ray absorption fine structure spectroscopy (NEXAFS) and thermal desorption spectroscopy (TDS). In addition the effect of OH-precoating on the adsorption was studied and the film ordering on pristine and defective ZnO surfaces was compared.

O 37.87 Tue 18:30 P2

**Superoxide and peroxide chemical states of adsorbed molecular oxygen on rutile TiO2 (110) surface** — •Hikmet Sezen, Alexei Nefedov, and Christof Wöll — Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

TiO2 is a highly attractive material due to its unique electron storage and transfer capabilities. In order to generate versatile chemical and physical interactions with the surface of TiO2, molecular oxygen was chosen because of its singlet and triplet electronic configurations. However, these properties of O2 have already been utilized as photo-oxidizing agent or electron scavenger,1-2 the nature of superoxide and peroxide states of molecule oxygen especially on metal oxide surfaces has not yet been understood. In this contribution, we demonstrate spectroscopic evidences about present of superoxide and peroxide species on rutile TiO2 (110) surface from both laboratory-based ultraviolet and X-ray photoelectron spectroscopies, and synchrotron-based X-ray photoelectron and near edge X-ray absorption fine structure spectroscopies.

1. I.X. Green, and J.T. Yates, The Journal of Physical Chemistry C 114, 11924 (2010). 2. M.A. Henderson, M. Shen, Z.-T. Wang, and I. Lyubinetsky, The Journal of Physical Chemistry C 117, 5774 (2013)

O 37.88 Tue 18:30 P2

**Water dissociation on $\alpha$-Al$_2$O$_3$(1102)** — •Sebastian Wlosczyk[1], Harald Kirsch[1], Jonas Wirth[2], Martin Wolf[1], Peter Saalfrank[2], and R. Kramer Campen[1] — [1]Fritz-Haber-Institut, Abt. Physikalische Chemie, 14195 Berlin, Germany — [2]Universitaet Potsdam, Institut fuer Chemie, 14476 Potsdam OT Golm, Germany

Alumina surfaces are ubiquitous in technologically relevant applications and a useful model system for more complicated, environmentally abundant, alumino-silicate phases. Because their properties change dramatically on interaction and reaction with water, water/Alumina chemistry has been studied, both experimentally and theoretically, for decades. In this work, we study the interaction of heavy water ($D_2O$) with the $\alpha$-Al$_2$O$_3$(1102) surface under ultra high vacuum (UHV) conditions. In-situ preparation of the carbon-free, well defined single crystal surfaces is checked by low energy electron diffraction (LEED) and Auger electron spectroscopy (AES). Hydroxylation of the Al$_2$O$_3$(1102) in UHV is performed by dosing $D_2O$ seeded in Helium with a molecular beam source (MBS). For characterization we employ vibrationally resonant sum frequency generation (VSF) spectroscopy to probe the OD stretch response of interfacial species and thermal desorption spectroscopy (TDS). The aim of the study is to investigate the adsorbate/substrate interaction and understand the effect of surface morphology on the hydroxylation process.

O 37.89 Tue 18:30 P2

**Preparation of single bismuth atoms on the silicon (111)-(7x7) surface** — •Alexander Kölker[1,2], Matthias Eltschka[1], Carola Strasser[1], Markus Etzkorn[1], Christian Ast[1], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Westfälische Wilhelms-Universität Münster, Fachbereich Physik, 48149 Münster, Germany — [3]Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Exploiting the nuclear spin for qubits is a possible route towards the realization of quantum computing. Bi in Si is a promising donor based quantum system due to the combination of its large nuclear spin (I = 9/2) and large hyperfine splitting that could be resolved by inelastic electron tunneling spectroscopy (IETS) [1].

In preparation of such a measurement we have investigated Bi in the sub monolayer regime on the Si (111)-(7x7) surface by scanning tunneling microscopy (STM). We observe the formation of isolated Bi impurities on the surface. Increasing the temperature of the Si sample during the evaporation of Bi we have observed a smaller height of the Bi atoms on the Si (111)-(7x7) surface, which indicates a stronger bound state of Bi atoms to the surface. First steps have been carried out to study the electronic properties of both systems at room temperature.

The ultimate goal is to observe single nuclear spin flips with an STM. As this energy scale is extremely small, we will investigate this using an STM operating at 15 mK for high energy resolution.

[1] F.Delgado Phys. Rev. Lett. 107, 076804 (2011)

O 37.90 Tue 18:30 P2

**Characterization of mass selected silver clusters produced in a supersonic nozzle expansion** — •Jens-Christian Meyer, David Engemann, and Heinz Hövel — Fakultät Physik / DELTA, Technische Universität Dortmund, 44227 Dortmund

The structures and properties of clusters are located in between molecules and solids and their properties are strongly dependent on their size.

Silver-cluster with a diameter distribution of $2R = 2 \pm 0.6$nm are produced in a cluster apparatus with a supersonic nozzle expansion source [1] and deposited into various matrices. These clusters are characterized by UV/VIS-spectroscopy, transelectron-microscopy (TEM) and small angle x-ray scattering technique (SAXS) to determine their structure.

To investigate in detail how the properties of silver-clusters are related to their size, a mass selector will be implemented to our cluster source. With an electric field, ionized clusters will be deflected dependent on their size.

[1] H. Hövel; S. Fritz; A. Hilger; U. Kreibig; M. Vollmer, Width of cluster plasmon resonances: Bulk dielectric functions and chemical interface damping. Phys.Rev.B, **48**, 18178, 1993.

O 37.91 Tue 18:30 P2

**Photovoltage on Metallic and Semiconducting Surfaces in Vicinity of Metallic Nanostuctures** — •Kevin Oldenburg, Kristian Sell, Stefan Polei, Sylvia Speller, and Ingo Barke — University of Rostock, Institute of Physics, 18051 Rostock, Germany

The effect of the local environment on the dynamics of electron-hole generation and decay is investigated by means of spatially resolved photovoltage measurements. For metallic surfaces such as Si(111)-(7x7) and Si(111)-(5x2)-Au a surprisingly low metal content results in saturation of the coverage-dependent photovoltage [1]. Experiments in progress include the comparison to samples with non-metallic surface states where pronounced spatial variations are expected. An experimental setup is presented that enables measurements at 405 nm wavelength, such that saturation conditions can be efficiently achieved with low thermal load. This is important to understand the spatial distribution of charge carriers at semiconducting surfaces in contact with clusters and metallic nanostructures.

[1] K. Sell, et al., Phys. Stat. Sol. (b) 247, 1087 (2010).

O 37.92 Tue 18:30 P2

**Growth and characterization of ultrasmall cobalt nanoislands on Cu(111)** — •David Gohlke and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

The ability to manipulate the magnetic properties of individual molecules and atoms is greatly affected by the substrate on which they rest. By adding nanoscale ferromagnetic regions to normal metal, one can vary the magnetic landscape for these adsorbates. It has previously been shown that Co adsorbed on the Cu(111) surface can self-assemble into spin-polarized triangular islands with lateral sizes between 5 and 30 nm. Here, we present a modified growth procedure for forming Co islands on this surface. By depositing metal on a cryogenic-temperature copper surface before annealing to room temperature, islands smaller than 5 nm are formed. These Co nanoislands bridge the size regime from the isolated adatom and few-atom clusters to the larger Co islands previously studied. Scanning tunneling microscopy (STM) allows for clear topographic characterization as well as a detailed examination of the electronic states of these islands, showing a continuation of the previously published downward trend in the energy of the highest occupied electronic state with decreasing island size.

O 37.93 Tue 18:30 P2

**Ab initio transport calculations of copper junctions in the presence of hydrogen chloride** — •Paul Schnäbele[1], Richard Korytár[1], Alexei Bagrets[1], Axel Gross[3], and Ferdinand Evers[1,2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany — [2]Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [3]Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Understanding nanoscale transport in the presence of a solvent is an important challenge in electrochemistry. To this end, we investigate transport properties of single-atom Copper junctions surrounded by hydrogen chloride. The components of this environment are partially adsorbed on the surface of the junction. In a first step we relax the geometry using density functional theory. (The chloride coverage is obtained from reference-calculations for flat surfaces [1].) This helps us to improve our understanding of the chemical bonds that occur in this situation. Furthermore, the optimized structure provides the basis for the investigation of transport properties. The calculations rely on a non-equilibrium Green's function (NEGF) approach and are implemented in the AITRANSS package that is being developed in our group [2,3]. We show that the solvent has a significant impact on the transmission and density of states.

[1] T. Roman, A. Groß, Phys. Rev. Lett. **110**, 156804 (2013)
[2] A. Arnold, F. Weigend, F. Evers, J. Chem. Phys. **126**, 174101 (2007)
[3] A. Bagrets, J. Chem. Theory Comput. **9**, 2801 (2013)

O 37.94 Tue 18:30 P2

**Controlled electromigration of copper wires and copper thin films** — •Julia Hauser[1], Jakob Schwichtenberg[1], Michael Marz[1], Christoph Sürgers[1], Hilbert v. Löhneysen[1,2], and Regina Hoffmann-Vogel[1] — [1]Karlsruher Institut für Technologie, Physikalisches Institut und DFG-Center for Functional Nanostructures, D-76131 Karlsruhe — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik, D-76021 Karlsruhe

Controlled electromigration (EM), i.e., thinning of a metallic wire by cyclic voltage ramping, offers the possibility to fabricate nanocontacts with gaps of a few nanometers in size [1]. We have investigated controlled EM of freely suspended Cu wires under ambient and UHV conditions. We are able to thin the contact down to a conductance of a few conduction quanta $G_0 = 2e^2/h$, in some cases even to $G_0$. The onset of the EM follows multiple constant-power curves, as reported earlier [1,2]. Under ambient conditions, we find a negative curvature of the envelope in the first cycles of the EM process before entering the constant-power envelope, which is not observed in UHV. Additionally, we have performed EM on thin Cu films on $SiO_2$ substrates under ambient conditions as well, in order to study the effect of the sample geometry on EM. We find that the films show qualitatively the same behavior as the 'ambient' wires. From the maxima of conduction histograms we infer preferred conduction values, whose number in the range of $0 < G \lesssim 10G_0$ depends on the initial thickness of the film.

[1] D. R. Strachan et al., Appl. Phys. Lett. **86**, 043109 (2005).
[2] D. Stöffler et al., Phys. Rev. B **85**, 033404 (2012).

O 37.95 Tue 18:30 P2

**Structural Transition in Atomic Chains Driven by Transient Doping** — •Stefan Polei[1], Paul Snijders[2], Steve Erwin[3], Franz Himpsel[4], Karl-Heinz Meiwes-Broer[1], and Ingo Barke[1] — [1]Department of Physics, University of Rostock, D-18051 Rostock, Germany — [2]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — [3]Center for Computational Materials Science, Naval Research Laboratory, Washington, DC 20375, USA — [4]Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

Transient, non-equilibrium electronic phases are of great interest for various fields of physics, as they open the door to hidden states of matter that are not accessible by static measurements. In this contribution we present scanning tunneling microscopy (STM) measurements of a reversible structural transition on Si(553)-Au from a 1x3 ground state to a 1x2 excited state upon electron injection from the tip to the surface [1]. It is shown that the 1x2 phase is created by temporary doping of the atom chains. Random telegraph fluctuations between two levels of the tunneling current provide direct access to the dynamics of the phase transition. An intriguing observation is the unusual temperature behavior that results in easier excitation at lower temperatures. As a consequence, the 1x3 ground state is not accessible by STM at low temperatures (e.g. T=5K). In a broader context this implies that a phase observed using STM at the lowest possible temperatures may not be the ground state of the system.

[1] Polei et al., PRL 111, 156801 (2013)

O 37.96 Tue 18:30 P2

**Vibration modes of Si(111)-$(7\times 7)$ and various reconstructed Au/Si(111) surfaces, studied by Raman spectroscopy** — Martin Liebhaber[1], Utz Bass[1], •Jean Geurts[1], Jochen Räthel[2], Eugen Speiser[2], Sandhya Chandola[2], Arne Baumann[2], and Norbert Esser[2] — [1]Universität Würzburg, Physikalisches Institut, Experimentelle Physik III, 97074 Würzburg — [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., 12489 Berlin

Ordered submonolayers of adsorbate atoms on semiconductor surfaces constitute a playground for electronic correlation effects, which are tightly connected with the local atomic arrangement and the corresponding vibration modes. We applied polarized Raman spectroscopy to Au-covered Si(111) surfaces, either with $(5\times 2)$ or with $(\sqrt{3}\times\sqrt{3})$ reconstruction, and to clean Si(111)-$(7\times 7)$ surfaces for reference. On the latter ones, six surface vibration modes appear between 7.7 meV and 52.1 meV, with different polarization dependence. Upon Au coverage, they are quenched and replaced by new modes, governed by the specific Au reconstruction. For $(5\times 2)$, five low-frequency Au-induced vibration modes emerge (3.2 meV to 18.7 meV). The $(\sqrt{3}\times\sqrt{3})$ Au reconstruction shares two of them, but also shows two new peaks in the same range. For the clean Si(111) $(7\times 7)$ surface, these results should enable refined calculations of the dynamic properties of the DAS structural model. For the Au-covered surfaces, the reconstruction-specific vibrations may help to clarify the atomic geometry, extending the base for more sophisticated calculations of atomic and orbital properties of ordered adatom arrangements for correlated-electron systems.

O 37.97 Tue 18:30 P2

**Unusual resistance-voltage dependence of ultra-high vacuum-electromigrated nanojunctions** — Dominik Stöffler[1], •Michael Marz[1], Birgit Kiessig[2], Tihomir Tomanic[1], Hilbert v. Löhneysen[1,2], and Regina Hoffmann-Vogel[1] — [1]Karlsruher Institut für Technologie, Physikalisches Institut und DFG-Center for Functional Nanostructures, D-76131 Karlsruhe Karlsruhe — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik, D-76021 Karlsruhe

Clean and well-defined electronic contacts in the nanometer-size range are one prerequisite for single-molecule-based electronics. Controlled electromigration (EM) [1], especially in ultra high vacuum (UHV), allows the preparation of sufficiently small and clean metallic contacts. Here we present measurements of the voltage dependance of the electrical resistance $R(V)$ subjected to EM in UHV. For large $R$ values an unexpected decrease of $R(V)$ with increasing bias is observed. Comparing with simple model calculations, we tentatively ascribe this behavior to tunneling in parallel to ohmic nanocontacs. In addition, we observe field emission, which additionally supports the idea that tunneling occurs in EM experiments performed in UHV.

[1] D. R. Strachan et al., Appl. Phys. Lett. 86, 043109 (2005).

O 37.98 Tue 18:30 P2

**Oligothiophene nanorings as electron resonators for whispering gallery modes** — •Gaël Reecht[1], Hervé Bulou[1], Fabrice Scheurer[1], Virginie Speisser[1], Fabrice Mathevet[2], and Guillaume Schull[1] — [1]IPCMS , Strasbourg, France — [2]Laboratoire de Chimie des Polymères, Paris, France

Recently, conjugated molecular wires were investigated using scanning tunneling microscopy (STM) [1]. These studies showed that the electronic structure of these oligomers can be approximated by a (nearly) free electron gas confined to a 1D box. Using a recent "on-surface" synthesis method [2], we obtained oligothiophene nanowires and nanocycles on a Au(111) surface. The electronic properties of these structures were energetically and spatially resolved using scanning tunneling spectroscopy (STS).This study reveals large differences between the electronic properties of the linear and cyclic structures. These differences find their origin in the close-ended nature of the cyclothiophene resonances which must be treated with periodic boundary conditions. A more detailed analysis shows that cyclothiophene must be considered as a ribbon (i.e., having an effective width) rather than a purely 1D structure. A fascinating consequence is that the molecular nanorings act as whispering gallery mode resonators for electrons, opening the way for new applications in quantum electronics [3].

[1]. Wang, S and al. Phys. Rev. Lett., 106, 206803 (2011)
[2]. Grill, L and al., Nature Nano, 2, 687 (2007)
[3]. Reecht, G and al. Phys. Rev. Lett., 110, 056802 (2013)

O 37.99 Tue 18:30 P2

**Composite wire metamaterial for broadband infrared superlensing** — •Mike Prämassing, Tobias Mass, and Thomas Taubner — I. Institute of Physics, RWTH Aachen University

Superlenses can either consist of natural [1] or metamaterials and enable subwavelength imaging beyond Abbes diffraction limit. Thereby, the evanescent near-fields are preserved and subwavelength information is transported [2]. We investigate a composite wire metamaterial consisting of parallel aligned metallic nanowires in a dielectric host medium. Its superlensing effect originates from strongly anisotropic optical properties [3,4]. Our theoretical investigations of the imaging properties concern the mid-infrared spectral range from 1 - 10$\mu$m. Furthermore we provide first fabrication attempts by means of electrochemical deposition [5].

[1] Taubner et al. *Science* **2006** 313(5793) 1595.
[2] Li et al. *ACS nano* **2012** 6(11), 10107-10114.
[3] Belov et al. *Phys. Rev.* **2006** E73, 056607.
[4] Elser et al. *Appl. Phys. Lett.* **2006** 89(26), 261102-261102.
[5] Noginov et al. *Appl. Phys. Lett.* **2009** 94(15), 151105.

O 37.100 Tue 18:30 P2

**Characterisation of Boron-doped Silicon Nanowires** — •Stefan Weidemann[1], Manfred Ramsteiner[2], Anna Mogilatenko[3], Klaus Rademann[4], and Saskia F. Fischer[1] — [1]Neue Materialien, Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany — [3]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, 12489 Berlin, Germany — [4]Nanostructured Materials, Institut für Chemie, Humboldt-Universität zu Berlin

Nanostructures of silicon possess a high surface to volume ratio and reveal new intrinsic properties like decreased thermal conductivity [1], which make them interesting for catalytic applications and electronic devices. Measuring simultaneously thermal and electronic transport properties of individual, structurally characterised, silicon nanowires still remains a challenge. Here we prepare silicon nanowires by the two-step metal-assisted chemical etching (MACE) [2].

In dependence of the boron doping concentration we obtain nanowires with lengths up to 110 $\mu$m (undoped Si, $\rho > 1$ k$\Omega$cm), 90 $\mu$m (medium doped, $\rho = 14 - 23$ $\Omega$cm) and about 40 $\mu$m (highly doped Si, $\rho < 0.01$ $\Omega$cm), with smooth, rough and porous surfaces, respectively. Fabrication on wafer scale is feasible. Surface and structural properties of nanowire ensembles and individual nanowires are investigated by scanning and transmission electron microscopy and Raman spectroscopy.

[1]A. I. Hochbaum *et al.*, Nature 451, 163 (2008)
[2]Z. Huang *et al.*, Adv. Mater., 23, 285-308 (2011)

O 37.101 Tue 18:30 P2

**Improving the performance of MW-CNT-based via interconnect systems - a conductive-AFM study** — •Marius Toader[1], Holger Fiedler[2], Sascha Hermann[2], Stefan E. Schulz[2,3], Thomas Gessner[2,3], and Michael Hietschold[1] — [1]Technische Universität Chemnitz, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany — [2]Technische Universität Chemnitz, Center for Microtechnologies, D-09126 Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nano Systems (ENAS), D-09126 Chemnitz, Germany

We have studied via interconnect systems based on vertically aligned multi-walled carbon nanotubes (MW-CNTs) grown on a copper-based metal line. Using c-AFM the corresponding overall performance can be accurately estimated based on the resistance of individual CNTs [1] in good agreement with the classical electrical measurements. By tuning the top metallic layer within the conductive line the corresponding CNT/metal contact quality could be considerably improved. Moreover, an improved performance as a result of exposure to HF vapours was observed as well.

[1] H. Fiedler, M. Toader, S. Hermann, R. D. Rodriguez, E. Sheremet, M. Rennau, S. Schulze, T. Waechtler, M. Hietschold, D.R.T. Zahn, S. E. Schulz and T. Gessner; Microelectron. Eng. 2013 (http://dx.doi.org/10.1016/j.mee.2013.07.007).

O 37.102 Tue 18:30 P2

**A Ruler for the Nanoworld: Scatterometry at the PTB** — •Victor Soltwisch, Anton Haase, Jan Wernecke, and Frank Scholze — Physikalisch-Technische Bundesanstalt

The continuous shrinking in feature size in industrial application is a huge challenge under metrology aspects. In- and ex-situ metrology solutions are needed which are fast enough, non-destructive and have capabilities for 3D structures. The PTB operates several Beamlines at BESSYII and the new MLS, with different endstations designed for highest accuracy of scatterometric measurements. EUV and GISAXS scatterometry is a part of the optical scatterometry (OCD) solutions. EUV scatterometry is designed for the next step in photolithography in the semiconductor industry with wavelengths around 13.5 nm. Scattering from surfaces enables to reconstruct geometric parameters from nm structured surfaces. The study of off-specular scattering from multilayers gives insight in the interface roughness. We present several practical application of different scatterometric experiments which were performed at the PTB.

O 37.103 Tue 18:30 P2

**Silicene on Ag(111): Reconstructions and first tests of laser-induced non-thermal deposition** — •Silke Hattendorf[1], Christian Kalupka[2], Martin Reininghaus[2], Marco Pratzer[1], and Markus Morgenstern[1] — [1]II.Institute of Physics B and JARA- FIT, RWTH Aachen — [2]Chair for Laser Technology, RWTH Aachen

Silicene, a buckled 2D honeycomb structure made of silicon, was predicted to be stable and exhibit an Dirac cone like graphene[1].
So far, it has been grown on Ag(111)[2], Ir(111)[3] and $ZrB_2$[4]. However, due to strong hybridization with the underlying substrate the Dirac cone is most likely strongly distorted and the silicene states are pushed far into the valence and conduction band[5] making it mandatory to transfer it to a less interacting substrate.
Silicene was grown on Ag(111) at rates between 0.05 and 0.16 ML/min and at a substrate substrate temperature of 200-250°C. The atomic structure was studied by scanning tunneling microscopy (STM) revealing the known reconstructions (e.g. 4 x 4, $\sqrt{13}$ x $\sqrt{13}$)[2].
We tried to transfer the silicene to mica using laser-induced non-thermal deposition [6]. However, possibly due to the strong interaction between the silver and silicene surfaces, this was not successful so far.
[1] S. Cahangirov et. al., PRL 102, 236804 (2009).
[2] P. Vogt et. al., PRL 108, 155501 (2012).
[3] L.Meng et. al., Nano Lett. 13, 685 (2013).
[4] A. Fleurence et. al., PRL 108, 245501 (2013).
[5] Y.Yuan et. al., Arxiv:1310.2420.
[6] M.Reininghaus, APL 100, 151606(2012).

O 37.104 Tue 18:30 P2

**Automated spray coating process for the fabrication of large-area opaline structures on textured substrates** — •Daniela Schneevoigt[1], Frederik Bub[1], Alexander Sprafke[1], and Ralf Wehrspohn[1,2] — [1]Martin-Luther-Universität, Halle-Wittenberg, Deutschland — [2]Fraunhofer IWM, Halle, Deutschland

3D photonic crystals, such as opaline structures, have been shown to have a high potential to increase the efficiency of solar cells by enabling advanced light management concepts. Our automated process for the spray induced self-assembly of large-area artificial opals presents a low-cost technique, which complies with the demands of the photovoltaic industry for the integration of such structures [1]. The process is based on spraying a dispersion of monodisperse nanoscaled colloids onto a substrate and subsequent crystallization of a 3D photonic crystal.

Here, we report on the successful fabrication of artificial opaline structures, such as opals and inverted opals, via spray coating on textured substrates.

With the intention to integrate opaline structures as back reflectors in $\mu$c-Si thin film solar cells, the crystallization of extensive artificial opals on different $\mu$c-Si surface textures was analyzed. The inversion of the opals was achieved with a conformal deposition of Al:ZnO (by atomic layer deposition) and a subsequent wet-chemical removal of the colloids. The optical, structural and electrical characteristics of these opaline structures were examined.

[1] Sprafke, A., Schneevoigt, D., Seidel, S., Schweizer, S. L., Wehrspohn, R., Optics Express, 21(26): 528, (2013).

O 37.105 Tue 18:30 P2

**Fabrication and application of nanosecond laser-induced surface nanostructures on polyimide** — •Lukas Bayer[1,2], Pierre Lorenz[1], Martin Ehrhardt[1], Klaus Zimmer[1], and Lutz Engisch[2] — [1]Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04315 Leipzig, Germany — [2]Hochschule für Technik, Wirtschaft und Kultur Leipzig, P.O. Box 301166, 04251 Leipzig, Germany

The formation of nanostructures on polymers, produced by laser irradiation near the ablation threshold, is well-known. In the last 20 years, the influence of laser parameters on the resultant structures has been manifold studied. However, applications for this kind of constant and good manageable surface structures are hardly known. In this study, the fabrication and application of KrF excimer laser-induced 3-D conical surface structures on polyimide is presented. The properties of the laser-induced surface structures that are dependent on the laser parameters are analysed by optical and scanning electron microscopy (SEM). Furthermore, some applications of these surface structures are presented. Particularly in the field of product safety there are many opportunities to bring these structures to use. There are both low and high security features possible. A low security feature could be a microscopic QR-code containing any desired data. For high security applications it is also possible to create pictures with very high resolution. In this case, the resolution is much higher than in conventional printing technologies.

O 37.106 Tue 18:30 P2

**Nanostructuring of stainless steel by pulsed laser interference lithography** — •Lukas Gröner, Martin Stärk, Elke Scheer, and Johannes Boneberg — Universität Konstanz, BW

In pulsed laser interference lithography a laser pulse is divided into several beams which are recombined on the sample to be structured. Due to interference one gets a periodic pattern of high and low intensities. Therefore samples will get hot only in the high intensity regions. We show that this temperature modulation leads to a change in etching resistance which can be used to structure stainless steel surfaces with periods in the micrometer range and depths up to several hundreds of nanometers. As the experiments show not all stainless steel types are usable for this process.

O 37.107 Tue 18:30 P2

**Processing and characterization of photonic crystals on flexible substrates for light absorption enhancement in solar cells** — •Frederik Bub[1], Daniela Schneevoigt[1], Alexander Sprafke[1], and Ralf Wehrspohn[1,2] — [1]Martin-Luther-Universität, Halle-Wittenberg, Germany — [2]Fraunhofer IWM, Halle, Germany

The success of the photovoltaic technology depends highly on two opposing improvements: saving material and therefore costs and increasing efficiency. One easy and cheap way to solve this conflict of interests is an advanced light management with photonic crystals to increase the light path in the absorber material.

Thus, we developed a production method for photonic crystals on flexible substrates based on a spray coating technique. The main advantage of this procedure is the fast assembly of photonic crystals consisting of polymeric colloids and the creation of a light management device separated from the solar-cell production line which allows easy integration into existing cell concepts. [1]

We produced photonic crystals respectively artificial opals on flexible substrates such as aluminum foil. The quality of the crystals was characterized optically, spectroscopically and mechanically. In detail we investigated the crystallization behavior of the artificial opals on flexible substrates by electron microscopy and analyzed the optical reflection. The stability and adhesion of the opaline films were qualified by applying mechanical stress to the flexible substrate.

[1] Sprafke, A, Schneevoigt, D, Seidel, S., Schweizer, S., Wehrspohn, R; Opt. Expr., 21(26): 528, (2013)

O 37.108 Tue 18:30 P2

**Simulation of ballistic glancing angle deposition** — •Christoph Grüner, Stefan G. Mayr, and Bernd Rauschenbach — Leibniz Institute of Surface Modification, Leipzig, Germany

Computer simulations can be a powerful tool to investigate physical vapor deposition processes. While molecular dynamics simulations can provide information about short range effects, long range effects have to be treated with different simulation techniques. Glancing angle deposition (GLAD) is based on the long range self-shadowing, which appears when a vapor beam reaches a substrate at a highly oblique condition [1]. This leads to the growth of a highly porous thin film, composed of many free-standing nanostructures. For a realistic modeling of this shadowing effect very large numbers of particles and large cell dimensions are required. Handling this large number of particles is very computationally intensive, so that on-lattice simulations are a common tool. However, this ballistic growth process is highly sensitive to the geometrical correctness of the simulation. Tanto et al. [2] have shown, that a simple approach, using cubic particles on a cubic lattice, introduces significant errors to the results of such simulations. A deeper investigation of these effects and a discussion of their impact on the modeling of the GLAD process are presented. Further a 'work-around' is proposed, that nearly eliminates the presented effects while it not increases the computation time to much.

[1] J.M. Nieuwenhuizen, H.B. Haanstra, Philips Tech. Rev. 27 87 (1966).

[2] B. Tanto, C. F. Doiron, T.-M. Lu, Phys. Rev. E 83, 016703 (2011).

O 37.109 Tue 18:30 P2

**A comparison of evaporation and sputter glancing angle deposition** — •Xubin Lu, Christoph Grüner, Jens Bauer, and Bernd Rauschenbach — Leibniz Institute of Surface Modification, Leipzig, Germany

It is well known, that different physical vapor deposition techniques lead to different micro structures of the deposited thin films. Particle energy and angular distribution during the process are the main factors influencing the growth behavior. While these parameters and their effects are well investigated for normal incidence deposition, the situation is much more unclear for oblique and glancing angle deposition (GLAD). Here the substrates normal and the incoming particle beam form a nearly right angle. This results in the growth of separated nanostructures, that form a porous thin film [1]. This process is mainly based on a self-shadowing effect between neighboring nucleation sites and later nanostructures. This self-shadowing during the growth is influenced by the divergence of the particle beam, while the shape of the individual nanostructures is sensitive to surface diffusion effects. A comparison of electron beam evaporation and sputter GLAD is shown, investigating growth speed and porosity of the film as well as size and tilt angle of the individual nanostructures.

[1] J.M. Nieuwenhuizen, H.B. Haanstra, Philips Tech. Rev. 27 87 (1966).

O 37.110 Tue 18:30 P2

**Structural and mechanical properties of graphene and polycrystalline carbon membranes** — •Maximilian Ammon, Yuri Koval, Michael Enzelberger-Heim, Christian Steiner, and Sabine Maier — Department of Physics, University of Erlangen-Nürnberg, Germany

Thin carbon membranes show interesting physical properties and are therefore promising materials for a variety of applications on the nano-scale ranging from chemical sensors to resonators. Here we discuss the structural and mechanical properties of two types of carbon membranes based on atomic force microscopy experiments in ambient condition. In one hand, we investigated the structure of electrochemically etched graphene membranes with an average graphene thickness of around 2-3 monolayers and a diameter of up to 30 $\mu$m. The morphology of these membranes shows a strong buckling with apparent heights of several tens of nanometers, which can be quantifiably connected to the pre-stress of the graphene after the growth on SiC at high temperatures. [1] On the other hand we studied polycrystalline carbon membranes with thicknesses down to about 3 nm obtained by the graphitization of polymers after low-energy ion irradiation. We determined the stiffness and Young's-Modulus of such polycrystalline membranes by force distance spectroscopy.

[1] D. Waldmann et al. ACS Nano, 7, 5, 4441-4448 (2013).

## O 38: Invited Talk (Stefan Heinze)

Time: Wednesday 9:30–10:15 Location: TRE Phy

**Invited Talk** O 38.1 Wed 9:30 TRE Phy
**Understanding STM experiments on single-atom junctions from first-principles** — •Stefan Heinze — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universtität zu Kiel, Germany

Today, scanning tunneling microscopy (STM) allows to create artificial nanostructures at surfaces atom-by-atom and to locally probe their structural, electronic, magnetic, and transport properties at the atomic level. In order to understand such experiments it is often indispensable to use a first-principles approach based on density functional theory. It is particularly intriguing to explore physical properties at the single atom limit. Here, I will show that it is possible to image the spin direction of single magnetic atoms on surfaces [1] and how the spin-valve effect in single-atom junctions can be explained [2]. We found that in such experiments the interaction between tip and adsorbed atom can become essential [3]. Surprisingly, it is also feasible to detect the spin-quantization axis of single atoms using non-magnetic STM tips [4] due to spin-orbit coupling. This effect – the so-called tunneling anisotropic magnetoresistance – can be implemented into a simple model of STM which allows fast simulation of spin-polarized and non-spin-polarized STM images [5].

[1] D. Serrate *et al.*, Nature Nanotech. **5**, 350 (2010).
[2] M. Ziegler *et al.*, New J. of Phys. **13**, 085011 (2011).
[3] C. Lazo *et al.*, Phys. Rev. B **86**, 180406 (R) (2012).
[4] N. Néel *et al.*, Phys. Rev. Lett. **110**, 037202 (2013).
[5] K. von Bergmann *et al.*, Phys. Rev. B **86**, 134422 (2012).

## O 39: Symposium Molecular Switches and Motors at Surfaces (O jointly with BP, CPP)

Time: Wednesday 9:30–12:15 Location: HSZ 02

**Invited Talk** O 39.1 Wed 9:30 HSZ 02
**Imaging and manipulation of single functional molecules on surfaces** — •Leonhard Grill — University of Graz, Department of Physical Chemistry, Graz, Austria

Functional molecules on surfaces and their assembly into pre-defined architectures are key challenges in nanotechnology and of interest in various fields from molecular electronics over novel materials to molecular machines. Various examples of functional molecules, studied by scanning tunneling microscopy under ultrahigh vacuum conditions will be discussed. Specifically designed molecular building blocks are connected to two-dimensional networks or one-dimensional chains [1,2], which can act as molecular wires [3,4]. On the other hand, chemical processes within individual molecular can be controlled via their environment. This was observed for molecular switches, where the atomic-scale surroundings cause drastic changes in their switching probability [5]. Recently, we could show that the rate of an intramolecular hydrogen transfer reaction can be tuned up and down by single atoms in the vicinity of the molecule [6]. Finally, a combination of the two approaches will be discussed, potentially leading to heterogeneous molecular nanostructures that contain functional molecules.

[1] L. Grill et al., Nature Nanotech. 2, 687 (2007); [2] L. Lafferentz et al., Nature Chem. 4, 215 (2012); [3] L. Lafferentz et al., Science 323, 1193 (2009); [4] M. Koch et al., Nature Nanotech. 7, 712 (2012); [5] C. Dri et al., Nature Nanotech. 3, 649 (2008); [6] T. Kumagai et al., Nature Chem., doi: 10.1038/nchem.1804.

**Invited Talk** O 39.2 Wed 10:00 HSZ 02
**Adiabatic quantum motors** — •Felix von Oppen — Dahlem Center for Complex Quantum Systems, Freie Universität Berlin

Microscopically, motion is frequently dominated by fluctuations, making it a challenge to generate directed motion at the nanoscale. This challenge has motivated recent experiments striving to realize nanomotors which convert electrical signals into unidirectional translational, vibrational, or rotational motion. Frequently, these experiments rely on ac actuation or current pulses to effect the directed motion of, say, a molecule or a carbon nanotube. In this talk, I will describe an alternative dc scheme to operate a nanomotor. Our proposed adiabatic quantum motor is effectively based on operating a quantum pump in reverse, a scheme whose macroscopic counterpart has been known since antiquity and is employed in current technology. Its quantum version has remained essentially unstudied despite enormous activity on adiabatic quantum pumps. Specifically, we consider a transport current which drives the periodic motion of an adiabatic degree of freedom. We relate the work performed per cycle on the motor degree of freedom to characteristics of the complementary quantum pump and discuss the motors' efficiency. We show that in principle, there exist motors which operate solely due to quantum interference, as well as ideal quantum motors with unit efficiency. The intrinsic damping of quantum motors has a lower bound which just involves Planck's constant. While most of our considerations are based on Gedankenmotors, we will also discuss possible realizations.

**Invited Talk** O 39.3 Wed 10:30 HSZ 02
**Operation of molecular devices and machines on surfaces** — •Saw Wai Hla — Center for Nanoscale Materials, Argonne National Lab, and Ohio University, USA.

A recent emergent research direction is the development of complex molecular machines suitable to operate on solid surfaces. Unlike biological counterparts, the synthetic molecular machines may tolerate a more diverse range of conditions, and thus be advantageous for the complex functions with low power consumption suitable to operate in solid state devices. Development of such molecular devices requires testing their operation mechanisms. We use low temperature scanning tunneling microscopy, spectroscopy, and molecular manipulation schemes to investigate fundamental operations of synthetic molecular switches and molecular motors on metallic surfaces. Using inelastic electron tunneling process, individual molecules can be switched from one state to another in a controlled manner [1-4]. Controlled directional rotation of molecular motors can also be performed using the same technique. Finally, this presentation will include our latest results of controlled synchronized rotation of molecular motors on surfaces.

[1] V. Iancu, A. Deshpande, S.-W. Hla, Nano Lett. 6, 820-823 (2006). [2] V. Iancu, and S.-W. Hla, Proc. Nat. Acad. Sci. 103, 13718-13721 (2006). [3] Y.-S. Fu et al. Nano Lett. 12, 3931-3935 (2012). [4] U.G.E. Perera et al. Nature Nanotechnology 5, 46-51 (2013).

**15 min. break**

**Invited Talk** O 39.4 Wed 11:15 HSZ 02
**Driving and Controlling Molecular Surface Rotors with a Terahertz Electric Field** — •Raymond Dean Astumian — Dept. of Physics, University of Maine, USA

Great progress has been made in the design and synthesis of molecular motors and rotors. Loosely inspired by biomolecular machines such as kinesin and the FoF1 ATPsynthase, these molecules are hoped to provide elements for construction of more elaborate structures that can carry out tasks at the nanoscale corresponding to the tasks accomplished by elementary machines in the macroscopic world. Most of the molecular motors synthesized to date suffer from the drawback that they operate relatively slowly (less than kHz). Here we show by molecular dynamics studies of a diethyl sulfide rotor on a gold(111) surface that a high- frequency oscillating electric field normal to the surface can drive directed rotation at GHz frequencies. The maximum directed rotation rate is 1010 rotations per second, significantly faster than the rotation of previously reported directional molecular rotors. Understanding the fundamental basis of directed motion of surface rotors is essential for the further development of efficient externally driven artificial rotors. Our results represent a step toward the design of a surface-bound molecular rotary motor with a tunable rotation frequency and direction.

**Invited Talk** O 39.5 Wed 11:45 HSZ 02
**Unidirectional motion by inelastic electron tunneling** — •Karl-Heinz Ernst — Empa, Swiss Federal Laboratories for Mate-

rials Science and Technology — Department of Chemistry, University of Zurich

Propelling single molecules in a controlled manner along an unmodified surface remains extremely challenging because it requires molecules that can use light, chemical or electrical energy to modulate their interaction with the surface in a way that generates motion. Biomolecular motors, such as the protein kinesin or the F1-ATPase, function as linear walkers or rotary motors. Chemists strive for synthesis of molecules that can perform unidirectional motion on surfaces. One successful approach was the use of ratchet-style unidirectional rotors based on overcrowded helical systems.

We show that excitation with inelastically tunneling electrons emanating from the tip of a scanning tunneling microscope (STM) very efficiently excites the rotors and leads to linear movement of the molecule on the surface for the right isomer. This requires a transient electron attachment into the LUMO, while vibronic excitation of the motor axles lead to reversible rearrangement without movement. We will discuss possible mechanisms and implication for further research and design of nanotechnological devices.

## O 40: Transport: Molecular Electronics I (TT jointly with O)

Time: Wednesday 9:30–13:00 Location: HSZ 304

O 40.1 Wed 9:30 HSZ 304

**Electrical transport through ferrocene molecules using MCBJ** — •Karthiga Kanthasamy, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik (ATMOS), Leibniz Universität Hannover

In order to understand the electrical behavior of molecules we fabricate a stable atomic gold contact by Mechanically Controllable Break Junction(MCBJ). We study the electrical transport through ferrocenedithiol (FDT) molecules because of its rotational flexibility with respect to two cyclopentadienyl(Cp) rings without activation threshold and high conductance.

The molecules are chemisorbed on the Au atomic contact, as confirmed by XPS characterization on Au thin film. After insertion of FDT molecules, measuring conductance versus contact distance at constant voltage 1 mV there are characteristic stepwise changes below 1 $G_0$ with a very pronounced plateau at 0.4 $G_0$. In the range 0.1 $G_0$ < conductance < 0.4 $G_0$, we measured IV-curves at room temperature and 80 K. Detailed analysis of IV-curves exhibit characteristic peak in the first derivative. The voltage at the maxima can be identified with the excitation of C-H bending, C-H stretching vibrational modes indicating resonantly enhanced conductance by vibrational excitation. The influence of different anchoring groups in the electronic transport will be shown.

O 40.2 Wed 9:45 HSZ 304

**Multi-orbital STM theory for $\pi$-conjugated molecules on thin insulating films** — •Benjamin Siegert, Andrea Donarini, and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg

We present a multi-orbital extension of our STM theory [1,2,3], based on the reduced density matrix formalism, which is capable of describing electronic transport through $\pi$-conjugated molecules on thin insulating films. In order to investigate spin-dependent transport effects using the example of a Cu-Phthalocyanine molecule, we set up an effective many-body Hamiltonian including exchange and spin-orbit interaction. The transport dynamics is calculated by evaluating a Generalized Master Equation including all diagonal and off-diagonal elements of the reduced density matrix of the molecule. Examples are shown of how many-body effects, like interference between degenerate many-body states, can affect the transport properties of $\pi$-conjugated molecules on thin insulating films in an STM setup.

[1] S. Sobczyk, A. Donarini, and M. Grifoni, PRB **85**, 205408 (2012).
[2] A. Donarini, B. Siegert, S. Sobczyk, and M. Grifoni, PRB **86**, 155451 (2012).
[3] B. Siegert, A. Donarini and M. Grifoni, pss (b) **250**, 2444 (2013)

O 40.3 Wed 10:00 HSZ 304

**Gate-controlled shift of CoPc orbitals on graphene in a STM junction** — •Samuel Bouvron[1], Philipp Erler[1], Alexander Graf[1], Romain Maurand[2], Luca Gragnaniello[1], Dirk Wiedmann[1], Fabian Pauly[1], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Department of Physics, University of Basel

One of the most promising aims of molecular electronics is the fabrication of a molecular transistor. Such a device necessarily requires a gate-electrode, which allows to set the molecule into a controllable electric field, therefore tuning the energy of the molecular orbitals relevant for charge transport. Moreover since the very first year of the development of the scanning tunneling microscope (STM), it has been proposed to use its extremely high lateral resolution to study molecules and record $I(V)$ or $I(z)$ characteristics of the tunnel contacts formed. However, the geometric constrains of the microscope make the implementation of a third gate-electrode challenging. Here we investigate the electronic properties of cobalt phthalocyanine (CoPc) molecules on graphene on $SiO_2$/Si, where graphene and Si serve as drain and gate electrode, respectively. We report on site-dependent and gate-dependent tunnel transport through the CoPc molecules. The influence of the gate voltage on the energy position of the molecular orbitals is discussed and the orbital structure is assigned. Finally this STM-tip/molecule/graphene/$SiO_2$/Si device geometry opens a possibility to combine the spatial resolution of the STM with the additional control of the electric field commonly used in transport measurements.

O 40.4 Wed 10:15 HSZ 304

**Laser pulse induced transient currents in a molecular junction** — •Yaroslav Zelinskyy[1,2] and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin — [2]Bogolubov Institute for Theoretical Physics, National Academy of Science of Ukraine

The investigation of transient phenomena in molecular junctions is of increasing interest. As an example, computations are presented on femtosecond laser pulse excitations and subsequent transient current formation. A single molecule sandwiched between two spherical leads is considered[1,2]. Optical excitation of the leads is accounted for by their collective plasmon excitations which may also couple to the molecular excitations. While this coupling may be strong the electron transfer coupling of the molecule to the leads is considered to be small to stay in the regime of sequential charge transmission. All the calculations of transient currents are performed in the framework of a density matrix theory. As a quantity detectable in the experiment the averaged dc–current resulting from a huge sequence of laser pulses is also calculated . The obtained transient currents are confronted with those induced by voltage pulses[3].

[1] L. Wang and V. May, Phys.Chem.Chem.Phys. 13, 8755 (2011)
[2] Y. Zelinskyy and V. May, Nano Lett. 12, 446 (2012)
[3] Y. Zelinskyy and V. May, J. Chem. Phys. (submitted)

O 40.5 Wed 10:30 HSZ 304

**Theory of molecular junction electroluminescence: plasmon-enhancement and emission narrowing due to multiple molecules** — •Yuan Zhang and Volkhard May — Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489, Germany

Photoemission of a molecular junction formed by up to five individual molecules and placed in the proximity of an Au nanosphere is studied theoretically. Charge transmission through the molecules at a finite applied voltage induces an electronic excitation while an energy transfer coupling to the nanosphere is responsible for plasmon excitation and enhancement effects. The consideration of several molecules and larger currents results in an increased electroluminescence intensity compared to earlier studies [1,2].The used density matrix description accounts for the entanglement of different molecular excitations due to their simultaneous coupling to the Au nanosphere. The obtained emission line narrowring with increasing number of molecules is related to the SPASER mechanism.

[1]Y. Zhang, Y. Zelinskyy, and V. May, J. Chem. C **116**, 25962 (2012)
[2]Y. Zhang, Y. Zelinskyy, and V. May, Phys. Rev. B **88**, 155426 (2013)

O 40.6 Wed 10:45 HSZ 304

**Polarization dependent, surface plasmon induced photoconductance in gold nanorod arrays** — Sandra Diefenbach[1], •Lisa Kugler[1], Nadine Erhard[1], Johannes Schopka[1], Alfonso Martin[2], Christoph Karnetzky[1], Daniela Iacopino[2], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München — [2]Tyndall National Institute, University College Cork, Lee Maltings Complex, Dyke Parade, Cork, Ireland

We report on the photoconductance properties of two-dimensional arrays of gold nanorods which are formed by a combination of droplet deposition and stamping methods. The photoconductance of the nanorod arrays is strongly enhanced through the excitation of longitudinal surface plasmons. Hereby, the photoconductance is polarization dependent with a maximum signal for the electric field of the exciting photon being aligned with the longitudinal axis of the nanorods [1]. We interpret the observations by a plasmonically induced, bolometric enhancement of the conductance, but we also discuss a possible hot-electron emission induced by the plasmons.

We gratefully acknowledge support from the European (FP7) 263091 project HYSENS.

[1] S. Diefenbach et al., arXiv:1311.1002 (2013)

**15 min. break.**

**Invited Talk** O 40.7 Wed 11:15 HSZ 304

**Quantum Transport at Molecular Scales** — •Ferdinand Evers — Karlsruhe Institute of Technology, Germany

The quantum transport on molecular scales is a wide and very complex research area. It connects to phenomena in experimental disciplines as diverse as the surface sciences, organic electronics, spintronics, catalysis, electrochemistry, strongly correlated systems and even the life sciences. An important motivation in the sub-discipline Molecular Electronics is to single out a single molecule and use it to investigate in detail aspects of the elementary charge transfer processes involved.

The first part of the presentation offers an overview about recent experimental and theoretical developments and new directions in Molecular Electronics. The second part will embark on effects of molecular magnetism. It will deal with the Kondo-effect in molecular adsorbates and explains, how a non-magnetic molecule (hydrogen-phtalocyanine) brings about a giant magnetoresistance.

O 40.8 Wed 11:45 HSZ 304

**Kondo-effect in binuclear metal-organic molecules** — •Dimitra Xenioti[1,2], Alexej Bagrets[1], Richard Korytár[1], Lei Zhang[1,3], Frank Schramm[1], Mébarek Alouani[2], Mario Ruben[1,2], Wulf Wulfhekel[1,3], and Ferdinand Evers[1,4] — [1]Institute of Nanotechnology (INT), KIT, Karlsruhe, Germany — [2]Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS), Strasbourg, France — [3]Physikalisches Institut (PI), KIT, Karlsruhe, Germany — [4]Institut für Theorie der Kondensierten Materie (TKM), Karlsruhe, Germany

Low-temperature STM measurements performed on a binuclear metal-organic molecule (Ni(hfacac)$_2$)$_2$(bpmd) ("Ni$_2$") deposited on a Cu surface reveal that the system undergoes a Kondo effect with $T_K \sim 10$K and a spin located nearby Ni atoms. The physics in play is intriguing, because the molecule does not have anchoring groups, which could be responsible for the formation of a chemical bond with the Cu surface. By comparing experimental data with simulated STM images, we have identified possible adsorption geometries. Our simulations show that some observed STM images and large $T_K$ could be attributed to a distorted "Ni$_2$" complex, which is bound to Cu(001) via the bipyrimidine (bpmd) unit. Other images may be interpreted as arising from molecular fragmentation, suggesting a Ni(hfacac)$_2$ moiety to be seen in the experiment. In the latter case our analysis of the DFT+$U$ (Kohn-Sham) spectral function show that the S=1 type Kondo effect arises mainly due to unpaired electrons populating $d_{xy}$ and $d_{z^2}$ orbitals of Ni$^{2+}$ ion. In the case of "Ni$_2$", our calculations suggest that the Kondo effect originates from a pair of weakly coupled S=1 Ni$^{2+}$ spins.

O 40.9 Wed 12:00 HSZ 304

**Heat dissipation and thermopower in atomic-scale junctions** — •Fabian Pauly — Department of Physics, University of Konstanz, Germany

In this talk, I will present recent combined experimental and theoretical efforts to understand the heat dissipation in atomic-scale junctions [1,2]. Using custom-fabricated scanning probes with integrated nanoscale thermocouples, we find that if the junctions have transmission characteristics that are strongly energy dependent, this heat dissipation is asymmetric (that is, unequal between the electrodes) and also dependent on both the bias polarity and the identity of the majority charge carriers. In contrast, junctions consisting of only a few gold atoms, whose transmission characteristics show weak energy dependence, do not exhibit appreciable asymmetry. Our results unambiguously relate the electronic transmission characteristics of atomic-scale junctions to their heat dissipation properties, establishing a framework for understanding heat dissipation in a range of mesoscopic systems where transport is elastic.

[1] W. Lee, K. Kim, W. Jeong, L. A. Zotti, F. Pauly, J. C. Cuevas, and P. Reddy, Nature 498, 209 (2013).

[2] L. A. Zotti, M. Bürkle, F. Pauly, W. Lee, K. Kim, W. Jeong, Y. Asai, P. Reddy, and J. C. Cuevas, New J. Phys. (accepted); arXiv:1307.8336.

O 40.10 Wed 12:15 HSZ 304

**Structure and conductance analysis of atomic-sized contacts** — •Manuel Matt[1], Fabian Pauly[1], Juan Carlos Cuevas[2], and Peter Nielaba[1] — [1]University of Konstanz, Department of Physics, 78457 Konstanz, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

We study the conductance histograms of different metals such as Au and Al. Our theoretical approach combines molecular dynamics simulations of the stretching of atomic-sized wires with the non-equilibrium Green's function formalism based on the tight-binding modelling of the electronic system. As compared to pervious work [1], we consider substantially larger wires and explore different lattice orientations. In combination with experiments we recently provided evidence that one can build a fatigue-resistant two-terminal switch with the reversible rearrangement of single atoms[2].

[1] M. Dreher, F. Pauly, J. Heurich, J. C. Cuevas, E. Scheer, and P. Nielaba, Phys. Rev. B 72, 075435 (2005)

[2] C. Schirm, M. Matt, F. Pauly, J. C. Cuevas, P. Nielaba and E. Scheer, Nature Nanotechnology 8, 645 (2013)

O 40.11 Wed 12:30 HSZ 304

**Large Fluctuation of Conductance in Oligo(phenylene ethynylene)-Based Molecular Junctions** — •Daijiro Nozaki[1], Cormac Toher[2], and Gianaurelio Cuniberti[1,3,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Department of Mechanical Engineering and Materials Science, Duke University — [3]Center for Advancing Electronics Dresden (cfAED), TU Dresden, 01062 Dresden, Germany — [4]Dresden Center for Computational Materials Science (DCCMS), TU Dresden, 01062 Dresden, Germany

Oligo(phenylene ethynylene)s (OPEs) are widely used as conductive building blocks in molecular electronics. It is known that a phenylene unit in OPEs has low energy barrier (100 meV) for its rotation along the axis of the molecule. We have modeled an OPE-based molecular junction where an OPE oligomer is connected between conducting leads, and calculated the conductance of the junction using gDFTB code [1]. We show that the conductance at the Fermi energy significantly changes as a function of rotation angle of the phenylene unit yielding the on/off ratio over $10^4$. We have also performed the ab initio MD at room temperature and obtained the similar result. This result implies that a special attention needs to be paid to the relationship between conductance and fluctuation of molecular framework.

[1] D. Nozaki, C. Toher, and G. Cuniberti, J. Phys. Chem. Lett. **4**, 4192 (2013)

O 40.12 Wed 12:45 HSZ 304

**A Simple Graphical Model to Predict and to Control of Quantum Interference in T-shaped Molecular Junctions** — •Daijiro Nozaki[1], Haldun Sevincli[2], Stanislav M. Avdoshenko[3], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1,4,5] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany. — [2]Department of Micro- and Nanotechnology, TU Denmark, DK-2800 Kgs. Lyngby, Denmark — [3]School of Materials Engineering, Purdue University, Indiana 47907, USA — [4]Center for Advancing Electronics Dresden (cfAED), TU Dresden, 01062 Dresden, Germany. — [5]Dresden Center for Computational Materials Science (DCCMS), TU Dresden, 01062 Dresden, Germany

Quantum interference (QI) effect in molecular devices introduces an abrupt dip in the transmission spectra, thus it can be used to a series of applications such as molecular switches and molecular thermoelectric devices. For the development of the QI-based molecular devices, it is important to give the guideline to predict and to control the shape and positions of QI in transmission spectra. For this purpose, we present a simple graphical approach (called as "parabolic model") to predict the appearance, shape, and energy position of the QI in transmission spectra for T-shaped molecular devices. We show that this "parabolic model" enables one to visualize the relationship between key electronic parameters and the shape of transmission functions without calculating transmission functions.

[1] D. Nozaki, *et al.*, Phys. Chem. Chem. Phys. **15**, 13951 (2013).

## O 41: Graphene: Transport (HL jointly with MA, O, TT)

Time: Wednesday 9:30–12:15 Location: POT 051

O 41.1 Wed 9:30 POT 051

**Ratchet effects in graphene with a lateral potential** — •Josef Kamann[1], Leonid Golub[2], Matthias König[1], Jonathan Eroms[1], Felix Fromm[3], Thomas Seyller[3], Dieter Weiss[1], and Sergey Ganichev[1] — [1]University of Regensburg, Germany — [2]Ioffe Physical-Technical Institute of the RAS, St. Petersburg, Russia — [3]Technical University of Chemnitz, Germany

We report on the observation of terahertz radiation induced ratchet effects in graphene with a lateral periodic potential. These effects generate a dc electric current from an ac electric field. To probe ratchet effects, a metal grating has been deposited on top of epitaxially grown graphene. This lattice contains periodically deposited stripes with different widths and spaces and, therefore, has no inversion symmetry.

We demonstrate that the ratchet effect is generated only in the modulated area and does not arise in unpatterned graphene. This proves the symmetry breaking induced by the asymmetric lateral potential. Additional effects like edge currents or the circular ac Hall effect are excluded by the geometry of the samples and by illumination under normal incidence. The ratchet signal is studied with respect to the polarization and the wavelength of the radiation. We show that the ratchet effect is sensitive to both linear and circular polarization and conducted calculations for different elastic-scattering processes to compare them to our experimental findings.

O 41.2 Wed 9:45 POT 051

**Magnetic quantum ratchet effect in graphene** — •Christoph Drexler[1], Sergey Tarasenko[2], Peter Olbrich[1], Johannes Karch[1], Marion Hirmer[1], Florian Müller[1], Martin Gmitra[1], Jaroslav Fabian[1], Rositza Yakimova[3], Samuel Lara-Avila[4], Sergey Kubatkin[4], Minjie Wang[5], Junichiro Kono[5], and Sergey Ganichev[5] — [1]THz Center, University of Regensburg, Germany — [2]Ioffe Physical-Technical Institute, St. Petersburg, Russia — [3]Linköping University, Sweden — [4]Chalmers University, Göteborg, Sweden — [5]Rice University, Houston, USA

We report on the experimental observation of the magnetic quantum ratchet effect in epitaxial- and CVD- grown graphene layers excited by pulsed terahertz (THz ) - laser radiation [1]. Our experimental findings can be well understood in terms of asymmetric carrier scattering in graphene in presence of an in-plane magnetic field yielding strong structure inversion asymmetry (SIA) in graphene. The SIA stems from the fact that graphene is deposited on a substrate and/or is sensitive to chemical bonding of adatoms on the surface. Considering hydrogen atoms on top of carbon we calculated the magnitude of the photocurrent being in good agreement with the data obtained from the experiments. The amplitudes of the current differ significantly for the used material systems whereas its sign can be influenced by the post-groth treatment of the samples. The ratchet current can be calibrated to measure the strength of the SIA, which plays an important role in graphene ferromagnetism and spintronics.

[1] C. Drexler et al, Nat. Nano. 8 104-107, 2013.

O 41.3 Wed 10:00 POT 051

**Spin transport in arrays of graphene nanoribbons** — Matthias Berl, Bastian Birkner, Andreas Sandner, Silvia Minke, Dieter Weiss, and •Jonathan Eroms — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany

We performed non-local spin valve and Hanle measurements in arrays of graphene nanoribbons in both single and bilayer graphene. Nanoribbons were patterned by electron beam lithography and oxygen-based reactive ion etching. By fabricating several sets of electrodes, we can compare spin transport data in bulk and nanoribbons on the same graphene flake. Due to band-gap opening in the nanoribbons at low temperatures, spin transport measurements were only possible at 200 Kelvin. For single layer graphene we observe that while nanopatterning decreases the electron mobility, the spin lifetime increases from 200 ps to 500 ps. This is consistent with a Dyakonov-Perel-like contribution to spin relaxation. In bilayer graphene, we observe a low electron mobility and high spin lifetimes of about 1 ns in both bulk and nanoribbons, again consistent with Dyakonov-Perel-like spin relaxation. Attempting to see an influence of possible magnetic moments at the sample edges, no clear signature was detected in the Hanle data at 200 Kelvin.

O 41.4 Wed 10:15 POT 051

**THz radiation interacting with epitaxial graphene** — •Christian Sorger, Sascha Preu, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We investigate the interaction between terahertz (THz) radiation and periodically doped graphene ribbons. We find a remarkable polarization dependence. The Drude response of graphene can be probed with THz electric fields parallel to the ribbons. This results in a high-pass filter-like behavior with a 3dB-frequency in the THz range. The exact value depends on carrier mobility and carrier concentration. For THz electric field perpendicular to the ribbons we detect rather high transmission as the response is dominated by plasmonic effects. Utilizing the material system epitaxial graphene on silicon carbide (SiC) we show that no lithographic patterning is required to couple light into the two-dimensional electron gas (2DEG). As the interaction strength depends on the geometry of the 2DEG and its electronic properties, respectively, this strategy allows for a characterization of the AC conductivity in epitaxial graphene.

O 41.5 Wed 10:30 POT 051

**Numerically exact approach to transport properties of disordered two-dimensional materials** — •Stefan Barthel[1,2], Malte Rösner[1,2], Fernando Gargiulo[3], Oleg V. Yazyev[3], and Tim O. Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Germany — [3]Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

We present a numerical method for modeling electron transport in disordered two-dimensional materials such as graphene with resonant impurities. Covalently bonded adatoms, such as hydrogen, modify the electronic structure and transport properties of graphene in the diffusive as well as localized regime in which quantum corrections become important. The electronic structure is described using a tight-binding model involving pz-orbitals on a honeycomb lattice, whereas the transport properties are evaluated in the linear response approximation (Kubo-Greenwood) using the kernel polynomial method as a solver. By combining these methods we gain access to large systems containing up to 10ˆ6 atoms. These results are compared to the ones obtained using the Landauer-Büttiker approach in the above-mentioned transport regimes.

O 41.6 Wed 10:45 POT 051

**Quantum Hall Effect in Chemically Functionalized Graphene: Defect-Induced Critical States and Breakdown of Electron-Hole Symmetry** — •Nicolas Leconte[1,2], Jean-Christophe Charlier[2], and Stephan Roche[1] — [1]ICN2 - Institut Catala de Nanociencia i Nanotecnologia, Campus UAB, 08193 Bellaterra (Barcelona), Spain — [2]Université catholique de Louvain (UCL), Institute of Condensed Matter and Nanoscience (IMCN), Chemin des étoiles 8, 1348 Louvain-la-Neuve, Belgium

Unconventional magneto-transport fingerprints in the quantum Hall regime (with applied magnetic field from one to several tens of Tesla) in chemically functionnalized graphene are reported. Upon chemical adsorption of monoatomic oxygen (from 0.5% to few percents), the electron-hole symmetry of Landau levels is broken, while a doublepeaked conductivity develops at low-energy, resulting from the formation of critical states conveyed by the random network of defects-induced impurity states. Scaling analysis suggests an additional zero-energy quantized Hall conductance plateau, which is here not connected to degeneracy lifting of Landau levels by sublattice symmetry breakage. This singularly contrasts with usual interpretation, and unveils a new playground for tailoring the fundamental characteristics of the quantum Hall effect. The study on oxygen is complemented with a study on a simplified divacancy model, confirming the percolation of impurity states leading to delocalized states.

### Coffee break (15 min.)

O 41.7 Wed 11:15 POT 051

**Ultra long spin decoherence times in graphene quantum dots with a small number of nuclear spins** — •Moritz Fuchs[1], John Schliemann[2], and Björn Trauzettel[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg — [2]Institut für Theoretische Physik, Universität Regensburg, 93053 Regensburg

We study the dynamics of an electron spin in a graphene quantum dot, which is interacting with a bath of less than ten nuclear spins via the anisotropic hyperfine interaction. Due to substantial progress in the fabrication of graphene quantum dots, the consideration of such a small number of nuclear spins is experimentally relevant. This choice allows us to use exact diagonalization to calculate the longtime average of the electron spin as well as its decoherence time. We investigate the dependence of spin observables on the initial states of nuclear spins and on the position of nuclear spins in the quantum dot. Moreover, we analyze the effects of the anisotropy of the hyperfine interaction for different orientations of the spin quantization axis with respect to the graphene plane. Interestingly, we then predict remarkable long decoherence times of more than 10ms in the limit of few nuclear spins.

O 41.8 Wed 11:30 POT 051

**Carrier dynamics in graphene under Landau quantization** — •Florian Wendler[1], Martin Mittendorff[2], Stephan Winnerl[2], Manfred Helm[2], Andreas Knorr[1], and Ermin Malic[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

We investigate the ultrafast dynamics of low-energetic Dirac electrons in graphene under Landau quantization [1]. In a joint experiment-theory study, we provide calculations based on the density matrix formalism [2] as well as measurements of the relaxation dynamics via differential transmission spectroscopy.

As a consequence of the linear dispersion at the Dirac points, graphene exhibits a non-equidistant Landau level spectrum which allows to address specific transitions by optical pumping. Exploiting this to selectively excite the energetically lowest Landau levels, we employ pump-probe spectroscopy to explore the carrier dynamics in this regime. A surprising sign reversal in differential transmission spectra is observed both in experiment and theory and provides evidence for strong Auger scattering on a picosecond timescale. Our calculations even predict the occurrence of a substantial carrier multiplication in Landau quantized graphene [3].

[1] M. Mittendorff et al., (in preparation).

[2] E. Malic, A. Knorr, Graphene and Carbon Nanotubes: Ultrafast Optics and Relaxation Dynamics, (Wiley-VCH, Berlin, 2013).

[3] F. Wendler, A. Knorr, and E. Malic, (submitted).

O 41.9 Wed 11:45 POT 051

**Polarization dependence of optical carrier excitation in graphene** — •Martin Mittendorff[1,2], Torben Winzer[3], Ermin Malic[3], Andreas Knorr[3], Harald Schneider[1], Manfred Helm[1,2], and Stephan Winnerl[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Technische Universität Berlin, Hardenbergstraße 36 10623 Berlin, Germany

We present near-infrared pump-probe measurements to investigate the polarization dependence of optical carrier excitation in graphene. Excitation with linearly polarized radiation leads to an anisotropic distribution of the nonequilibrium carriers in momentum space. This anisotropy can be revealed by the comparison of pump-probe signals for different polarization configurations. In parallel configuration the probe beam has the same polarization with respect to the pump beam, for the perpendicular configuration the polarization of the probe beam is rotated by 90°. The signal amplitude of the parallel configuration is about twice as large as compared to the perpendicular configuration. The initial relaxation process is faster for the parallel polarized probe beam, which leads to identical signals about 150 fs after excitation. At this time delay an isotropic carrier distribution is reached by electron-phonon scattering. These findings are confirmed by microscopic calculations.

O 41.10 Wed 12:00 POT 051

**Anisotropic photoinduced current injection in graphene** — •Julien Rioux[1], John Sipe[2], and Guido Burkard[1] — [1]University of Konstanz — [2]University of Toronto

Quantum-mechanical interference effects are considered in carrier and charge current excitation in gapless semiconductors using coherent optical field components at frequencies $\omega$ and $2\omega$. Due to the absence of a bandgap, excitation scenarios outside of the typical operation regime are considered; we calculate the polarization and spectral dependence of these all-optical effects for single- and bilayer graphene. For linearly-polarized light and with one-photon absorption at $\omega$ interfering with $2\omega$ absorption and $\omega$ emission, the resulting current injection is five times stronger for perpendicular polarization axes compared to parallel polarization axes. This additional process results in an anisotropic current as a function of the angle between polarization axes, in stark contrast with the isotropic current resulting from the typical interference term in graphene [Rioux et al., PRB 83, 195406 (2011)]. Varying the Fermi level allows to tune the disparity parameter $d = \eta_I^{xyyx}/\eta_I^{xxxx}$ closer to typical values in GaAs [$|d| \approx 0.2$, Rioux and Sipe, Physica E 45, 1 (2012)]: from $-1$, when the additional process is fully Pauli-blocked, to $-3/7$, when it is fully accessible, thus facilitating polarization sensitive applications.

# O 42: Topological Insulators: Theory (HL jointly with MA, O, TT)

Time: Wednesday 9:30–11:15 Location: POT 151

O 42.1 Wed 9:30 POT 151

**Stabilizing Chern and fractional Chern insulators** — •Adolfo G. Grushin, Johannes Motruk, and Frank Pollmann — Max Planck Institute for the Physics of Complex Systems, Dresden

The experimental realization of Chern insulators (CI) and fractional Chern insulators (FCI), zero field lattice analogues of the integer and fractional Hall effects respectively, is still a major open problem in condensed matter. For the former, it was proposed that short range interactions at the mean-field level can drive a trivial insulator into a CI. For the latter, the effect of band dispersion and sizes of the single-particle gaps with respect to the interaction strength have been argued to be important to stabilize an FCI state. In this talk we will examine the robustness and fate of these statements both with exact diagonalization and infinite density matrix renormalization group (iDMRG).

O 42.2 Wed 9:45 POT 151

**Point contacts and localization in generic helical liquids** — •Christoph P. Orth, Grégory Strübi, and Thomas L. Schmidt — University of Basel, Switzerland

We consider two helical liquids on opposite edges of a two-dimensional topological insulator, which are connected by one or several local tunnel junctions. In the presence of spatially inhomogeneous Rashba spin-orbit coupling, the spin of the helical edge states is momentum dependent, and this spin texture can be different on opposite edges. We demonstrate that this has a strong impact on the electron transport between the edges. In particular, in the case of many random tunnel contacts, the localization length depends strongly on the spin textures of the edge states.

O 42.3 Wed 10:00 POT 151

***ab-initio* investigation of topological states and symmetry inversion in HgTe-CdTe Quantum wells** — •Sebastian Kuefner, Juergen Furthmueller, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

Topological insulators (TIs) recently attracted a high level of attention in solid state physics due to their unique physical properties. Generally, a TI is a material that is insulating in the bulk but exhibits metallic surface or edge states. These states are topologically protected which means that they are independent of surface orientation and passivation. The edge states usually have linear band dispersion forming Dirac cones.

The electromagnetic properties of the edge states might be used for the realisation of topological superconducting phases. In two dimensions the edge states build the quantum spin Hall state (QSH). In 2006, Bernevig et al. predicted the occurence of the QSH in HgTe-CdTe superlattices theoretically by an **kp**-approch which was later verified by König et al. experimentally.

However, these results have not yet been discussed in the framework of a reasonable electronic structure theory based on *ab-initio* methods but account for quasiparticle effects and spin-orbit coupling. Using density-functional theory together with the Tran-Blaha approximation we discuss the occurence of topological quantum-well states and investigate the topological transition in atomic structures.

O 42.4 Wed 10:15 POT 151

**Nontrivial Interface States Confined Between Two Topological Insulators** — •Tomáš Rauch[1], Markus Flieger[1], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle (Saale), Germany

By *ab initio*-based tight-binding calculations, we show that nontrivial electronic states exist at an interface of a $\mathcal{Z}_2$ topological insulator and a topological crystalline insulator. At the exemplary (111) interface between $Bi_2Te_3$ and SnTe, the two Dirac surface states at the Brillouin zone center $\overline{\Gamma}$ annihilate upon approaching the semi-infinite subsystems but one topologically protected Dirac surface state remains at each time-reversal invariant momentum $\overline{\mathrm{M}}$. This leads to a highly conducting spin-momentum-locked channel at the interface but insulating bulk regions. For the $Sb_2Te_3/Bi_2Te_3$ interface we find complete annihilation of Dirac states because both subsystems belong to the same topology class.

O 42.5 Wed 10:30 POT 151

**Natural three-dimensional topological insulators in $Tl_4PbTe_3$ and $Tl_4SnTe_3$** — •Chengwang Niu[1,2], Ying Dai[1], Baibiao Huang[1], Gustav Bihlmayer[2], Yuriy Mokrousov[2], Daniel Wortmann[2], and Stefan Blügel[2] — [1]School of Physics, Shandong University, Jinan, China — [2]Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The recently discovered three-dimensional topological insulators have attracted much interest due to their exceptional properties of possessing insulating bulk but time-reversal symmetry protected metallic surfaces with Dirac-like band structure [1,2]. The search for new topological insulators is critical for both fundamental and practical interests. Based on first-principles calculations, we reveal that both $Tl_4PbTe_3$ and $Tl_4SnTe_3$ are strong topological insulators with different band inversion behaviors at Γ point [3]. The mechanisms of band inversion in $Tl_4PbTe_3$ and $Tl_4SnTe_3$, as well as in $Bi_2Se_3$ and $Sb_2Se_3$, are investigated and classified. The $Z_2$ topological invariants and topological surface states are investigated to confirm the topologically non-trivial phase. Our calculations further indicate that the electron- or hole-type Dirac fermion can be effectively engineered by hole doping, which is necessary for device applications of topological insulators.

[1] M. Hasan and C. Kane, Rev. Mod. Phys. **82**, 3045 (2010).
[2] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).
[3] C. Niu et al., in preparation.

O 42.6 Wed 10:45 POT 151

**Electronic properties of the topological crystalline insulator SnTe and its (001) and (111) surfaces: an ab-initio study** — •Matthias Drüppel, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster

The insulator SnTe belongs to the recently discovered class of materials in which a crystalline symmetry ensures the existence of topologically protected surface states. We report on the properties of these states at the (001) and (111) surfaces. To this end, we have employed density-functional theory.

The bulk band structure of SnTe is characterized by inversion at the four equivalent L points giving rise to a mirror Chern number $n_m = -2$. The (001) surface exhibits two mirror planes and shows four Dirac cones at non-time-reversal-invariant points along the $\pm\overline{\Gamma}\overline{\mathrm{X}}$ and $\pm\overline{\Gamma}\overline{\mathrm{X}}'$ lines, respectively. Here we explore the influence of lattice deformations on the stability of the surface states. Our results reveal that distortions of the topmost layers which break a mirror symmetry locally at the surface do *not* lead to an opening of the surface band gap. We find that only*bulk* lattice deformations, e.g. rhombohedrial distortions, that break one or both mirror symmetries also in the bulk part of the system give rise to a surface band gap. Our calculations show that the Sn terminated (111) surface exhibits Dirac cones centered at $\overline{\Gamma}$ and $\overline{\mathrm{M}}$. In particular at the $\overline{\mathrm{M}}$ point, these topologically protected states are distinctly extended into the bulk. Interestingly, we observe for the Te terminated (111) surface a gap-closing Dirac state only at the $\overline{\Gamma}$ point

O 42.7 Wed 11:00 POT 151

**Adsorbate- and vacancy-induced band bending in $Bi_2Se_3$: ab-initio calculations** — •Tobias Förster, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

$Bi_2Se_3$ is one of the first topological insulators ever discovered. It has been widely studied both experimentally und theoretically, due to its simple electronic structure with only one Dirac point at $\overline{\Gamma}$. In experiments, a downward band bending and an ageing effect are frequently observed. This has been attributed to an intrinsic n-doping and to coverage with adsorbates. Models for the band bending mostly focussed on the intrinsic doping.

Using DFT calculations, we show that a long-ranged potential also occurs for an adsorbate-covered surface, even without intrinsic doping. As a prototype adsorbate, we have investigated potassium at various coverages. The resulting changes in the charge density, the potential, and the band structure can be attributed to two distinct origins: short-ranged adsorbate-specific changes and the formation of a long-ranged potential (which is independent of the specific adatom). We will explain how the band bending is related to the layered structure of $Bi_2Se_3$. Similar effects result from our calculations for different types of adsorbates as well as for selenium vacancies in the surface layer.

# O 43: Organic Electronics and Photovoltaics IV (CPP jointly with DS, HL, O)

Polymers, Solar Cells, OFETs, OLEDs, Spectroscopy

Time: Wednesday 9:30–12:45 Location: ZEU 260

O 43.1 Wed 9:30 ZEU 260

**Structural Degradation of Polymer Solar Cells** — •Christoph J. Schaffer[1], Claudia M. Palumbiny[1], Martin A. Niedermeier[1], Christian Jendrzejewski[1], Gonzalo Santoro[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department - LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]DESY, Notkestr. 85, 22607 Hamburg

A major challenge in organic photovoltaics (OPV) is to elongate their lifetimes. Several mechanisms of organic solar cell degradation have been proposed in literature within the last years. However, insufficient research has been done on determining the role of transitions in the nanomorphology of the active layer of bulk-heterojunction (BHJ) polymer solar cells as an aspect of degradation. These transitions would strongly affect the properties of solar cells since the active layer morphology plays a crucial role in the energy conversion process.

We present a direct evidence of morphological degradation on a nanometer scale in polymeric solar cells by simultaneous in-situ GISAXS and current-voltage tracking on a running P3HT:PCBM solar cell. The loss of short-circuit current with time is fully modeled by the observed morphological transitions [1].

[1] C. J. Schaffer et al., *Adv. Mater.* **2013**, DOI: 10.1002/adma.201302854

O 43.2 Wed 9:45 ZEU 260

**Controlling nanomorphology in bulk heterojunction solar cells via addition of third component** — •Eva M. Herzig[1], Ammara R. Akhtar[2], Anna Naumann[2], Shuai Guo[2], Gregory Tainter[2], Jianqi Zhan[2], Jan Perlich[3], Stephan V. Roth[3], Christine M. Papadakis[2], and Peter Müller-Buschbaum[2] — [1]TU München, MSE, Lichtenbergstr. 4, 85748 Garching — [2]TU München, Physik-Department,, James-Franck-Str. 1, 85748 Garching — [3]DESY, Notkestr. 85, 22603 Hamburg

Nanomorphology and effciency of organic solar cells are closely linked. It is therefore desirable to have control over the self-assembly process responsible for the morpholgy formation of the active material. Employing grazing incidence small and wide angle x-ray scattering(GISAXS & GIWAXS) as well as spectroscopy and microscopy methods allows us to characterize organic thin films on the nanoscale with high statistical relevance. Using these methods we thoroughly investigate the morphological changes upon the addition of a third polymeric component showing that the self-assembly process is altered. We find that the amount of the third component controls the phase separation in the bulk heterojunction active layer. Adjusting the preparation route to support crystallization of the active material leads to an increased solar cell performance for a tuned ternary solar cell system.

O 43.3 Wed 10:00 ZEU 260

**Layer by layer solution processing of nanostructured all-polymer solar cells** — •Thomas Pfadler, Mihael Coric, Jonas Weickert, Karl-Philipp Strunk, and Lukas Schmidt-Mende — University of Konstanz

Organic solar cells have the potential to become an important low-cost alternative to conventional solar cells. However, before this can happen, the energy harvesting potential of organic solar cells must become more comparable with that of the pervading technology. This research is focusing on nanoimprint lithography (NIL), a low-cost lithographic method for high-throughput patterning applicable to organic semiconductors. This technique can be used to tailor an organic solar cells active material on a nanometer scale. A promising application of NIL aims to control the nanostructure of a donor-acceptor interface in an organic all-polymer device. The electron accepting polymer is structured. A stiff polymer network featuring a nanostructured topography is developed by the usage of a photoactivable crosslinker molecule (sFPA). The crosslinked polymer matrix is not dissolved during spincoating the donor polymer allowing fully solution processed device fabrication with controlled nanostructured donor-acceptor interfaces. Target of this approach is to investigate nanostructured bi-layer devices with controlled interfaces to finally enhance the overall efficiency by maximizing the interfacial area, increasing the exciton separation yield and ensuring direct pathways to the electrodes.

O 43.4 Wed 10:15 ZEU 260

**The role of processing additives in Organic Solar Cells after the preparation process** — •Stefan Väth[1], Andreas Baumann[1], Andreas Sperlich[1], Carsten Deibel[1], Milutin Ivanovic[2], Heiko Peisert[2], Thomas Chassé[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Eberhard Karls University Tübingen, 72076 Tübingen — [3]ZAE Bayern, 97074 Würzburg

Processing additives are widely used in the preparation of new high performance bulk heterojunction organic solar cells to improve the power conversion efficiency (PCE) significantly. They act as selective solvent for fullerenes and are therefore improving the morphology of the active area. Nevertheless the question wether or not these cosolvents remain in the organic solar cells after the preparation process occurs. This question could be solved by investigating blends consisting of the material system PTB7:$PC_{60}BM$ processed with the additives diiodooctane (DIO), octanedithiol (ODT) and without additives as reference. We used the spin sensitive measurement technique light induced Electron Paramagnetic Resonance (LESR) to distinguish between positive polarons on the polymer and negative charges on the fullerene by their different g-factors. Together with Photoelectron Spectroscopy (PES) measurements we could show that the additive DIO remains partly inside the active layer of organic solar cells even after a high vacuum preparation step. We propose that they do not only lead to an improved morphology, but also to a doping effect.

O 43.5 Wed 10:30 ZEU 260

**Radiative and non-radiative recombination in organic solar cells** — •Kristofer Tvingstedt, Philip Pelchmann, Vladimir Dyakonov, and Carsten Deibel — Experimental Physics VI Julius Maximilian University of Würzburg 97074 Würzburg

Although several organic solar cells has reached close to unity internal quantum efficiency at short circuit conditions, the open circuit voltage is still very far from its potential upper limit due to substantial charge recombination of various types, which remains to be accurately determined. In this work we evaluate the limiting mechanisms in OPVs by employing complementary steady state measurements of recombination as a function of charge carrier density by thoroughly evaluating the diode ideality factor. The diode ideality is directly related to the order of recombination and we first assess it via light intensity dependent open circuit voltage characterization under the influence of a varying temperature. We focus our study on the ratio between radiative and non-radiative recombination via the interfacial charge transfer state as determined by absolute CT electroluminescence efficiency measurements, also as a function of temperature. The charge transfer state governs the radiative recombination in OPV bulk heterojunctions and is therefore crucial to evaluate in this context. Improving the radiative efficiency of OPVs will substantially increase the open circuit voltage and eventually put these promising photovoltaic converters in efficiency parity with their inorganic counterparts.

O 43.6 Wed 10:45 ZEU 260

**Electronic Structure of Fullerene Heterodimer in Bulk-Heterojunction Blends** — •Andreas Sperlich[1], Oleg G. Poluektov[2], Jens Niklas[2], Kristy L. Mardis[3], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg and ZAE Bayern, 97074 Würzburg — [2]Chemical Sciences and Engineering Division, ANL, Argonne, Illinois 60439, USA — [3]Department of Chemistry and Physics, Chicago State University, Chicago, Illinois 60628, USA

To increase performance of organic solar cells, the optimization of the electron-accepting fullerenes has received less attention. Here, we report an electronic structure study of a novel covalently linked $C_{60}$-$C_{70}$-heterodimer in blend with the polymer PCDTBT. Upon optical excitation of polymer:heterodimer solid films, the electron is shared between both $C_{60}$ and $C_{70}$ cages. In contrast, in the solution the electron is localized on one half of the dimer. Electronic structure calculations reveal that for the heterodimer two nearly iso-energetic minima exist, essentially the cis and trans conformers. These conformers have different edge-to-edge distance between the two cages and therefor the electron is either shared between two dimer halves (cis) or localized on one half of the heterodimer (trans). By comparison with the experimental data, we conclude that the cis conformation is preferable in films, and the trans conformation in solution. These findings demonstrate how electronic coupling of the fullerene acceptor molecules is influenced by their packing in blends, which may have an impact on the charge carrier generation efficiency in solar cells.

**15 min. break**

O 43.7 Wed 11:15 ZEU 260

**Cyclic potential growth mechanism for electropolymerized polythiophenes as anode buffer layers in P3HT-PCBM solar cells** — •Sidhant Bom, Marlis Ortel, and Veit Wagner — Research Center for Functional Materials and Nanomolecular Science, Jacobs University, Bremen, Germany

A new method for electro-polymerization of polythiophenes as anode buffer layer (ABL) is presented. The ABL is used in a bulk-heterojunction solar cell with P3HT-PCBM as active material. Electro-polymerized thiophenes (ePT) are grown electrochemically with a standard three electrodes system on conductive contacts. We find a distinct impact of the time variation of the growth potential on the obtained layer properties. A new time dependent cyclic potential electro-polymerization method is systematically compared to a standard constant potential method. AFM topography reveals that a uniform homogeneous film of ePT is obtained by the time dependent cyclic potential growth method. The devices were fabricated with a 10 nm ePT between the active layer and PEDOT:PSS with aluminum as cathode. With a cyclic potential method, about 20% enhancement in short circuit current was observed in contrast to 10% enhancement with constant potential method. Improvements by the ePT layer are attributed to better band alignment of the HOMO levels and a LUMO offset of 0.2eV which gives its electron blocking characteristics. In summary, the cyclic potential method results in a better quality of ePT layers with good homogeneity and area coverage leading to further improvements in device performance.

O 43.8 Wed 11:30 ZEU 260

**Intrinsic charge carrier mobility in PCDTBT:$PC_{71}$BM blend thin films investigated by simultaneous transient absorption and transient microwave conductivity measurements** — •Andreas Fritze[1], Jeremias Weinrich[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

PCDTBT is a promising low-bandgap polymer for photovoltaic applications that has demonstrated unique recombination dynamics compared to the model P3HT system. Usually, the recombination dynamics in organics blends is expected to be proportional to the macroscopic charge carrier mobility, which is influenced by trapping and therefore potentially depends on the charge carrier concentration. For PCDTBT blends, we want to determine if the recombination dynamics are indeed governed exclusively by the low macroscopic mobility or if it is dominated by the, high local mobility. Therefor, we performed simultaneous measurements of transient absorption (TAS) and transient microwave conductivity on PCDTBT:$PC_{71}$BM thin films on a 10 ns to 1 ms time scale. TAS probes the charge carrier density, whereas the microwave experiment is sensitive to the intrinsic, high frequency conductivity. By investigating the charge carrier dynamics and conductivity at different laser pump intensities and temperatures, we can separate the effects of mobility relaxation from carrier concentration dependent mobility in order to understand the dominant loss mechanism in organic solar cells.

O 43.9 Wed 11:45 ZEU 260

**On the role of the effectiv mass, ground state complexes and interfacial dipoles on exciton dissocitation in organic donor-acceptor systems** — •Anna Köhler — University of Bayreuth, Bayreuth, Germany

Efficient exciton dissociation at a donor-acceptor interface is a necessary condition for obtaining high efficiency polymeric solar cells. Despite its importance, this step is still not fully understood. A central question is how and why, after photoexcitation of the donor and transfer of an electron onto the acceptor, the the e-h pair can overcome their considerable mutual Coulomb potential. Possibilities that are currently discussed include the degree of delocalization of both an exciton and a charge in a conjugated polymer, ground state charge transfer complexes as well as interfacial dipoles that may exist at the donor-acceptor interface in the ground state, and the degree of energetic and structural order/disorder. In this talk I will show how we combine insight gained from ultrafast pump-probe spectroscopy, field dependent photocurrent measurements, photoemission measurements and modeling to assess which factors control the dissociation process.

O 43.10 Wed 12:00 ZEU 260

**Non-photochemical self-quenching mechanism in conjugated polymers revealed by control of chain length and morphology** — •Florian Steiner, Jan Vogelsang, and John M. Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D- 93040 Regensburg

Unraveling the complex photophysics of multichromophoric systems like conjugated polymers (CPs) is an ongoing interdisciplinary task. Some of the pressing questions in CP photophysics are: (i) what unit absorbs and emits the light in a CP? (ii) What processes take place between the absorption and emission event? And (iii) what is the interplay between excitation energy transfer between chromophores and non-radiative fluorescence decay? Answering these questions will lead to a fundamental understanding of the photophysics of CPs, which in turn can highlight important loss mechanisms regarding the efficiency in CP-based devices, such as self-quenching.

We illustrate that control of size and morphology in combination with several single-molecule techniques leads to a universal picture of the self-quenching mechanism in CPs by addressing these questions. As a model system we chose the device-relevant prototypical CP poly(3-hexylthiophene). Morphological control, combined with well-defined sub-populations of different sizes, enabled us to correlate a diverse set of photophysical observables (brightness, emission polarization, emission spectra, photon antibunching) with each other and the size. Finally, the increasing fluorescence self-quenching with size and morphological order is rationalized with a comprehensive photophysical model.

O 43.11 Wed 12:15 ZEU 260

**Conformations and electronic structure of Oligo-PPEs Investigated by Pulsed Electron Paramagnetic Resonance Spectroscopy** — Patrick Korf, Friederike Schütze, Christian Hintze, Stefan Mecking, and •Malte Drescher — Department of Chemistry, University of Konstanz, Germany

Poly(para-phenyleneethynylene)s (PPE) are versatile polymers that are synthetically easily accessible.

Owing to their application in organic electronics and cell microscopy their microscopic and electronic properties are of high interest.

Herein we report the investigation of the electronic structure including the photo-excited triplet state of rod-like Oligo-PPEs. The lifetime, relaxation rates and populations of the triplet sublevels are quantitatively analyzed at cryogenic temperatures in a glassy toluene matrix via time-resolved EPR with synchronized UV laser flash excitation. The photo-physical properties are studied depending on the size of the delocalized $\pi$-electron system by varying the number of repeat units in the Oligo-PPEs.

In addition, their microscopic material properties are studied in particles with confined size constituted by block coplymers of PEGylated Oligo-PPEs. The molecular conformation is investigated by EPR distance measurements in solution, in bulk material as well as in particles. The data suggest that the rod-like Oligo-PPEs are present in a collapsed state in the particles.

O 43.12 Wed 12:30 ZEU 260

**Structural and electrical characterization of Hex-5T-Hex**

**oligothiophene thin films during film formation** — •Eduard Mikayelyan[1], Linda Grodd[1], Ullrich Pietsch[1], Artem. V. Bakirov[2], Maxim. A. Shcherbina[2], Sergei N. Chvalun[2], and Souren Grigorian[1] — [1]University of Siegen — [2]Enikolopov Institute of Synthetic Polymeric Materials of Russian Academy of Sciences

Organic semiconductors are attractive for electronics due to the low cost processing methods and their high electrical conductivity. Thiophene based polymers and oligomers are demonstrating relatively high mobility, excellent luminescence properties which used for application in solar cells, radio-frequency identification, etc. [1, 2]. We have investigated the thiophene based oligomer Hex-5T-Hex. Structural characterization has been performed by grazing incidence x-ray diffraction (GIXD)method, in particular we probed the crystallite orientations in prefabricated thin films. The 3D structure of Hex-5T-Hex oligomer evaluated from the in-plane (010), (020) and (021) reflections is consistent with 2D structure suggested from 5T based oligomer self-assembled monolayer (SAM) [3]. Additionally, we found the (100) and (100)' reflections in out-of-plane direction characterizing two different stacking along thiophene backbone axis. In order to correlate the structural properties of oligothiophene thin films with the electrical characteristics both properties were probed simultaneous during film formation. This work was supported by BMBF, project number 05K10PSC.

## O 44: Low-Dimensional Systems: 2D - Theory (TT jointly with O)

Time: Wednesday 9:30–13:00 Location: BEY 81

O 44.1 Wed 9:30 BEY 81

**Critical theory of the spin quantum Hall transition** — •Roberto Bondesan — Institute of theoretical physics, Köln, Deutschland

The spin quantum Hall (SQH) transition is a 2+1 dimensional Anderson transition between topological phases distinguished by different integer values of the spin conductance. In contrast to the celebrated integer quantum Hall transition, in the SQH case, critical exponents governing low moments of observables are known exactly. In this talk I will address the problem of characterizing completely the exponents of the theory beyond low moments. For this puropouse I will explain recent insights on the classification of scaling fields at Anderson transitions, which allow to perform efficient numerical studies and conjecture the multifractal spectrum of the theory.

O 44.2 Wed 9:45 BEY 81

**Pure scaling operators at the integer quantum Hall plateau transition** — Roberto Bondesan, •Daniel Wieczorek, and Martin Zirnbauer — Universität zu Köln, Institut für theoretische Physik, Zülpicher Straße 77, 50937 Köln

Despite considerable effort, the conformal field theory underlying the integer quantum Hall plateau transition is still not known. We circumvent the fact that conductances in the Chalker-Coddington model do not show pure scaling behaviour by introducing a new family of scattering observables corresponding to n-point functions of conformal primary fields at the plateau transition. Disorder averages of these observables correspond to lattice pure scaling operators in the supersymmetric vertex model. We also present numerical results for the multifractal spectra of 2 and 3 point functions.

O 44.3 Wed 10:00 BEY 81

**Plasmons due to the interplay of Dirac and Schrödinger fermions** — •Stefan Jürgens, Paolo Michetti, and Björn Trauzettel — Institute of Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

We study the interplay between Dirac and Schrödinger fermions in the polarization properties of a two-dimensional electron gas (2DEG). Specifically, we analyze the low-energy sector of narrow-gap semiconductors described by a two-band Kane model. In the context of quantum spin Hall insulators, particularly, in Hg(Cd)Te quantum wells, this model is named Bernevig-Hughes-Zhang model. Interestingly, it describes electrons with intermediate properties between Dirac and Schrödinger fermions. We calculate the dynamical dielectric function of such a model at zero temperature within random phase approximation. Surprisingly, plasmon resonances are found in the intrinsic (undoped) limit, whereas they are absent – in that limit – in graphene as well as ordinary 2DEGs. Additionally, we demonstrate that the optical conductivity offers a quantitative way to identify the topological phase of Hg(Cd)Te quantum wells from a bulk measurement.

O 44.4 Wed 10:15 BEY 81

**Correlated spinless fermions on the honeycomb lattice** — •Martin Hohenadler[1] and Maria Daghofer[2] — [1]University of Würzburg, Germany — [2]IFW Dresden, Germany

We study the phase diagram of spinless fermions on the honeycomb lattice with nearest– ($V_1$) and next-nearest neighbour repulsion ($V_2$) using numerical methods. At the mean-field level, this model has been shown to describe an interaction-generated quantum anomalous Hall (QAH) phase with nonzero Chern index [Raghu *et al.*, PRL **100**, 156401 (2008)]. Our exact results reveal that this phase is completely suppressed by quantum fluctuations. However, for small $V_2$, we find that $V_2$ enhances bond order correlations that resemble the mean-field bond order in the QAH phase. This weak-coupling tendency toward a QAH state suggests that the phase may be realized in other models.

O 44.5 Wed 10:30 BEY 81

**The $\pi$ flux honeycomb lattice: a topological crystalline insulator.** — •Martin Bercx, Martin Hohenadler, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg

We consider the Kane-Mele-Hubbard model with intrinsic spin-orbit coupling $\lambda$ supplemented by a $\pi$ flux threading each honeycomb plaquette. At $U = 0$ and in each spin sector the band structure is characterized by a Chern number $C = \pm 2$. Furthermore fine tuning of $\lambda$ leads to a point of quadratic band crossing associated with a topological phase transition. Bulk quantum Monte Carlo simulations reveal a magnetically ordered phase which extends to weak couplings at the value of $\lambda$ where the quadratic band crossing occurs. Although the spinful model carries two helical edge states and is explicitly shown to be a $Z_2$ trivial insulator, its edge states are robust due to protection by lattice translation symmetry. We present quantum Monte Carlo calculations which reveal that well defined edge states remain even in the case of strong interactions.

O 44.6 Wed 10:45 BEY 81

**Density Functional Description of Two-Dimensional Fermi Gases** — •Martin-Isbjörn Trappe[1], Hui Khoon Ng[1], Cord Axel Müller[2], and Berthold-Georg Englert[1] — [1]Centre for Quantum Technologies, National University of Singapore — [2]Department of Physics, University of Konstanz, Germany

Several methods suggest the gradient corrections beyond the Thomas-Fermi (TF) kinetic energy functional to vanish for two-dimensional systems at zero temperature. However, the TF functional does not coincide with the exact functional, implying the existence of corrections. We present a systematic derivation of such first order gradient corrections by means of the Wigner function and test the result employing the exactly known particle density of spin-1/2-fermions in a two-dimensional harmonic trap.

O 44.7 Wed 11:00 BEY 81

**Renormalization group approach to non-analytic corrections in Fermi liquid theory** — •Casper Drukier[1,2], Philipp Lange[1,2], and Peter Kopietz[1,2] — [1]Institut für Theoretische Physik, J.W.Goethe-Universität Frankfurt, Frankfurt am Main, Germany — [2]Department of Physics, University of Florida, Gainesville, Florida, USA

We calculate the leading non-analytic magnetic field dependence of the free energy and spin-susceptibility of a two-dimensional Fermi liquid using functional renormalization group methods, with bosonized particle-hole fluctuations. At weak coupling we recover the perturbative results of Maslov and Chubukov [PRB 79, 075112 (2009)]. We go beyond perturbation theory by including self-energy and vertex corrections within a truncated vertex expansion and present explicit results for the leading non-analytic correction to the spin-susceptibility and other Fermi liquid parameters as a function of interaction strength.

**15 min. break.**

O 44.8 Wed 11:30 BEY 81

**From infinite to two dimensions through the functional renormalization group** — Ciro Taranto[1], Sabine Andergassen[2], Johannes Bauer[3], Karsten Held[1], Andrey Katanin[4], Walter Metzner[5], Georg Rohringer[1], and •Alessandro Toschi[1] — [1]Institute for Solid State Physics, Vienna University of Technology 1040 Vienna, Austria — [2]Faculty of Physics, University of Vienna, 1090 Vienna, Austria — [3]Department of Physics, Harvard University, 17 Oxford St., MA 02138, USA — [4]Institute of Metal Physics, Russian Academy of Sciences and Ural Federal University, Ekaterinburg, Russia — [5]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

We present a novel scheme[1] for an unbiased and non-perturbative treatment of strongly correlated fermions. The proposed approach combines two of the most successful many-body methods, i.e., the dynamical mean field theory (DMFT) and the functional renormalization group (fRG). Physically, this allows for a systematic inclusion of non-local correlations via the flow equations of the fRG, after the local correlations are taken into account non-perturbatively by the DMFT. To demonstrate the feasibility of the approach, we present numerical results for the two-dimensional Hubbard model at half-filling.
[1] C. Taranto, S. Andergassen, J. Bauer, K. Held, A. Katanin, W. Metzner, G. Rohringer, and A. Toschi, arXiv: 1307.3475.

O 44.9 Wed 11:45 BEY 81

**Efficient 2D density matrix renormalization group in mixed real- and momentum-space representation** — •Johannes Motruk[1], Michael P. Zaletel[2], Roger S. K. Mong[3], and Frank Pollmann[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]Department of Physics, University of California, Berkeley, California 94720, USA — [3]Department of Physics, California Institute of Technology, Pasadena, California 91125, USA

Density matrix renormalization group (DMRG) is a powerful numerical technique for both 1D and 2D systems. The traditional implementation for a 2D system requires an ordering of sites to form an effective 1D chain for simulation. We present a variation of the DMRG technique that utilizes a real-space representation in one direction and momentum-space representation in the perpendicular direction of the lattice. We demonstrate how the mixed representation reduces the computational costs by using momentum as a conserved quantity—and as a by product—produces the momentum-resolved entanglement spectrum. As an application, we map out the phase diagram of a tight-binding model of spinless fermions with nearest-neighbour interactions on the square lattice. For this model, we give performance benchmarks comparing the mixed basis to the traditional real-space basis.

O 44.10 Wed 12:00 BEY 81

**Dimensional-Crossover-Driven Mott Transition: A Variational Cluster Approach** — •Benjamin Lenz and Thomas Pruschke — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

The dimensional-crossover-driven Mott transition has been studied recently for a frustrated Hubbard model with next-nearest neighbor hopping at finite temperatures [Raczkowski, Assaad, PRL 109 (2012)]. Here, we study this crossover from one to two dimensions at zero temperature by means of the variational cluster approximation (VCA) for fixed frustration as function of the interaction. The transition at zero temperature is found to be continuous, and results for various dynamic and static quantities are discussed as a function of cluster size.

O 44.11 Wed 12:15 BEY 81

**Superconductivity in the two-dimensional $t$-$t'$-Hubbard model** — •Andreas Eberlein and Walter Metzner — Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Using a recently developed renormalization group method for fermionic superfluids, we determine conditions for d-wave superconductivity in the ground state of the two-dimensional Hubbard model at moderate interaction strength, and we compute the pairing gap in the superconducting regime. A pairing instability signaled by a divergent flow in the Cooper channel leads to a superconducting state in all studied cases. The next-to-nearest neighbor hopping $t'$ plays a crucial role in the competition between antiferromagnetism and superconductivity. A sizable $t'$ is necessary to obtain a sizable pairing gap.

O 44.12 Wed 12:30 BEY 81

**Unconventional superconductivity in the two dimensional Edwards model** — •Dai-Ning Cho and Steffen Sykora — Institute for Theoretical Solid State Physics, IFW Dresden, D-01069 Dresden, Germany

The nature of charge transport within a correlated background medium can be described by spinless fermions coupled to bosons in the model introduced by Edwards. Employing the analytical projector-based renormalization method (PRM), we obtain a solvable effective Hamiltonian $\tilde{\mathcal{H}}$ which consists of a decoupled system of renormalized conduction electrons and a bosonic term with renormalized dispersion $\tilde{\omega}_{\mathbf{q}}$ which is generated naturally within the renormalization procedure. This method has been applied successfully to the 1D Edwards model where unbiased numerical results could be confirmed by the PRM. For the 2D model we show results for the effective one-particle dispersions of electrons and bosons in the whole Brillouin zone and for different values of the electron filling. In particular, we find strong dispersion of boson modes indicating a quantum phase transition to an unconventional superconducting state mediated by strong charge fluctuations. We show that the pairing changes its character from s- to d-wave symmetry.

O 44.13 Wed 12:45 BEY 81

**Phase diagram of the square lattice bilayer Hubbard model: A Variational Monte Carlo study** — Robert Rüger[1,2], •Luca Fausto Tocchio[1,3], Roser Valentí[1], and Claudius Gros[1] — [1]University of Frankfurt, Germany — [2]Scientific Computing & Modelling NV, Amsterdam, The Netherlands — [3]SISSA, Trieste, Italy

We investigate the phase diagram of the square lattice bilayer Hubbard model at half filling with the variational Monte Carlo method for both the magnetic and the paramagnetic case as a function of interlayer hopping $t_\perp$ and on-site Coulomb repulsion $U$. With this study we resolve some discrepancies in previous calculations based on the dynamical mean field theory, and we are able to determine the nature of the phase transitions between metal, Mott insulator and band insulator. In the magnetic case we find only two phases: An antiferromagnetic Mott insulator at small $t_\perp$ for any value of $U$ and a band insulator at large $t_\perp$. At large $U$ values we approach the Heisenberg limit. The paramagnetic phase diagram shows at small $t_\perp$ a metal to Mott insulator transition at moderate $U$ values and a Mott to band insulator transition at larger $U$ values. We also observe a reentrant Mott insulator to metal transition and metal to band insulator transition for increasing $t_\perp$ in the range of $5.5t < U < 7.5t$. Finally, we discuss the obtained phase diagrams in relation to previous studies based on different many-body approaches.

# O 45: Spintronics I (HL jointly with MA, O, TT)

Time: Wednesday 10:15–12:00 Location: POT 006

O 45.1 Wed 10:15 POT 006

**Spin dynamics on the metallic side of the metal to insulator transition** — •Jan G. Lonnemann, Kim Niewerth, Jens Hübner, and Michael Oestreich — Leibniz Universität Hannover - Abteilung Nanostrukturen, Hannover, Germany

Several theoretical works treat the spin dynamics in zinc-blende semiconductors, like GaAs, around the metal-to-insulator transition. Most of them fail to explain the extremely long lifetimes experimentally observed [1]. Recently, it was argued that the Dyakonov-Perel mechanism (DP), usually only applicable in the conduction band, can be extended towards hopping transport (HT) present in the impurity band [2]. The theoretical calculations predict a dependence on the carrier density differing strongly from the DP spin relaxation expected for the conduction band electrons. We present extremely low excitation Hanle depolarization measurements on precisely n-doped MBE grown samples in the range of carrier concentrations from 2 to $10 * 10^{16}$ cm$^{-3}$. The density dependence of the spin lifetimes extracted from our measurements indicates that the dephasing due to HT is not the dominant mechanism. Remarkably, there is no significant difference in the spin lifetimes obtained from measurements on MBE material, with extremely low compensation ratios, as compared with samples from commercial wafers. This further indicates that dephasing due to HT is not the dominant mechanism, since HT depends strongly on the compensation ratio.

[1] M. Römer et al.; *Phys. Rev. B*, **81**, 075216 (2010).
[2] G.A. Intronati et al.; *Phys. Rev. Lett.*, **108**, 016601 (2012).

O 45.2 Wed 10:30 POT 006

**Nanomechanical read-out and manipulation of a single spin** — •Heng Wang and Guido Burkard — University of Konstanz, Department of Physics

The single electron spin in quantum dot is a promising candidate as a qubit for quantum computation and quantum information. We investigate detection as well as manipulation of the single spin in a suspended carbon nanotube quantum dot. The detection and the manipulation are based on the spin-mechanical coupling induced from the intrinsic spin-orbit coupling. We use a Jaynes-Cummings model with a quantized flexural mode of the resonator to describe the system. An external electric field is used to drive the resonator and to induce an the interaction between the single electron in the quantum dot and the external driving field. The spin states can be identified by measuring the mechanical motion of the nanotube, which is detected by observing the current through a nearby charge sensor. Arbitrary-angle rotations about arbitrary axes of the single electron spin can be achieved by varying the frequency and the strength of the external electric driving field.

O 45.3 Wed 10:45 POT 006

**Time-resolved electrical detection of the inverse spin Hall Effect after ps optical excitation** — •Manfred Ersfeld[1], Ivan Stepanov[1], Sammy Pissinger[1], Christopher Franzen[1], Sebastian Kuhlen[1], Mihail Lepsa[2], and Bernd Beschoten[1] — [1]2nd Institute of Physics, RWTH Aachen University, Germany — [2]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich GmbH, Germany

Electrical detection of spin currents give an insight into the microscopic mechanisms of spin transport and play an important role in spin electronics. In previous experiments spin currents due to spin Hall effect have been imaged in optical measurements as spin accumulation.[1]

Here we report on the first time-resolved electrical detection of spin precession in n-InGaAs in time-resolved measurements of the inverse spin Hall effect. Net spin currents are achieved by applying electric fields and by polarization of the electrons with circularly polarized picosecond laser pulses. Electron spin precession in an external magnetic field can be monitored using a phase-triggered sampling oscilloscope as an oscillating voltage perpendicular to the applied electric field. Temperature dependent measurements of the spin Hall effect are presented. Time-resolved Faraday rotation measurements on the same sample under identical experimental conditions show good agreement between the measured spin dephasing times and the g-factor in the spin Hall measurements.

This Work has been supported by DFG through FOR 912

[1] Y. K. Kato et al., Science 306, 1910 (2004)

O 45.4 Wed 11:00 POT 006

**Terahertz out-of-plane resonances due to spin-orbit coupling** — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP)Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

A microscopic kinetic theory is developed which allows to investigate non-Abelian SU(2) systems interacting with mean fields and spin-orbit coupling under magnetic fields in one, two, and three dimensions. The coupled kinetic equations for the scalar and spin components are presented and linearized with respect to an external electric field. The dynamical classical and quantum Hall effect are described in this way as well as the anomalous Hall effect for which a new symmetric dynamical contribution to the conductivity is presented. The coupled density and spin response functions to an electric field are derived including arbitrary magnetic fields. The magnetic field induces a staircase structure at frequencies of the Landau levels. It is found that for linear Dresselhaus and Rashba spin-orbit coupling a dynamical out-of-plane spin response appears at these Landau level frequencies establishing terahertz resonances. (EPL, 104 (2013) 2700)

O 45.5 Wed 11:15 POT 006

**Resonant spin amplification in intrinsic bulk germanium** — •Jan Lohrenz, Timo Paschen, and Markus Betz — Experimentelle Physik 2, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund

Recent experiments have revealed the possibility to optically orient electron spins in bulk germanium via indirect optical transitions. However, the temporal limitations to both the spin lifetime and the coherence of photogenerated electrons have remained unexplored so far. Here we demonstrate resonant spin amplification in intrinsic bulk germanium using a 90 MHz femtosecond pulse train at 0.8 eV central photon energy. Most importantly, we find remarkably long spin lifetimes exceeding 50 ns at temperatures of up to 60 K, limited by Elliott Yafet type processes. Consistent with model simulations we also find pronounced signatures of the g-factor anisotropy in germanium in the resonant spin amplification data.

O 45.6 Wed 11:30 POT 006

**Ultrahigh Bandwidth Spin Noise Spectroscopy** — •Fabian Berski, Hendrik Kuhn, Jan G. Lonnemann, Jens Hübner, and Michael Oestreich — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

We advance all optical spin noise spectroscopy (SNS) in semiconductors to detection bandwidths of several hundred gigahertz by employing a sophisticated scheme of pulse trains from ultrafast laser oscillators as an optical probe [1]. The ultrafast SNS technique avoids the need for optical pumping and enables nearly perturbation free measurements of extremely short spin dephasing times. We apply the technique to highly-n-doped bulk GaAs where magnetic field dependent measurements show unexpected large g-factor fluctuations. Calculations suggest that such large g-factor fluctuations do not necessarily result from extrinsic sample variations but are intrinsically present in every doped semiconductor due to the stochastic nature of the dopant distribution.

[1] Berski, F., et al., Phys. Rev. Lett. **111**, 186602 (2013).

O 45.7 Wed 11:45 POT 006

**Effect of Nuclear Quadrupole Moments on Electron Spin Coherence in Semiconductor Quantum Dots** — •Erik Welander[1], Evgeny Chekhovich[2], Alexander Tartakovskii[2], and Guido Burkard[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Department of Physics and Astronomy, University of Sheffield, United Kingdom

We theoretically investigate the influence of the fluctuating Overhauser field on the spin of an electron confined to a quantum dot. The fluctuations arise from nuclear spin being exchanged between different nuclei via the nuclear magnetic dipole coupling. We focus on the role of the nuclear interaction from electric quadrupole moments (QPM), which generally cause a reduction in internuclear spin transfer efficiency. By dividing the nuclear problem into subcells we are able to describe $10^4 - 10^5$ nuclei, which are realistic numbers for a quantum dot. The effects on the electron spin coherence time are studied by modeling an electron spin echo experiment. We find that the QPM cause an increase in the electron spin coherence time and that an inhomogeneous distribution, where different nuclei have different QPM, causes an even larger increase than a homogeneous distribution.

# O 46: Plasmonics and Nanooptics I

Time: Wednesday 10:30–13:00 Location: TRE Phy

O 46.1 Wed 10:30 TRE Phy

**Tailored nano-antennas for directional Raman studies of individual carbon nanotubes** — •Nicola Paradiso, Fatemeh Yaghobian, Christoph Lange, Tobias Korn, Christian Schüller, Ruper Huber, and Christoph Strunk — Institut für Experimentelle und Angewandte Physik, University of Regensburg

We exploit patterned nano-antennas to investigate the Raman spectra of otherwise not optically detectable carbon nanotubes (CNTs). We demonstrate that a top–down approach is particularly promising when applied to CNTs, owing to the sharp dependence of the scattered signal on the angle between incident light polarization and CNT axis. In contrast to tip enhancement techniques, our method enables us to control the light polarization in the sample plane, locally amplifying and rotating the incident field in order to optimize the Raman signal. Such promising features are confirmed also by the numerical simulations presented here. From the analysis of the $G$ modes we deduced that the CNT under study is semiconducting and chiral, and we estimated its diameter and chiral angle. Measurements on arrays with different orientation with respect to the CNT revealed that thin metal strips allow not only to magnify, but also to rotate the electromagnetic field, thus introducing a new degree of freedom for SERS applications. The relative ease of fabrication and alignment makes this technique suitable for the realization of integrated devices that combine scanning probe, optical, and transport characterization.

O 46.2 Wed 10:45 TRE Phy

**Yttrium hydride nanoantennas for reconfigurable plasmonics** — •Nikolai Strohfeldt[1], Andreas Tittl[1], Martin Schäferling[1], Frank Neubrech[1], Uwe Kreibig[2], Ronald Griessen[3], and Harald Giessen[1] — [1]Universität Stuttgart, Germany — [2]RTWH Aachen, Germany — [3]Vrije Universiteit Amsterdam, The Netherlands

A key challenge for the development of active plasmonic devices is the lack of materials with fully controllable plasmonic properties. In this work we demonstrate that a plasmonic resonance in top-down nanofabricated yttrium antennas can be completely and reversibly turned on and off using hydrogen exposure. We fabricate arrays of yttrium nanorods and optically observe in extinction spectra the hydrogen-induced phase transition between the metallic yttrium dihydride and the insulating trihydride. Whereas the yttrium dihydride nanostructures exhibit a pronounced particle plasmon resonance, the transition to yttrium trihydride leads to a complete vanishing of the resonant behavior. Our fully reversible plasmonic switch can be tuned over a wide wavelength range by simply varying the size of the nanostructures. Furthermore, we developed an analytical diffusion model with which we are able to explain the temporal behavior of the reconfiguration process observed in our experiments and gain information about the thermodynamics of our device. Thus, our nanorod system serves as a versatile basic building block for reconfigurable plasmonic devices ranging from reconfigurable perfect absorbers to active local heating control elements.

O 46.3 Wed 11:00 TRE Phy

**Large-Area Low-Cost Resonant Nano-Antenna Enhanced SEIRA Substrate Using Interference Lithography** — •Shahin Bagheri, Frank Neubrech, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

We manufactured large-area plasmonic antenna arrays by laser interference lithography for surface-enhanced infrared absorption. Geometrical parameters of the homogeneous antennas can be precisely defined by changing the interference condition in each exposure process independent of the underlying wafer. Such antennas with tunable and high quality resonances from near- to mid-infrared (1 to 7 $\mu$m) are well suited as substrates for surface-enhanced infrared absorption studies. We show the broad applicability of these substrates by enhancing the infrared vibrational signals of a monolayer octadecanethiol and monitoring the ultraviolet degradation of a polymer via the decrease of its specific vibrational modes. Large-area and fast fabrication process make our approach suited as a low-cost sensing platform for a variety of different SEIRA real-world applications.

O 46.4 Wed 11:15 TRE Phy

**Resonant surface-enhanced Raman scattering in nanoparticle dimer structures** — •Matthias Hensen[1], Ingo Heesemann[2], Elina Oberlander[3], Adelheid Godt[2], Thomas Huser[3], and Walter Pfeiffer[1] — [1]Molecular and Surface Physics, Department of Physics, Bielefeld University, 33615 Bielefeld, Germany — [2]Organic Chemistry and Polymer Chemistry, Department of Chemistry, Bielefeld University, 33615 Bielefeld, Germany — [3]Biomolecular Photonics Group, Department of Physics, Bielefeld University, 33615 Bielefeld, Germany

Surface-enhanced Raman scattering (SERS) benefits from the local field enhancement in the vicinity of plasmonic nanoantennas. We experimentally investigate rodlike acetyl-protected dithiol molecules that specifically link two gold nanoparticles with a diameter of 40 nm and gap dimensions of about 1 nm. Raman spectroscopy using excitation between 473 nm and 785 nm wavelength reveals a resonant enhancement of the linker molecule related Raman signals for excitation around 650 nm. This coincides with the gold dimer resonance, as predicted by FDTD calculations, and we conclude that the resonant excitation of gold-nanoparticle dimers enhances the Raman signal. Furthermore, based on a quantitative analysis of particle and aggregate concentrations we derive Raman enhancement factors in comparison to dithiol molecules in acetone. About 100 linker molecules in the gap of a nanoparticle dimer contribute to the signal and a Raman enhancement factor of about $10^6$ is obtained for resonant excitation.

O 46.5 Wed 11:30 TRE Phy

**Resonance enhanced local thermionic emission** — •Felix Becker, Dominik Differt, Matthias Hensen, Christian Strüber, and Walter Pfeiffer — Molecular and Surface Physics, Department of Physics, Bielefeld University, 33615 Bielefeld, Germany

In the interaction of intense laser pulses with nanostructures or optical antennas the electron emission is commonly discussed in the context of multi-photon processes and strong field phenomena. However, resonant excitation and the related field enhancement also significantly increase the locally absorbed energy density leading to a transient local heating of the electron gas. Thermionic emission dominates the electron yield for sufficiently strong excitation. This has been demonstrated recently for nanoantenna induced currents in metal-insulator-metal junctions and for photonic resonances in nanotextured amorphous silicon layers. Based on electron-electron and electron-phonon scattering rates transient electron energy distributions after short pulse excitation and the related thermionic emission over an internal tunnel barrier and for electron emission into the continuum are simulated. Variation of both scattering rates determines the ratio between sequential multiphoton photoemission and thermionic emission following the Richardson-Dushman equation. Despite the incoherent character of thermionic emission it can be exploited as a probe for this energy concentration process.

O 46.6 Wed 11:45 TRE Phy

**Third harmonic spectroscopy of single Au- nanoantennas fabricated by helium ion beam milling** — •Heiko Kollmann[1], Martin Esmann[1], Simon F. Becker[1], Xianji Piao[2], Chuong Huynh[3], Lars-Oliver Kautschor[3], Guido Bösker[3], Henning Vieker[4], Armin Gölzhäuser[4], Namkyoo Park[2], Martin Silies[1], and Christoph Lienau[1] — [1]University of Oldenburg, Germany — [2]Seoul National University, Korea — [3]Carl Zeiss Microscopy GmbH, Jena, Germany — [4]University of Bielefeld, Germany

Metallic nanoantennas are able to localize far-field electromagnetic waves in volumes of a fraction of their wavelength. Standard tools for fabricating these structures with sub-20-nm feature sizes are Electron Beam Lithography or Ga-based Focused Ion Beam (FIB) milling. Here, we combine Ga- and He-ion based milling (HIM) for the fabrication of gold bow-tie antennas with few-nanometer gap sizes. Using polarization-sensitive Third-Harmonic (TH) spectroscopy, we compare the nonlinear optical properties of single HIM-antennas with sub-6-nm gaps with those produced by Gallium-based FIB. We find a pronounced enhancement of the intensity and a greatly improved polarization contrast of the TH for He-ion produced antennas in comparison with state-of-the-art Ga-FIB antennas. Our experimental findings are strongly supported by FEM calculations and demonstrate electric field localization in the few-nanometer gap of the bow-tie antenna. This makes He-ion beam milling a highly attractive and promising new tool for the fabrication of plasmonic nanoantennas with few-nanometer feature sizes.

O 46.7 Wed 12:00 TRE Phy

### Tayloring the third harmonic response of plasmonic nanoantennas by incorporation of dielectric nanocrystals

— •Bernd Metzger[1], Mario Hentschel[1,2], Thorsten Schumacher[1,2], Markus Lippitz[1,2], Xingchen Ye[3], Christopher B. Murray[3], Bastian Knabe[4], Karsten Buse[4], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Department of Chemistry, University of Pennsylvania, Philadelphia, USA — [4]Fraunhofer Institute for Physical Measurement Techniques IPM, Freiburg, Germany

The electric field strength in the hot-spot of a plasmonic nanoantenna [1] can surpass the far-field amplitude by more than an order of magnitude, which caused scientists to envision enhanced conversion efficiencies for nonlinear optical effects [2]. Hence, we incorporate indium tin oxide (ITO) nanocrystals into the hot-spot of plasmonic gold gap-antennas and investigate the nonlinear third harmonic (TH) response of the hybrid nanostructure arrays. We find an enhancement by about a factor of two of the TH emission when comparing the hybrid to bare gap-antenna arrays, where no dielectric nanocrystals have been incorporated. Surprisingly, we find that the enhancement is not due to the third order susceptibility of the ITO nanocrystals, but due to the optical nonlinearity of the gold and predominantly due to an enhanced dipole moment of the plasmonic oscillations in the gold gap-antennas. [1] L. Novotny and N. van Hulst, Nature Photon. 5, 83 (2011). [2] M. Kauranen and A. V. Zayats, Nature Photon. 6, 737 (2012).

O 46.8 Wed 12:15 TRE Phy

### Gold strip gratings for surface enhanced infrared spectroscopy

— Tao Wang[1], •Tobias W. W. Mass[1], Vu Hoa Nguyen[2], Andreas Buchenauer[2], Uwe Schnakenberg[2], and Thomas Taubner[1,3] — [1]I. Institute of Physics (IA), RWTH Aachen University — [2]Institute of Materials and Electrical Engineering I, RWTH Aachen University — [3]Fraunhofer Institute for Laser Technology (ILT)

Metallic nanoantennas efficiently couple light into a region of subwavelength size. Antenna arrays designed for surface enhanced infrared absorption spectroscopy enable the detection of molecular vibration with high sensitivity [1,2]. In contrast to the cost-intensive and low-throughput fabrication of nanostructures e.g. via e-beam lithography, gold strip gratings fabricated with standard optical UV-lithography offer great potential for future commercial applications. The grating structures are analysed using FTIR-spectroscopy and exhibit grating resonances depending on the period and the refractive index of the environment. Accordingly, the grating resonances can be tuned over a broad spectral range in order to match and enhance the absorption bands of interest. We demonstrate enhancement factors of more than 6000 and significantly amplify the well defined absorption band of a 30 nm thick PMMA layer at about 5.8 $\mu$m [3].

[1] Adato et al. *PNAS* **2009** 106(46), 19227-19232.
[2] Neubrech et al. *Phys.Rev.Lett.* **2008** 101(15), 157403.
[3] Wang et al. *Opt. Express* **2013** 21(7), 9005-9010.

O 46.9 Wed 12:30 TRE Phy

### Distinction between horizontal and vertical plasmonic modes in 3D nanostructures

— •Monika Fleischer[1], Julia Fulmes[1], Christian Schäfer[1], Dieter Kern[1], Mikael Renault[2], Anne-Laure Baudrion[2], and Pierre-Michel Adam[2] — [1]Eberhard Karls University Tübingen, 72076 Tübingen, Germany — [2]University of Technology Troyes, 10000 Troyes, France

The dark-field scattering or extinction spectra of plasmonic nanostructures, such as e.g. nanorods, exhibit distinct peaks that indicate the resonances of the localized surface plasmon polaritons excited in the structures [1]. For three-dimensional nanostructures, vertical modes may occur as well. These are however rarely reported due to the predominant excitation and detection of in-plane modes. Here gold nanocone antennas with different aspect ratios are fabricated by two strategies using top-down lithography [2,3], and their plasmon resonance spectra in the far-field are analyzed by single-particle dark field scattering spectroscopy [4,5], variable angle UV-vis extinction spectroscopy, and total internal reflection spectroscopy. The study shows that both in-plane and out-of-plane modes of the 3D nanostructures can be excited, and that their relative spectral positions can be individually engineered via the nanocone geometry [3]. The experiments are compared with simulations for the same geometries.

[1] W. Gotschy et al., Opt. Lett. 21, 1099 (1996); [2] M. Fleischer et al., Nanotechnol. 21, 065301 (2010); [3] J. Fulmes et al., in preparation (2013); [4] C. Sönnichsen et al., New J. Of Physics 4, 93 (2002); [5] C. Schäfer et al., Nanoscale 5, 7861 (2013).

O 46.10 Wed 12:45 TRE Phy

### Higher multipolar mode contributions to nonlinear nanoantenna response

— Jan Renger[1], •Pablo M. de Roque[1], Nikos Fayard[1,2], Marta Castro-Lopez[1], Nicolo Accanto[1], and Niek F. van Hulst[1] — [1]ICFO-Institut de Ciencies Fotoniques, 08860 Castelldefels (Barcelona), Spain — [2]Institut Langevin, ESPCI ParisTech, France

Nanoantennas, such as metallic nanorods featuring localized surface plasmon resonances (LSPR), are attractive for application such as optical sensing of chemicals or biomedical markers because of their wide spectral-tunability and strong mode confinement and enhancement. The latter one together with the intrinsically strong nonlinearity of metals allows these antennas to act as coherent nano light sources. For a short gold nanorod, the dipolar LSPR occurring in the visible spectral range will dominate the optical response. This resonance rapidly shifts towards the near infrared for a longer nanorod and additional multipolar modes contribute in the visible and NIR wavelength range. We identified the resonance conditions for the different multipolar modes by tracking the linear and nonlinear optical properties of nanorods for increasing lengths and to demonstrate that dark and bright multipolar modes of metallic nanorods contribute equally to the nonlinear optical emission via two-photon photoluminescence (TPPL) and second harmonic generation (SHG).

# O 47: Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale IV

Time: Wednesday 10:30–13:15 Location: TRE Ma

**Topical Talk** O 47.1 Wed 10:30 TRE Ma

**From Rydberg Crystals to Bound Magnons - Probing the Non-Equilibrium Dynamics of Ultracold Atoms in Optical Lattices** — •Immanuel Bloch — Max-Planck Institut für Quantenoptik, Garching, Germany — Ludwig-Maximilians-Universität, Munich, Germany

Ultracold atoms in optical lattice form an ideal testbed to probe the non-equilibrium dynamics of quantum many-body systems. In particular recent high-resolution imaging and control techniques allow to probe dynamically evolving non-local correlations in an unprecedented way. As an example, I will focus in my talk on the dynamical excitation of spatially ordered Rydberg structures that are formed through laser exctiation from ground state Mott insulating atoms. In addition, I will show how single-spin and spin-pair impuritites can be used to directly reveal polaron dynamics in a strongy interacting superfluid or the bound state of two magnons in a Heisenberg ferromagnet - a problem discussed first theoretically more than 80 years ago by H.A. Bethe. New atom interferometric schemes to directly probe the Green's function of a many-body system through the impurity dynamics will be discussed.

O 47.2 Wed 11:00 TRE Ma

**Correlated Light-Matter Interactions in Cavity QED** — •Johannes Flick[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

In the electronic structure community, the quantized nature of the electrons is usually (approximately) incorporated, whereas the electromagnetic field is mostly treated classically. In contrast, in quantum optics, matter is typically simplified to models with a few levels, while the quantized nature of light is fully explored. In this work, we aim at treating both, matter and light, on an equal quantized footing.

We present exact solutions for fully quantized prototype systems consisting of atoms or molecules placed in optical one- or two-dimensional high-Q cavities and coupled to the quantized electromagnetic modes in the dipole or quadrupole coupling regime. We focus on spontaneous emission, strong-coupling phenomena, dipole-dipole couplings including van-der-Waals interactions, and Förster resonance energy transfer (FRET), all beyond the rotating-wave approximation.

This work has implications for a future development of a time-dependent density functional theory formulation of QED [1,2] for correlated multi-photon configurations.

[1] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011).
[2] I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).

O 47.3 Wed 11:15 TRE Ma

**Optimized effective potential approach to time-dependent density functional theory for many-electron systems interacting with cavity photons** — •Camilla Pellegrini[1], Johannes Flick[2], Heiko Appel[2], Ilya V. Tokatly[1,3], and Angel Rubio[1,2] — [1]Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, E-20018 San Sebastían, Spain — [2]Fritz-Haber Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany — [3]IKERBASQUE, Bilbao, Spain

In a recent paper [1] time dependent density functional theory has been generalized to many-electron systems strongly coupled to quantum electromagnetic modes of a microcavity. Here we construct an approximation for the corresponding exchange-correlation (xc) potential by extending the optimized effective potential (OEP) method to the electron-photon system. The derivation of the OEP equation employing the non-equilibrium Green's function formalism, and the first order approximation for the electronic self-energy is presented. Beyond the mean field level, the electron-photon coupling generates a time non-local photon-mediated interaction between the electrons, whose propagator enters the exchange-like diagram. We further show the approximated xc-potential for a model two-level diatomic molecule with one electron coupled to photon modes. The comparison between the obtained results and the exact numerical ones in the different coupling regimes (from weak up to ultra-strong) is discussed. [1] I.V. Tokatly, Phys. Rev. Lett. 110, 233001(2013)

O 47.4 Wed 11:30 TRE Ma

**Correlated photon-electron wavefunctions in cavity Quantum Electrodynamics** — •Heiko Appel[1], Johannes Flick[1], Rene Jestaedt[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Experimental progress in recent years has enabled the fabrication of Fabry-Perot resonators with high optical quality factors (high-Q). Such cavities allow to study the interaction of matter with a quantized light field at the single-photon level (Nobel prize 2012). In this talk we present the real-time evolution of correlated photon-electron wavefunctions in optical one- and two-dimensional high-Q cavities. We discuss implications for a multi-component density functional theory for Quantum Electrodynamics [1,2] based on the time-dependent electron density and the photon energy density.
[1] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011).
[2] I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).

O 47.5 Wed 11:45 TRE Ma

**Photoelectron driven plasmaron excitations in (2x2)K/Graphite** — •Bo Hellsing — Department of Physics, Gothenburg University, Sweden

A new type of plasmarons formed by the compound of photoelec- trons and acoustic surface plasmon (ASP) excitations is investigated in the system p(2 * 2)-K/Graphite. The physics behind these types of plasmarons, e-plasmarons, is different from the ones re- cently found in graphene and quantum well systems, where the loss features results from the photohole-plasmon interaction in the material, h-plasmarons. Based on the first principles scheme, Time dependent density functional (TDDFT), we calculated the linear response due to the presence of the escaping photo-electron and determine the ASP dispersion. The coupling between the photoelectron and the ASP gives rise to excitation of the e- plasmarons manifested by a broad dispersive feature shifted about 0.5 eV below parabolic K induced quantum well band (QWB) in agreement with the ARPES experiment by Agdal et al. The e-plasmarons should be considered as a source of the loss satellite structure in ARPES for 2D systems. In addition they are important to take into account in theoretical studies of different compounds as they reflect an additional channel for excitations of plasmons. This could then increase the photon-plasmon conversion yield which obviously is of interest in the field of plasmonics.

O 47.6 Wed 12:00 TRE Ma

**Charge-transfer excitations in organic systems from many-body perturbation theory** — •Xavier Blase[1], Carina Faber[1,2], Paul Boulanger[1], Claudio Attaccalite[1], and Ivan Duchemin[2] — [1]Institut Néel, CNRS and UJF, Grenoble, France — [2]L_SIM/INAC, CEA, Grenoble, France

Charge-transfer excitations in organic systems lies at the heart of a large variety of physical phenomena, from photosynthesis to photovoltaics, photocatalysis or DNA denaturation. From a theoretical point of view, such nonlocal excitations are well known to lead to difficulties within the TDDFT framework, leading to the development of range-separated hybrids. We present here the merits of the Bethe-Salpeter formalism and demonstrate its ability to reproduce *cold* and *hot* Frenkel or charge-transfer excitations with remarkable accuracy [1-3]. Our calculations are based on a recent Gaussian basis implementation of the GW and Bethe-Salpeter formalism, the Fiesta initiative [1-4], allowing all-electron or pseudopotential excited states calculations for systems comprising several hundred atoms. Recent developments towards discrete and continuous embedding techniques within the many-body perturbation framework will be presented.

References: [1] C. Faber, I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. B, 86, 155315 (2012). [2] I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. 109, 167801 (2012). [3] I. Duchemin and X. Blase, Phys. Rev. B 87, 245412 (2013). [4] X. Blase, C. Attaccalite, V. Olevano, Phys. Rev. B 83, 115103 (2011).

O 47.7 Wed 12:15 TRE Ma

**Charge transfer from first principles: self-consistent *GW* applied to donor-acceptor systems** — •Fabio Caruso[1,2], Viktor Atalla[1], Angel Rubio[1,3], Matthias Scheffler[1], and Patrick Rinke[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]University of Oxford, UK — [3]Universidad del País Vasco, San Sebastián, Spain

Charge transfer in donor-acceptor systems (DAS) is determined by the relative alignment between the frontier orbitals of the donor and the acceptor. Semi-local approximations to density functional theory (DFT) may give a qualitatively wrong level alignment in DAS, if the ionisation potential of one molecule erroneously ends up above the electron affinity of the other. An unphysical fractional electron transfer will then result in weakly interacting DAS [1]. *GW* calculations based on first-order perturbation theory ($G_0W_0$) correct the level alignment. However, the ground state is unaffected by the $G_0W_0$ approach, and the charge-transfer properties remain on the level of the initial DFT calculation [1]. We demonstrate that self-consistent *GW* (sc*GW*) – based on the iterative solution of the Dyson's equation – provides an ideal framework for the description of charge transfer in DAS. The sc*GW* level alignment is in agreement with experimental reference data. In addition ground- and excited-state properties are described at the same level of theory. As a result, the electron density in DAS is consistent with the level alignment between donor and acceptor, leading to a qualitatively correct description of charge-transfer properties.

[1] V. Atalla, M. Yoon, F. Caruso, P. Rinke, and M. Scheffler, Phys. Rev. B **88**, 165122 (2013).

O 47.8 Wed 12:30 TRE Ma

**What Koopmans' compliant orbital-density dependent functionals can do for you: a comprehensive benchmark of the G2-set** — •Giovanni Borghi[1], Ngoc Linh Nguyen[1], Andrea Ferretti[2], Ismaila Dabo[3], and Nicola Marzari[1] — [1]École Polytechnique Fédérale de Lausanne, Lausanne (VD), CH — [2]Centro S3, CNR–NANO, Modena, IT — [3]Department of Materials Science and Engineering, Penn State University, University Park (PA), USA

In this talk we present the results of benchmark calculations of the structure and electronic-structure of all molecules in the g2 set, using different flavours for Koopmans' compliant (KC) functionals. Results are compared not only to LDA and PBE, but also to orbital-density dependent calculations with the Perdew-Zunger self-interaction correction.

Our results assess the accuracy of Koopmans' compliant functionals in improving semilocal functionals to predict electronic eigenvalues and in particular ionization energies, with an accuracy that for molecules seems to be comparable or superior to that of many-body (GW) approaches. We also highlight how the Koopmans' condition tends to preserve the potential energy surface of the underlying functional, with higher reliability than e.g. PBE in structural predictions, while also providing good estimates of atomization energies.

The talk will also provide a general introduction to the theory of Koopmans' compliant functionals and their implementation in existing electronic structure codes.

**Ref.** Dabo *et al.*, PRB 82, 115121 (2010), and Psik highlight (2012).

O 47.9 Wed 12:45 TRE Ma

**The electronic structure of quinacridone: Optimally tuned range-separated hybrid functional versus GW results** — Daniel Lüftner[1], Sivan Refaely-Abramson[2], Michael Pachler[1], Michael G. Ramsey[1], Leeor Kronik[2], and •Peter Puschnig[1] — [1]Institut für Physik, Karl-Franzens-Universität Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, Israel

Quinacridone is an organic molecule (C20H12N2O2) utilized in the formation of organic pigments. It has also been discussed for usage in organic electronics particularly due to its stability under ambient conditions and its tendency to form self-assembled supramolecular networks. Here, we report on its electronic structure, both, for the isolated molecule as well as for the alpha- and beta- bulk molecular crystal polymorphs. We employ an optimally tuned range-separated hybrid functional (OT-RSH) within density functional theory as well as GW corrections within a many-body perturbation theory framework. A comparison of the theoretical results obtained with the different levels of theory and a subsequent comparison with experimental data from angle-resolved photoemission spectroscopy emphasize the need for going beyond simple semi-local DFT-functionals in order to obtain the correct orbital ordering. Furthermore the comparison indicates that the results obtained with OT-RSH greatly improve those of standard DFT functionals and achieve an agreement with experiment at the level of GW calculations, thus making the OT-RSH an alternative to the computationally more expensive GW approach.

O 47.10 Wed 13:00 TRE Ma

**GW many-body perturbation theory for electron-phonon coupling calculations** — •Carina Faber[1,2], Paul Boulanger[1], Ivan Duchemin[1,2], and Xavier Blase[1] — [1]Institut Néel, CNRS, Grenoble, France — [2]INAC, CEA, Grenoble, France

We study within many-body perturbation theory the electron-phonon coupling in organic systems, taking as paradigmatic examples the fullerene molecule and the pentacene crystal [1,2]. We show that the strength of the electron-phonon coupling potential is dramatically underestimated at the LDA level, while GW calculations offer an excellent agreement with experiments [1]. Further, combining GW calculations of the electronic band structure and of the electron-phonon coupling in crystalline pentacene, we show that the hole bands dispersion can be reconciled with photoemission experiments, by solving non-perturbatively (DMFT) the effect of electron-phonon coupling on the electronic self-energy [2]. We finally explore various approximations that may allow to combine the GW formalism with convenient linear response formalisms beyond the frozen-phonon techniques. Our calculations are performed with the Fiesta package, a Gaussian based GW and Bethe-Salpeter code allowing all-electron or pseudopotential calculations with various resolution of the identity techniques and without any plasmon pole approximation [3,4].

[1] C. Faber et al., Phys. Rev. B 84, 155104 (2011) [2] S. Ciuchi et al., Phys. Rev. Lett. 108, 256401 (2012) [3] C. Faber, I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. B, 86, 155315 (2012). [4] I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. 109, 167801 (2012).

# O 48: Scanning Probe Methods I

Time: Wednesday 10:30–13:15 Location: GER 38

O 48.1 Wed 10:30 GER 38

**Correction of non linear lateral distortions of scanning probe microscopy images** — •Michael Schnedler, Phillip Weidlich, Verena Portz, Dieter Weber, Rafal E. Dunin-Borkowski, and Philipp Ebert — Peter Grünberg Institut, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The inverse piezo electric effect is commonly utilized to position the tip or cantilever with atomic precision in scanning probe microscopes (SPM). Although the properties of modern piezo electric materials are well known, their application in SPMs requires a calibration of their lateral and vertical positioning, which is usually achieved by acquiring images of atomic lattices and comparing them with the perfect periodical arrangement of the atoms of a crystalline surface. Hence, the calibration is optimized for a nanometer scan range. However, sometimes the measurement requires scanning parameters that exceed the designated linear range of the calibration. Then, nonlinear effects of the piezoceramic actuators, like hysteresis creep, drift, and a nonlinear dependence of the displacement on the applied voltage often result in image distortions. Therefore, a methodology for the correction of scanning probe microscopy image distortions occuring in large scanning ranges is demonstrated. It is based on the determination of displacement vectors from the measurement of a calibration sample. By moving the pixels of the distorted scanning probe microscopy image along the displacement vectors an almost complete correction of the nonlinear, time independent distortions is achieved.

O 48.2 Wed 10:45 GER 38

**Detecting the Dipole Moment of a Molecule with Atomic Force Microscopy** — •Alexander Schwarz, Arne Köhler, Josef Grenz, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany

Using non-contact atomic force microscopy (NC-AFM) in the constant $\Delta f$ mode with metallic tips enabled us to detect the permanent electrostatic dipole moment of single CO molecules adsorbed on three very different substrates, i.e., Cu(111), NiO(001) and Mn/W(001). The observed characteristic distance dependent contrast, which changes from a simple protrusion to a donut-shape for decreasing tip-sample separations, can be explained by an interplay between the attractive van der Waals interaction and a repulsive electrostatic interaction. The latter stems from antiparallel aligned dipoles present in CO as well as at the tip apex [1]. Our results suggest that the dipole-dipole interaction has to be considered when using metallic or CO functionalized tips to study polar molecules. They can also be responsible for complex and tip-dependent contrast patterns reported recently, which have been interpreted in terms of so-called *subatomic* features [2].

[1] G. Teobaldi, et al., Phys. Rev. Lett. **106**, 216102 (2011).

[2] J. Welker and F. J. Giessibl, Science **336**, 444, (2012).

O 48.3 Wed 11:00 GER 38

**Tuning Fork Force Sensor: Spring Constant and Q-Factor in Experiment and Simulation** — •Marvin Stiefermann[1], Jens Falter[1], Harald Fuchs[2], Henrik Hölscher[3], and André Schirmeisen[1] — [1]Institute of Applied Physics (IAP), Justus-Liebig-University Giessen, Germany — [2]Center for Nanotechnology (CeNTech) and Institute of Physics, University of Münster (WWU), Münster, Germany — [3]Institute of Microstructure Technology (IMT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany

Force spectroscopy in non contact-atomic force microscopy (nc-AFM) has recently been used to determine absolute forces on individual atoms and molecules. Particular impressive results at cryogenic temperatures have been achieved using tuning fork based sensors in the "qPlus" design. However, reliable interpretation of force spectroscopy results require a precise calibration of the tuning fork spring constant. Here we present a comprehensive and straightforward calibration analysis based on experimental determination and FEM simulation of the tuning fork spring constant. We find that the beam formula widely used in the literature systematically overestimates the spring constant. However, we show that a origin shift of the beam can be used to correct this effect for most cases. Further, we find that already a small tilt angle of the tip glued to the prong strongly influences the spring constant, explaining the large scatter of our experimental calibration values. Further we present FEM simulations monitoring the influence of different tuning fork setups, adhesives and tip positions on the Q-Factor.

O 48.4 Wed 11:15 GER 38

**Reconstruction of field ion microscopy characterized tungsten tips of AFM tuning fork sensors at the atomic level** — •Sören Zint[1], Jens Falter[2,1], Dirk Dietzel[1], and André Schirmeisen[1] — [1]Institute of Applied Physics (IAP), Justus-Liebig-University Giessen — [2]TransMIT-Center for Adaptive Cryotechnology and Sensors

Non-contact atomic force microscopy (ncAFM) has proven to be a valuable tool for surface characterization with atomic-resolution. For a quantitative comparison between force spectroscopy experiments and corresponding analytical models, knowledge of the true tip geometry is required. One method for gaining information about the geometry of metallic tips is the field ion microscopy (FIM) technique. In order to determine the tip geometry with FIM we employ the reconstruction of ball models based on the field ion micrograph. For this purpose we developed specific software which allows for the creation of hemispherical ball models, the determination of atoms imaged brightly in FIM and the possibility of both the addition and removal of tip atoms. In order to ascertain the tip geometry of a FIM characterized tip we compare the field ion micrograph and the projection of the tip model at the atomic level. This new approach allows us to precisely determine the tip radius with an error of less than two lattice constants.

O 48.5 Wed 11:30 GER 38

**Advances in Scan Movement Linearization for High-Speed AFM Imaging** — •Anne-D. Müller and Falk Müller — Anfatec Instruments AG, Melanchthonstr. 28, 08606 Oelsnitz

In the past decade, several approaches have been undertaken to speed up the raster scan of an Atomic Force Microscope into the 100 Hz range or even higher with the aim to produce artifact free images. From the hardware side, specialized stiff scanner designs with very high resonance frequencies have been developed, some of them even using a push-pull technique. The most promising method, however, is the resonance compensation by a dedicated shaping of the scan ramp output first realized by a simple notch filter, whose parameters are adapted to the scanner [1].

This contribution presents a smarter and more flexible design method for a filtered and linearized scan control of high-speed AFMs, that works for all kind of scanners, even if they have strong nonlinearities, large hysteresis and multiple resonances. Moreover, a first approach for the reduction of resonances in z-direction is presented.

[1] DJ Burns, K Youcef-Toumi, and GE Fantner. Nanotechnology. 22.31 (2011).

O 48.6 Wed 11:45 GER 38

**SubSurface-AFM: unravelling the contrast formation mechanism** — Gerard J. Verbiest[1] and •Marcel J. Rost[2] — [1]JARA-FIT and II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Kamerlingh Onnes Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands

Subsurface-AFM is realized by Heterodyne Force Microscopy (HFM), in which two ultrasonic signals of slightly different frequencies are sent through the sample and the cantilever, respectively. The sound wave through the sample contains subsurface information. The nonlinear interaction between the cantilever's tip and the sample generates a low-frequency heterodyne force that is detected in the cantilever's motion, if one tunes this force below its fundamental resonance frequency.

Despite some reported subsurface observations that clearly demonstrate the power of this technique, a decent quantitative understanding of the physical contrast mechanism was (until now) still missing.

Our recent insight in the working principles of HFM [1-3] enabled us to perform a quantitative analysis of our measurements on a well-characterized sample and to determine the physical contrast mechanism. Totally unexpected, the contrast is neither related to ultrasonic Rayleigh scattering nor elasticity variations in the sample, but to the *rattling* motion (and the involved friction) of *shaking* nanoparticles [4].

[1] G.J. Verbiest et al., Ultramicroscopy 135, 113 (2013)

[2] G.J. Verbiest et al., Nanotechnology 24, 365701 (2013)

[3] G.J. Verbiest, and M.J. Rost, Nature Physics submitted

[4] G.J. Verbiest and M.J. Rost, http://arXiv/abs/1307.1292

O 48.7 Wed 12:00 GER 38

**Visualizing the Subsurface of Soft Matter: Simultaneous Topographical Imaging, Depth Modulation, and Compositional Mapping with Triple Frequency Atomic Force Microscopy** — •Daniel Ebeling[1,2], Babak Eslami[2], and Santiago D. Solares[2] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Giessen, Germany — [2]Department of Mechanical Engineering, University of Maryland, College Park, Maryland, United States

Characterization of subsurface morphology and mechanical properties with nanoscale resolution and depth control is of significant interest in soft matter fields like biology, polymer science, where buried structural and compositional features can be important. However, controllably "feeling" the subsurface is a challenging task for which the available imaging tools are relatively limited. In this paper, we propose a trimodal atomic force microscopy (AFM) imaging scheme, whereby three eigenmodes of the microcantilever probe are used as separate control "knobs" to simultaneously measure the topography, modulate sample indentation by the tip during tip-sample impact, and map compositional contrast, respectively. We illustrate this multifrequency imaging approach through computational simulation and experiments conducted on ultrathin polymer films with embedded glass nanoparticles in ambient air. By actively increasing the tip*sample indentation using a higher eigenmode of the cantilever, we are able to gradually and controllably reveal glass nanoparticles which are buried tens of nanometers deep under the surface, while still being able to refocus on the surface.

O 48.8 Wed 12:15 GER 38

**Origin of sharp apparent intermolecular bonds in AFM and STM experiments** — •Prokop Hapala[1], Georgy Kichin[2], Stefan Tautz[2], Ruslan Temirov[2], and Pavel Jelinek[1] — [1]Institute of Physics , Academy of Sciences of the Czech Republic, Cukrovarnická 10, Prague, 16253, Czech Republic — [2]Institut fur Bio- und Nanosysteme 3, Forschungszentrum Julich, 52425 Julich, Germany

In recent years sub-molecular resolution in STM and AFM was achieved and enabled visualization of individual bonds between atoms. These techniques are based on usage of functionalized probe consisting a simple molecule or atom (such as CO, CH3, Xe, H2, Cl-) attached to the tip apex. Recently, several groups also reported direct observation of intermolecular bonds between molecules by the same technique [1],[2],[3]. In literature this observations used to be explained as visualization of electron density in the bond due to Pauli repulsion. It was already shown, that the measured images are strongly distorted and sharpened by relaxation of molecular probe [4]. Here we show, that sharp features measured in these experiments, especially apparent intermolecular bonds, can be explained almost exclusively by simple geometrical model using pairwise potential (Lennard-Jones, Morse) when relaxation of probe position is considered.

1. J.Zhang, et al., Science 342, 611-4 (2013).
2. C.Weiss, et al., J. Am. Chem. Soc. 132, 11864-5 (2010).
3. G.Kichin, et al., J. Am. Chem. Soc. 133, 16847-51 (2011).
4. L.Gross, et al., Science 337, 1326-9 (2012).

O 48.9 Wed 12:30 GER 38

**The influence of the tip geometry on picking up a CO molecule** — •Daniel Meuer and Franz J. Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, D-93053 Regensburg, Germany

CO tip termination allows increased AFM resolution of carbon based molecules and structures by imaging, for instance, carbon back bonds [1,2]. Furthermore it has been shown that a measure of the bond order and the length of covalent bonds is possible with CO functionalized tips [2]. Our group has shown that it is possible to identify the orientation of the front most tip atom, using a CO molecule chemisorbed to a Cu(111) surface [3]. This allows us to investigate the influence of the metal tip geometry on the likelihood of picking up a CO molecule.

References

[1] L. Gross et al., Science 325, 1110 (2009)

[2] L. Gross et. al., Science 337, 1329 (2012)

[3] J. Welker and F. J. Giessibl, Science 336, 444 (2012)

O 48.10 Wed 12:45 GER 38

**Looking for the Origin of Power Laws in Electric Field Assisted Tunneling** — •H. Cabrera, D.A. Zanin, L.G. De Pietro, A. Vindigni, U. Ramsperger, and D. Pescia — Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland

We have measured the voltage vs distance characteristics at constant current $I$ of a tunnel diodelike junction consisting of an electron emitting sharp tip placed at a variable distance $d$ from a planar anode. Such a junction is used e.g. in Scanning Tunneling Microscopy (STM) and in the topografiner technology. By mounting the tip onto a piezocrystal, which can move the tip perpendicularly to the surface, the distance $d$ can be varied, its value can be also double checked by an optical sensor device. At sufficiently large distances, i.e. in the regime of electric field assisted quantum tunneling, the $V-d$ characteristic curves for different currents follow approximately a power law, the exponent $\lambda$ being independent of the current. Here we compare and discuss the origin of the observed power law and the measured value of it in terms of electrostatic properties of the tip-plane junction, taking the geometry of the tip as a hyperboloid of revolution.

O 48.11 Wed 13:00 GER 38

**Investigations on the imaging dynamics of carbon nanotube based probes in intermittent-contact AFM** — •Moid Bhatti — Institut für Experimentalphysik, Universität des Saarlandes, 66041 Saarbrücken, Germany

High speed (video rate and beyond) atomic force microscopy (AFM) requires not only fast feedback with a bandwidth exceeding 100 kHz – for which solutions are emerging – but also cantilever resonant frequencies in the MHz range. Nanocantilevers (NC) or nanowires (NW) can fulfill this requirement motivating an understanding of their interaction with the sample.

We are studying contact mechanics of the cantilever-sample system in the dynamic mode AFM using: (1) nanowires (NW) grown on a substrate whose dynamic behavior is equivalent to an AFM cantilever with a NW attached to it (AFM-NW), (2) carbon nanotubes (CNT) attached to an AFM cantilever (AFM-CNT), and (3) focused-ion-beam-(FIB)-structured NC (AFM-NC).

Single-walled AFM-CNT have been in use as a super tip. A CNT adds to the complexity of the contact mechanics of the probe-sample system because it can stick, slip, adhere, kink, and buckle as it interacts with the sample surface leading to imaging artifacts. We describe here the imaging dynamics of AFM-NW by using a long and shortened multi-walled CNT and explain the interaction dynamics using cantilever trajectories, distance-dependent resonance curves, and amplitude-distance curves which differ from those of the conventional AFM tips in a marked way.

# O 49: Surface Chemical Reactions and Heterogeneous Catalysis III

Time: Wednesday 10:30–13:00 Location: PHY C 213

O 49.1 Wed 10:30 PHY C 213

**Hydrogen adsorption on bimetallic PdAg/Pd(111) surface alloys** — •Luis Mancera and Axel Gross — Institute of Theoretical Chemistry, University of Ulm, D-89069 Ulm, Germany

Hydrogen adsorption on metallic surfaces has been a very active field of research due to the wide range of technical applications, in areas such as heterogeneous catalysis, energy storage and energy conversion. Bimetallic surface alloy catalysts have in various cases been found to show superior catalytic properties compared to those of the individual species, with the additional advantage of being tunable by doing changes in their compositions. In this contribution, we investigate hydrogen adsorption on PdAg/Pd(111) bimetallic surface alloys, a system that has been found to be thermodynamically stable and to exhibit a catalytic performance that is related to the size of the palladium ensembles [1]. We use periodic density functional theory (DFT) in order to elucidate mechanisms for molecular hydrogen dissociation and to identify active sites for adsorption as a function of palladium ensemble size and hydrogen coverage. In most of cases, similarly to adsorption on pure Pd(111), hydrogen atoms adsorb preferentially at threefold-coordinated hollow sites of palladium ensembles, while adsorption of molecular hydrogen is observed only at top position of isolated Pd atoms in the surface alloy.

[1] L. Mancera *et al.*, Phys. Chem. Chem. Phys. **15**, 1497 (2013).

O 49.2 Wed 10:45 PHY C 213

**Degree of hydrogenation of the reconstructed Si(001)-surface under MOVPE-conditions - A DFT study** — •Phil Rosenow and Ralf Tonner — Philipps-Universität Marburg, Fachbereich Chemie, Hans-Meerwein-Str. 4, 35032 Marburg

In order to model the metal organic vapor phase epitaxy of III/V-semiconductors on the silicon surface for the integration of laser devices in electronic circuits, the properties of the surface under the relevant conditions must be known beforehand. Especially the extent of hydrogenation is important for the reactivity of the surface. A DFT-based thermodynamics study has been performed on the reconstructed Si(001) surface in order to assess the validity of the theoretical approach compared to experimental observations and prepare for further adsorption studies.

The frequently used *ab initio*-thermodynamics approach which usually neglects surface contributions to thermodynamic quantities is compared to full phonon calculations. It can be shown that *ab initio*-thermodynamics overestimates the stability of the hydrogenated surface compared to full phonon calculations. The difference between the two can be used as a fitting parameter to obtain an expression for the extent of hydrogenation dependent on any MOVPE-conditions, in accord with experienced observations and allowing for a consistent computational treatment of the adsorption process on an atomistic scale.

O 49.3 Wed 11:00 PHY C 213

**Interaction and reactivity between $H_2O$ and CO on Au(310)** — •Matthijs van Spronsen[1], Angela den Dunnen[2], Maarten van Reijzen[2], Christine Hahn[2], Kees-Jan Weststrate[3], and Ludo Juurlink[2] — [1]Kamerlingh Onnes Laboratory, Leiden University, PO Box 9504, 2300 RA, Leiden, The Netherlands — [2]Leiden Institute of Chemistry, Leiden University, PO Box 9502, 2300 RA, Leiden, the Netherlands — [3]Technische Universiteit Eindhoven, Postbus 513, 5600 MB, Eindhoven, the Netherlands

Important discoveries show significant activity of supported Au nanoparticles in the oxidation of CO [1]. Furthermore, it also has been showed recently that water promotes the reactivity [2]. Both the remarkable activity of the Au nanoparticles and the promoting effect of water have not been completely understood. To study the effect of low coordinated Au atoms, the interaction between $H_2O$ and CO has been studied on the stepped Au(310) by Temperature Desorption Spectroscopy and high resolution X-ray Photoelectron Spectroscopy under Ultra High Vacuum conditions. In contrary to the Au(111) surface, desorption of $H_2O$ occurs in two peaks indicating stronger interaction of $H_2O$ with the low coordinate sites in the Au(310) surface. However, no fragmentation or reaction with CO has been detected. Electron irradiation of the adsorbed $H_2O$ layers creates a mixture of $H_2O$, OH and O. In this mixture both OH and O show high reactivity to CO oxidation even at temperatures as low as 123 K.

[1] M. Haruta, et al, Chemistry Letters, no. 2, pp. 405-408, 1987. [2] M. Daté,et al, Angewandte , vol. 43, pp. 2129-2132, Apr. 2004.

O 49.4 Wed 11:15 PHY C 213

**Functional Azobenzene based Self-Assembled Monolayers: molecular composition effects and photo switchable properties** — •Swen Schuster[1], Andreas Terfort[2], and Michael Zharnikov[1] — [1]Applied Physical Chemistry, Heidelberg University, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany — [2]Institute for Inorganic und Analytical Chemistry, Frankfurt University, Max-von-Laue-Straße 7, 60438 Frankfurt, Germany

Control adjustment of work function of surfaces and interfaces by external stimuli is a challenging task. In this context, we designed novel photoresponsive, azobenzene-based self-assembled monolayers (SAMs) on gold and characterized them by synchrotron based high resolution x-ray photoelectron spectroscopy (HRXPS) and near-edge x-ray absorption fine structure spectroscopy (NEXAFS). The SAM precursors consisted of the thiol headgroup, a short aliphatic linker, azobenzene unit, and a functional tail group carrying a certain dipole moment. The length of the linker was varied to control the packing density in the monolayers, based on so called odd-even effect in monomolecular assembly. It was expected that the change in the orientation of the tail group upon the photoisomerization will result in a change of the work function of the entire system. The respective effects were monitored in situ by an ultra-high vacuum (UHV) Kelvin Probe. A clear signature of the photoisomerization behavior accompanied by the pronounced changes in the work function was found. The extent of the observed changes was related to the molecular structure (character of the tail group) and packing density in the SAM.

O 49.5 Wed 11:30 PHY C 213

**On-Surface Azide-Alkyne Cycloaddition on Au(111)** — •Oscar Díaz Arado[1], Harry Mönig[1], Hendrik Wagner[2], Jörn-Holger Franke[1], Gernot Langewisch[1], Philipp Held[2], Armido Studer[2], and Harald Fuchs[1] — [1]Physikalisches Institut and Center for Nanotechnology, WWU, Münster, Germany — [2]Organisch-Chemisches Institut, WWU, Münster, Germany

Two dimensional chemical reactions have been an uprising field of research in the recent years to obtain new polymeric networks directly at surfaces under ultrahigh vacuum (UHV) conditions [1,2]. Here we present the successful cycloaddition reaction between azides and alkynes on a Au(111) surface at room temperature and under UHV conditions [3]. High-resolution scanning tunneling microscopy images reveal that these on-surface cycloadditions occur highly regioselectively to form the corresponding 1,4-triazoles. Density functional theory simulations confirm that the reactions can occur at room temperature, where the Au(111) surface does not participate as a catalytic agent in alkyne C-H activation but acts solely as a two-dimensional constraint for the positioning of the two reacting moieties. Our results provide new insights about the necessity of copper catalysts for on-surface azide-alkyne "click" chemistry. The on-surface azide-alkyne cycloaddition has great potential for the development and fabrication of functional organic nanomaterials on surfaces.

[1] D. F. Perepichka, F. Rosei, Science 2009, 323, 216 [2] L. Grill et.al., Nature Chemistry, 2012, 4 (3), pp. 215-220 [3] O. Díaz Arado et.al., ACS Nano, 2013, 7 (10), pp. 8509-8515

O 49.6 Wed 11:45 PHY C 213

**Chemical reactions and electronic structure of single molecules at surfaces** — •Alexander Riss[1,2], Sebastian Wickenburg[1], Liang Z. Tan[1,3], Hsin-Zon Tsai[1], Patrick Gorman[1], Dimas G. de Oyteza[1,4], Yen-Chia Chen[1,3], Steven G. Louie[1,3], Felix R. Fischer[1,3], and Michael F. Crommie[1,3] — [1]University of California, Berkeley, USA — [2]Institute of Applied Physics, Vienna University of Technology, Austria — [3]Lawrence Berkeley National Laboratory, Berkeley, USA — [4]Centro de Física de Materiales CSIC/UPV-EHU-Materials Physics Center, San Sebastián, Spain

We investigated intra- and intermolecular reactions by imaging the chemical structure of single molecules by non-contact atomic force microscopy (nc-AFM). Additionally we used scanning tunneling microscopy and spectroscopy (STM/STS) to probe how coupling of molecules affects their electronic properties. In our studies we:

- resolved the structural changes and bond rearrangements associated with complex cyclization cascades of enediyne molecules [1],
- revealed multiple steps of cyclization and coupling reaction mechanisms by real-space identification of intermediate species, and
- probed the combined structural and electronic properties of conjugated polymers formed through radical coupling reactions. We observed the formation of a low-energy 1D conducting channel along the backbone of polymer chains, which can be explained by pi-orbital overlap between monomer building blocks [2].

[1] D.G. de Oteyza et al.; Science 340, 1434–1437 (2013)

O 49.7 Wed 12:00 PHY C 213

### Substrate induced dehydrogenation: Transformation of octaethylporphyrin into tetrabenzoporphyrin

— •Merlin Schmuck[1], Dennis van Vörden[2], Manfred Lange[2], Johannes Schaffert[2], Maren Cottin[2], Christian Bobisch[2], and Rolf Möller[2] — [1]Department of Physical Chemistry I, Ruhr-University Bochum, 44801 Bochum — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstr. 1-21, 47048 Duisburg, Germany

Solids of organic molecules can exhibit semiconducting properties but have many more possibilities to manipulate their electronic properties than compound semiconductors. That makes them interesting for numerous technical applications. One of such organic molecules is the porphyrin molecule, which is already in use for solar cells. Its electronic properties can be manipulated through different metallic core atoms and different ligands like ethyl groups or benzene rings or even more complex side groups. During the characterization of octaethylporphyrin iron (lll) chloride via topographical STM imaging, we observed the thermally induced transformation of such a porphyrin derivative on a Cu(111) substrate to tetrabenzoporphyrin (TBP) by annealing the sample at about 450 K. The TBP was identified by comparing the newly formed molecules with iron phthalocyanine in mixed layers. Furthermore, an activation energy of this process was determined by counting the number of events for various temperatures. (D. van Vörden et al., J. Chem. Phys. 138, 211102 (2013))

O 49.8 Wed 12:15 PHY C 213

### Structure and Reactivity of K[VO($O_2$)Hheida]: DFT Studies on the Interpretation of IR and NEXAFS Spectra

— •Lili Sun and Klaus Hermann — Inorganic Chemistry Department, Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin

The identification of structural details of catalyst particles is important for a reliable description of structure-reactivity relationships. Here we consider an oxoperoxovanadium(V) compound chelated with N-(2-hydroxyethyl) iminodiacetic acid, [VO($O_2$)Hheida]. This complex is an efficient functional model for the vanadium haloperoxidase enzyme which acts as a halide oxidant. It includes various oxygen species next to its vanadium atom in very different local coordination. Thus, the [VO($O_2$)Hheida] complex offers an ideal test case for examining differently coordinated oxygen in the same system.

DFT calculations are performed to obtain the equilibrium geometry of the [VO($O_2$)Hheida]$^-$ ion and the results agree well with experiments for a K[VO($O_2$)Hheida] single crystal where potassium ions form the positive counterpart. The analysis of vibrational modes allows an identification of differently coordinated oxygen species, such as vanadyl and di-oxo, although corresponding modes are not well localized. The theoretical spectrum fits with experimental data from IR and Raman measurements. Theoretical O 1s NEXAFS spectra are also evaluated. The corresponding partial NEXAFS spectra show substantial differences amongst the different oxygen species which allows an easy discrimination. These results confirm the experimental O K-shell NEXAFS data.

O 49.9 Wed 12:30 PHY C 213

### Surface reaction steps of dicyclohexylmethane/diphenylmethane on Pt(111)

— •Christoph Gleichweit[1], Oliver Höfert[1], Nicole Brückner[2], Peter Wasserscheid[2], Hans-Peter Steinrück[1], and Christian Papp[1] — [1]University Erlangen-Nuremberg, Chair of Physical Chemistry II, Egerlandstr. 3, 91058 Erlangen, Germany — [2]University Erlangen-Nuremberg, Institute of Chemical Reaction Engineering, Egerlandstr. 3, 91058 Erlangen, Germany

The liquid organic hydrogen carrier pair dicyclohexylmethane (DHM) and diphenylmethane (DPM) was studied on Pt(111) by high-resolution X-ray photoelectron spectroscopy and temperature programmed desorption (TPD) in order to elucidate the reaction steps. Using physical vapor deposition, the molecule was first adsorbed under ultra high vacuum conditions, and subsequently the surface reaction was monitored during heating. The signals of the individual surface species during the reaction of the loaded carrier (DHM) are compared to the ones of the unloaded carrier (DPM), giving information on the dehydrogenation mechanism. During adsorption, the development of monolayer and multilayer signals is observed clearly in the C 1s region for both DHM and DPM. When heating the sample continuously, the multilayer of DHM desorbs at about 230 K. Subsequently, the dehydrogenation of DHM follows successively in the range of 250 to 320 K. For comparison, we measured TPD of the unloaded carrier DPM showing dehydrogenation at the $CH_2$ group above 310 K, leading to the first decomposition product. Upon further heating up to 800 K complete decomposition to carbon fragments happens.

O 49.10 Wed 12:45 PHY C 213

### Computational screening study towards redox-active metal-organic frameworks

— •Jelena Jelic[1], Dmytro Denysenko[2], Dirk Volkmer[2], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Universität Augsburg, Germany

The metal-organic framework (MOF) MFU-4l containing Co(II) centers and $Cl^-$ ligands [1] has recently shown promising redox activity. Aiming for further improved MOF catalysts for oxidation processes employing molecular oxygen we present a density-functional theory (DFT) based computational screening approach to identify promising metal center and ligand combinations within the MFU-4l structural family [2]. Using the $O_2$ binding energy as a descriptor for the redox property, we show that relative energetic trends in this descriptor can reliably be obtained at the hybrid functional DFT level and using small cluster (scorpionate-type complex) models. Within this efficient computational protocol we screen a range of metal center / ligand combinations and identify several candidate systems that offer more exothermic $O_2$ binding than the original Co/Cl-based MFU-4l framework.

[1] S. Biswas *et al.*, Dalton Trans. 6487 (2009).

[2] J. Jelic *et al.*, New Journal of Physics **15**, 115004 (2013).

# O 50: Oxide and Insulator Surfaces I

Time: Wednesday 10:30–13:00 Location: WIL A317

O 50.1 Wed 10:30 WIL A317

**Elementary steps of water dissociation on $\alpha$-$Al_2O_3$(0001)** — •Harald Kirsch[1], Jonas Wirth[2], Yujin Tong[1], Martin Wolf[1], Peter Saalfrank[2], and R. Kramer Campen[1] — [1]Fritz-Haber-Institut, Abt. Physikalische Chemie, 14195 Berlin, Germany — [2]Universitaet Potsdam, Institut fuer Chemie, 14476 Potsdam OT Golm, Germany

Alumina surfaces are ubiquitous in technologically relevant applications and a useful model system for more complicated, environmentally abundant, alumino-silicate phases. Because their properties change dramatically on interaction and reaction with water, water/Alumina chemistry has been studied, both experimentally and theoretically, for decades. In this work, we study the interaction of heavy water ($D_2O$) with the $\alpha$-$Al_2O_3$(0001) surface under ultra high vacuum (UHV) conditions. Hydroxylation of the $Al_2O_3$(0001) in UHV is performed by dosing $D_2O$ seeded in Helium with a molecular beam source (MBS). For characterization we employ vibrationally resonant sum frequency generation (VSF) spectroscopy to probe the OD stretch response of interfacial species. This technique allows us to distinguish several different OD-species in the OD-stretching region. Comparison of the resulting measured spectra with frequencies and geometries claculated from periodic density functional theory allows us to identify, for the first time, the products of the two theoretically predicted dissociation pathways: we observe the elementary steps of water dissociation on $\alpha$-$Al_2O_3$(0001).

O 50.2 Wed 10:45 WIL A317

**Optical Characterization of $\alpha$-$Al_2O_3$(0001) Surface Structure and Reactivity in Ambient Conditions** — •Yujin Tong, Harald Kirsch, and R. Kramer Campen — Fritz-Haber-Institut, Abt. Physikalische Chemie, 14195 Berlin, Germany

The surface chemistry of alumina is important in fields such as heterogeneous catalysis, geo- and environmental chemistry. Often these surfaces are not merely passive participants in interfacial chemistry: reaction between species present in adjoining phases at the surface can lead to correlated changes in surface structure and reactivity. While much important chemistry at alumina surfaces occurs in ambient conditions, simultaneously probing surface reconstruction and reactivity in these environments is challenging. In this study, we employ surface specific vibrational sum frequency (VSF) spectroscopy to characterize the reaction of water with the the $\alpha$-$Al_2O_3$(0001) surface in ambient conditions. Starting with a Al-terminated surface prepared under UHV in the absence of water, we use the evolution of the interfacial OH stretch spectral response to track the presence of dissociatively adsorbed water and that of the surface phonon spectral response to track the accompanying surface reconstruction. All changes in spectral observables are clearly shown to be reversible on heating. We demonstrate that the observed phonon modes are surface specific by their frequencies and symmetry and assign them based on comparison to computation.

O 50.3 Wed 11:00 WIL A317

**Water Adsorption at the Tetrahedral Titania Surface Layer of $SrTiO_3$(110)-(4×1): An STM and Photoemission Study.** — •Stefan Gerhold[1], Zhiming Wang[1], Xianfeng Hao[1], Zbynek Novotny[1], Cesare Franchini[2], Eamon McDermott[3], Karina Schulte[4], Michael Schmid[1], and Ulrike Diebold[1] — [1]Institute of Applied Physics, Vienna University of Technology, Austria — [2]Center for Computational Materials Science, University of Vienna, Austria — [3]Institute of Materials Chemistry, Vienna University of Technology, Austria — [4]MAX IV Laboratory, Lund University, Sweden

The interaction of water with oxide surfaces is of great interest for both fundamental sciences and applications. We present a combined theoretical [density functional theory (DFT)] and experimental [Scanning Tunneling Microscopy (STM), photoemission spectroscopy (PES)] study of water interaction with the two-dimensional titania overlayer that terminates the $SrTiO_3$(110)-(4 × 1) surface and consists of $TiO_4$ tetrahedra. STM, core-level and valence band PES show that $H_2O$ neither adsorbs nor dissociates on the stoichiometric surface at room temperature, while it dissociates at oxygen vacancies. This is in agreement with DFT calculations, which show that the energy barriers for water dissociation on the stoichiometric and reduced surfaces are 1.7 and 0.9 eV, respectively. We propose that two-dimensional tetrahedrally coordinated titania overlayers are generally hydrophobic. In addition, enhanced reactivity due to deposited Sr adatoms is discussed. This work was supported by the Austrian Science Fund (FWF, project F45).

O 50.4 Wed 11:15 WIL A317

**Sub-Monolayer Water Adsorption on Alkaline Earth Metal Oxide Surfaces: A First-Principles Study** — •Xunhua Zhao, Saswata Bhattacharya, Luca M. Ghiringhelli, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft

In the present work, we predict atomic structures of adsorbed complexes that should appear on alkaline earth metal oxide (001) terraces in thermodynamic equilibrium with water and oxygen gases. Density-functional theory with the hybrid exchange-correlation functional HSE06 combined with the self-consistent many-body dispersion approach [1] is used to calculate total energies. The choice of this functional is validated by renormalized second-order perturbation theory [2]. An unbiased search for global minima of $H_xO_y$ adsorption is performed using first-principles genetic algorithm for periodic models. $x$ and $y$ as a function of temperature and pressure are determined using *ab initio* atomistic thermodynamics. We find a range of $H_2O$ chemical potentials where one-dimensional adsorbed water structures are thermodynamically stable on CaO(001). On MgO(001) and SrO(001), such structures are not found. The formation of the one-dimensional structures is explained by the balance between water-water and water-surface interactions.—[1] A. Tkatchenko, R. A. DiStasio, Jr., R. Car and M. Scheffler, Phys. Rev. Lett. **108**, 236402 (2012); [2] X. Ren, P. Rinke, G. E. Scuseria, M. Scheffler, Phys. Rev. B **88**, 035120, (2013).

O 50.5 Wed 11:30 WIL A317

**A first principles study of halogenated adsorbates on ice** — •Michel Bockstedte and Philipp Auburger — Lst. Theor. Festkörperphysik, Universität Erlangen-Nürnberg, 91058 Erlangen

Fluid water, water clusters, and water ice possess the fascinating ability to solvate ions and electrons. On ice, the solvated electron facilitates electron-induced reactions of adsorbates via dissociative electron attachment (DEA) that for instance take place in atmospheric chemistry. The simultaneous interaction of the electron with the molecule and the ice surface enhances the cross section as compared with the gas phase. The current understanding of the physical mechanisms at work is rather incomplete, in particular a picture on the molecular scale is missing. Here we investigated the interaction of halogenated hydrocarbons and HCl with prototypical electron traps at the ice surface in the framework of density functional theory (DFT), hybrid DFT, and many body perturbation theory. For the hydrocarbons clear chemical trends across the halogen series, F, Cl, and Br, are found concerning favorable adsorption sites. Depending on the halogen and the electron trap, electron affinity of antibonding adsorbate levels is enhanced. A quenching of electron traps by HCl or $Cl^-$, as form during the DEA, is discussed.

O 50.6 Wed 11:45 WIL A317

**impact of the vapour pressure of water on the equilibrium shape of zinc oxide nanoparticles: An ab-initio study** — •stephane kenmoe, mira todorova, p.ulrich biedermann, and joerg neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1,40237 Düsseldorf ,Germany

ZnO powders and nanoparticles are used as catalysts and have potential applications in gas-sensing and solar energy conversion. A fundamental understanding ofthe exposed crystal facets, their surface chemistry and stability as function of environmental conditions is essential for rational design and improvement of synthesis and properties. Using density-functional theory calculations we study the adsorption of water on the non-polar low-index (10-10) and (11-20) surfaces of ZnO. Observing both molecular and dissociative H2O adsorption, we analyse the contributions of water-surface and water-water interactions to the energies of the stable structure.Based on this insight we compute and analyse the impact of water adsorption on surface energies and the equlibrium shape of nanoparticles in a humid environment

O 50.7 Wed 12:00 WIL A317

**The role of surfaces and interfaces in the phase separating Li intercalation material $\mathbf{Li_xFeSiO_4}$** — •Nicolas G. Hörmann$^{1,2}$ and Axel Gross$^{1,2}$ — $^1$Helmholtz Institute Ulm (HIU) Electrochemical Energy Storage, Albert-Einstein-Allee 11, 89069 Ulm — $^2$Universität Ulm, Institut für Theoretische Chemie, Albert-Einstein-Allee 11, 89069 Ulm

Phase separating behavior of electrode materials of secondary Li battery materials is typically assumed to cause low rate capability due to a nucleation and growth process. Nevertheless, cathodes made of $LiFePO_4$ can show fast charging rates if they consist of nanoscale particles. Several mechanisms have been proposed for this observation, most of which are related to finite size effects such as interfaces or strain [1]. It is, however, still under debate whether e.g. the alignment of phase interfaces is mainly driven by "lattice" or "chemical mismatch" and how the actual interface looks like.

We present ab-initio studies tackling related issues for the promising material $Li_xFeSiO_4$ [2] based on density functional theory (DFT). In particular, Li binding energies for different chemical environments - in bulk and near surfaces or interfaces - are determined. Effects of strain are considered by decomposing the interface energy into contributions due to coherency strain and change of the chemical environment. Subtleties such as charge localisation are analysed as well.

[1] Malik, R et al., *J. Electrochem. Soc.*, **160**, 5, A3179-A3197, **2013**

[2] Hörmann, N.G. and Groß, A. , *J. Solid State Electrochem.*, accept.

O 50.8 Wed 12:15 WIL A317

**In-situ x-ray investigation of solid oxide fuel cell model electrodes** — •Sergey Volkov$^{1,2}$, Markus Kubicek$^3$, Vedran Vonk$^1$, Dirk Franz$^{1,2}$, Jürgen Fleig$^3$, and Andreas Stierle$^{1,2}$ — $^1$Deutsches Elektronen-Synchrotron DESY, 22603 Hamburg, Germany — $^2$Fachbereich Physik, Universität Hamburg, 20355 Hamburg, Germany — $^3$Institut für Chemische Technologien und Analytik, Technische Universität Wien, 1060 Vienna, Austria

The performance of high temperature solid oxide fuel cell (SOFC) electrodes depends strongly on the structure and composition of yttria stabilized zirconia (YSZ) surfaces. In addition, on the fuel cell cathode side the interface between the perovskite electrode and the YSZ electrolyte plays an important role during the oxygen incorporation process. Our studies focus on the cathode side of SOFCs, which is mimicked by the YSZ (100) surface, as electrolyte, and pulsed laser deposition grown La0.8Sr0.2MnO3, as electrode, were studied. In order to track structural changes in-situ surface x-ray diffraction experiments were performed at the ESRF, beamline ID03. A special x-ray diffraction chamber was developed, which allows contacting the electrode and applying a controlled voltage across the electrolyte. Anomalous scattering at the Y and Zr K-edges was used to enhance the scattering contrast. The analysis of the crystal truncation rod data has revealed a noticeable change in intensity depending on different oxygen pressure, temperature and voltage conditions. These intensity changes mostly refer to the changes in the composition and vacancy concentration below the electrode, what will be presented in detail.

O 50.9 Wed 12:30 WIL A317

**Structural, electronic and thermodynamic properties of $\mathbf{YBaCo_4O_{7+\delta}}$ from DFT+U calculations** — •Jakub Goclon and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

In the past decade, one of the main goals in solid oxide fuel cell (SOFC) research was to develop intermediate-temperature SOFCs (IT-SOFCs) operating at 600–800 °C. Recently, a new family of layered cobalt oxide compounds based on the $YBaCo_4O_7$ structure has been proposed for application as cathode material in IT-SOFCs. The compounds are able to adsorb in a reversible way up to $\delta$=1.5 oxygen atoms per unit formula, both at low and high temperatures.

We performed DFT+U calculations for different $YBaCo_4O_7$ bulk structures based on structural models proposed in the literature. We then focused on the bulk properties of the oxygen-rich phases after oxygen incorporation, searching for the most favorable positions of the additional oxygen atoms. In the second part of this work we determined the most stable termination (structure, chemical composition) of the $YBaCo_4O_7$(001) surface based on thermodynamic analysis. Analogical calculations were performed for oxygen adsorption on $YBaCo_4O_8$(001). The local electronic structure and the local distribution of the cobalt cations in close vicinity of the additional oxygen atoms has been carefully analyzed and will be discussed. In addition, results from corresponding calculations for the bulk and low-index surfaces of $Co_3O_4$ will be shown as reference.

O 50.10 Wed 12:45 WIL A317

**Ab-initio study of the wurtzite terminated rocksalt CoO(111) polar surface: Facing a DFT bulk dilemma** — Florian Mittendorfer and •Josef Redinger — Inst. f. Applied Physics, Vienna University of Technology, Vienna, Austria

Evidenced by LEED, the polar (111) surface of CoO is terminated by a wurtzite like top Co-O bilayer, which from experimental and theoretical evidence is believed to become metallic to compensate polarity [1]. An ab-initio DFT investigation of such a mechanism is not only complicated by the polarity of the surface, but also by the correlated nature of the Co 3d electrons, which have to be treated by PBE+U type approaches or by employing hybrid functionals like HSE06. Using the VASP code slabs of various thickness have been treated and the preference for a wurtzite like termination could be established. However, this outcome should be taken with caution, since already for the CoO bulk system PBE+U and HSE06 find a preference for the wurtzite (or zincblende) structure over the experimental slightly distorted rocksalt structure, similar to the case of MnO [2]. We present an analysis of our HSE06 and PBE+U results also for different double counting corrections and conclude that only for unreasonably high values of U the correct bulk phase order can be established.

[1] K Heinz and L Hammer, J. Phys.: Condens. Matter **25**, 173001 (2013 Review)

[2] A. Schrön, C. Rödl, and F. Bechstedt, Phys. Rev. B **82**, 165109 (2010)

## O 51: Surface and Interface Magnetism I (O jointly with MA)

Time: Wednesday 10:30–13:00 Location: WIL C107

O 51.1 Wed 10:30 WIL C107

**Tracing the RKKY-interaction in pairs of adatoms via the peak splitting of a Kondo resonance** — Alexander Ako Khajetoorians$^1$, •Manuel Steinbrecher$^1$, Mohammed Bouhassoune$^2$, Samir Lounis$^2$, Markus Ternes$^3$, Jens Wiebe$^1$, and Roland Wiesendanger$^1$ — $^1$Institute of Applied Physics, Universität Hamburg, 20355 Hamburg, Germany — $^2$Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — $^3$Max-Planck Institut für Festkörperphysik, 70569 Stuttgart, Germany

Ruderman-Kittel-Kasuya-Yoshida (RKKY)-interaction is an indirect exchange interaction between localized magnetic moments in a host mediated by conduction electrons, which oscillates between ferromagnetic and anti-ferromagnetic coupling as a function of distance [L. Zhou *et al.*, Nat. Phys. **6**, 187 (2010)]. We performed scanning tunneling spectroscopy at 300 mK on a Fe-H complex and a clean Fe atom, both adsorbed on Pt(111), for different spacing between the atom and the complex. While the Fe atom shows the well known spin excitation [A. A. Khajetoorians *et al.*, Phys. Rev. Lett. **111**, 157204 (2013)], the hydrogen complex shows a Kondo resonance. As a result of the RKKY-interaction the Kondo resonance reveals a distance dependent peak splitting. Fitting the spectra to model calculations including the coupling to the substrate electrons in third order perturbation enables to determine the distance dependency of the RKKY-interaction, which we compare to our first principles calculations.

O 51.2 Wed 10:45 WIL C107

**Controllable Kondo Effect of Fe on Alkali Substrates** — •Malte Schüler$^{1,2}$, Tim O. Wehling$^{1,2}$, Sandra Gardonio$^3$, and Carlo Carbone$^4$ — $^1$Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, D-28359 Bremen, Germany — $^2$Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany — $^3$Materials Research Laboratory, University of Nova Gorica, Vipavska 13, 5000 Nova Gorica, Slovenia — $^4$Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Basovizza, I-34149 Trieste, Italy

The interaction between a magnetic impurity and a non-interacting bath presents a characteristic case of a multiorbital Kondo system. Prototypical realizations are Fe adatoms on alkali-surfaces (in our case Li, Na, K, Cs). The different substrates lead to different hybridization strengths, caused by the decrease of electron density with the increase of the lattice constant.

The electronic configuration and the magnetization of the impurity are measured by XMCD and XAS. Multiplet-broadening and a decrease of magnetic moment with increasing electronic density are observed. The simulation of this behavior leads to understanding how orbital degree of freedom influences the Kondo effect: The orbital resolved hybridization is obtained by fully relaxed DFT calculations and is used as a starting point to model the impurity problem with different complexity. These models are solved by numerical renormalization group, exact diagonalization and quantum Monte Carlo methods and compared to the experimental data.

O 51.3 Wed 11:00 WIL C107

**Spin-orbit coupling and spin dynamics of magnetic adatoms** — •Manuel dos Santos Dias and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

The control and manipulation of magnetic nanostructures hinges on understanding of their spin dynamics, which have been phenomenologically described for many systems using the Landau-Lifshitz-Gilbert equation (LLGe). Here we investigate the validity and possible extension of this equation down to the single atom limit. The magnetic excitation spectrum is derived from the dynamical magnetic susceptibility of the electronic system, employing Time–Dependent Density Functional Theory, as implemented in the Korringa–Kohn–Rostoker Green function method [1]. We include spin-orbit and Zeeman couplings in our calculations, and explore the key parameters in the LLGe, the precessional frequency and damping, for $3d$ adatoms deposited on the Cu(111) and Pt(111) surfaces. See [2] for an example of a theoretical and experimental investigation of Fe adatoms on Pt(111).

Work supported by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] S. Lounis, A. T. Costa, R. B. Muniz and D. L. Mills, Phys. Rev. Lett. **105**, 187205 (2010), Phys. Rev. B **83**, 035109 (2011)

[2] A. A. Khajetoorians, *et al.*, Phys. Rev. Lett. **111**, 157204 (2013)

O 51.4 Wed 11:15 WIL C107

**Exchange coupling and Magnetic anisotropies in 3d atomic chains adsorbed on $Cu_3N - Cu$(110) molecular network** — •Dmitry I. Bazhanov[1,2], Oleg V. Stepanyuk[1,2], and Valeri S. Stepanyuk[2] — [1]Faculty of Physics, Moscow State University, GSP-1, Lenin Hills, 119991 Moscow, Russia — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Based on first-principles calculations we study the magnetic states and exchange coupling in transition metal Mn, Fe, Co atomic chains deposited on a self-corrugated $Cu_3N - Cu$(110) molecular network. The various adsorption sites on a bumping area of $Cu_3N$ layer are investigated where the atomic chains grow at the initial stage of nanowires growth [1]. We demonstrate, that the exchange coupling, magnetic order and anisotropies in atomic chains depend sensitively on their chemical composition and adsorption sites on $Cu_3N$ network. We find that the exchange interactions in atomic chains could lead to ferromagnetic or antiferromagnetic coupling depending on the position of the chain on the surface. The dynamics of classical spins is investigated by means of kinetic Monte Carlo method based on transition-state theory. Also using an *ab initio* determined exchange parameters and spin moments we evaluate the Heisenberg-Dirac-Van Vleck quantum spin Hamiltonian for calculations of the magnetic susceptibility, which is used for indicating the existence of quantum entanglement in the antiferromagnetic atomic chains.

This work was supported by the RFBR grant $N$13-02-01322.

[1] X.-D. Ma *et al.* , Phys. Rev. Lett. 102, 205503 (2009)

O 51.5 Wed 11:30 WIL C107

**Complex trend of magnetic order in Fe clusters on Rh(111) and Ru(0001)** — •Sören Krotzky[1], Fabian Otte[2], Violetta Sessi[3], Carsten Tieg[3], Paolo Ferriani[2], Stefan Heinze[2], Marta Wasniowska[1], Jan Honolka[1,4], and Klaus Kern[1,5] — [1]Max Planck Institute for Solid State Research, Stuttgart Germany — [2]Institute of Theoretical Physics and Astrophysics, University of Kiel, Kiel Germany — [3]European Synchrotron Radiation Facility, Grenoble France — [4]Institute of Physics of the ASCR, Prague Czech Republic — [5]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, Switzerland

We investigate the spin configurations in Fe clusters and monolayers on Ru(0001) and Rh(111) by means of X-ray magnetic circular dichroism experiments, first-principles calculations and Monte Carlo simulations. The importance of Fe $3d$ state itinerancy and its hybridization with partly filled $4d$ substrate bands will be studied for monoatomic height Fe clusters of different atomic size $N$ and various geometries. Randomly positioned single Fe atom spins in the dilute regime ($N = 1$) indirectly interact via the Rudermann-Kittel-Kasuya-Yoshida mechanism, which shows inverted character on Ru(0001) and Rh(111). For Fe dimers we prove the antiferromagnetic (Ru) to ferromagnetic (Rh) cross-over of the nearest-neighbour exchange coupling constant $J_1$. For larger clusters (i.e. $2 \leq N \leq 4$) we show the onset of cluster geometry dependent compensated magnetic structures. Finally, we present experimental evidence for the formation of compensated spin textures both for Ru(0001) and Rh(111) in fully ordered epitaxial Fe islands.

O 51.6 Wed 11:45 WIL C107

**Impact of the large substrate polarization on the magnetic anisotropy energy of $3d$ adatoms on Pt(111)** — •Mohammed Bouhassoune, Manuel dos Santos Dias, David S. G. Bauer, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

It has been shown recently, from first-principles and experimentally with inelastic tunneling spectroscopy, that the magnetic anisotropy energy (MAE) of single Fe adatoms deposited on Pt(111) surface depends strongly on the adsorption site. Surprisingly the sign of the MAE changes once an Fe adatom is moved from an fcc site to a hcp site, thus favoring an in-plane orientation of the moment instead of the out-of-plane orientation [1]. We perform ab-initio calcualtions utilizing the full-relativistic full-potential Korringa-Kohn-Rostoker Green function method [2] for Cr, Mn, Fe and Co adatoms, analyse the contribution of the neighboring shells of Pt atoms and demonstrate that the large polarisation cloud of the Pt-substrate impacts strongly on the MAE.

This work is supported by the HGF-YIG Programme FunSiLab –Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] A. A. Khajetoorians, T. Schlenk, B. Schweflinghaus, M. dos Santos Dias, M. Steinbrecher, M. Bouhassoune, S. Lounis, J. Wiebe, R. Wiesendanger, PRL **111**, 157204 (2013)

[2] D. S. G. Bauer, PhD thesis, RWTH-Aachen (2013)

O 51.7 Wed 12:00 WIL C107

**Emergent phenomena induced by spin orbit coupling in photoemission from ultrathin ferromagnetic films** — •L. Plucinski[1,2], M. Eschbach[1], I. Aguilera[3], G. Bihlmayer[3], S. Blügel[3], and C. M. Schneider[1,2] — [1]PGI-6, FZ Jülich — [2]Fakultät f. Physik, Uni Duisburg-Essen — [3]PGI-1 and IAS-1, FZ Jülich

The existence of easy magnetization axis reduces the crystal symmetry and may manifest itself in lifting the degeneracy of electronic band dispersions along otherwise symmetrical directions in reciprocal space.

In non-magnetic materials spin orbit coupling (SOC) may cause the lifting of the spectral degeneracy of certain surface or bulk bands by means of Rashba or Dresselhaus effects. However, only combining SOC with ferromagnetism offers the possibility of remanent magnetic swapping of the non-degenerate directions which results in discrete switching of the electronic states for certain wave vectors in the Brilloin zone.

We will show the prediction of such phenomena for several monolayers thick films of Fe(001), which have 4-fold in plane easy magnetization axis. The energy scale of the predicted effect (from 20 to 200 meV) is several times larger than the resolution of the state-of-the-art angle-resolved photoemission (ARPES) experiment when performed on cryocooled samples.

Reciprocal space constant energy contours measured by ARPES will be compared with the electronic band structures of Fe calculated using the LDA and GW approximations. Interplay between initial state and photoemission dichroic effects will be discussed.

O 51.8 Wed 12:15 WIL C107

**Oscillatory orbital magnetic moment via $d$-band quantum well states in Fe(001) films** — •Thiago R. F. Peixoto[1],

Maciej Dabrowski[1], Mariusz Pazgan[1], Aimo Winkelmann[1], Takeshi Nakagawa[2], Yasumasa Takagi[2], Toshihiko Yokoyama[2], Uwe Bauer[1], Fikret Yildiz[1], Francesco Bisio[1,3], Marek Przybylski[1,4], and Jürgen Kirschner[1,5] — [1]MPI of Microstructure Physics, Halle, Germany — [2]Institute for Molecular Science, Okazaki, Japan — [3]CNR-SPIN, Genova, Italy — [4]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland — [5]Naturwissenschaftliche Fakultät II, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Iron films grown on silver surfaces have shown an intriguing thickness-dependent oscillatory magnetic anisotropy [1,2]. We explored the effect of electron confinement on the magnetocrystalline anisotropy of *bcc* Fe films via a combination of spin-resolved photoemission spectroscopy ($h\nu = 6$ eV), x-ray magnetic circular dichroism, and magneto-optical Kerr effect measurements. The thickness-dependent variations in the magnetocrystalline anisotropy are ascribed to periodic changes in the density of states at the Fermi level, induced by confinement of electronic states derived from majority $d_{xz}$, $d_{yz}$ out-of-plane orbitals. Our results confirm a direct correlation between QWS, the orbital magnetic moment and the magnetocrystalline anisotropy.

[1] U. Bauer and M. Przybylski, Phys. Rev. B 81, 134428 (2010).
[2] J. Li *et al.*, IEEE Trans. on Magn. 47, 1603 (2011).

O 51.9 Wed 12:30 WIL C107

**Spin dynamics of a single magnetic adatom coupled to nano-mechanical oscillator operating on the atomic scale** — •Michael Schüler[1], Andrey Klavsyuk[2], and Jamal Berakdar[1] — [1]Martin-Luther University Halle-Wittenberg, Institute for Physics, Karl-Heinrich-von-Fritsch-Straße 3, 06120 Halle, Germany — [2]M. V. Lomonosov Moscow State University, Faculty of Physics, Vorob'evy gory, 119899 Moskow, Russia

Great advances have been achieved recently in fabricating, manipulating, and imaging in a controlled way the properties of small magnetic systems. One of the most versatile approaches is the scanning tunnelling microscopy (STM) or spectroscopy (STS) setup, allowing to access the dynamics of single magnetic adatoms on the surface. Within a simple model system, we demonstrate how the transport properties and the relaxation spin dynamics are related to the anisotropic environment. As a second step, we have computed the magnetic anisotropy parameters for the typical Fe@Cu(001) systems by ab initio methods which allows to compare the calculations including the STM tip with the result in absence of the tip. As it turns out, the presence of the tip has a considerable influence on the anisotropy energy. Therefore, depositing the tip apex on a nano-scaled cantilever yields a nanomechanical oscillator coupled to a single spin - a kind of hybrid systems that are subject of recent experimental investigations. We analyse the resulting spin dynamics and point out how the magnetic moment of the Fe atom can be controlled coherently.

O 51.10 Wed 12:45 WIL C107

**Surface electronic properties of Ni(111) investigated by low-temperature scanning tunneling spectroscopy** — •Andreas Krönlein, Jeannette Kemmer, Pin-Jui Hsu, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Although the general electronic properties of Ni(111) have been intensively investigated theoretically and experimentally, the exact position of the majority and minority surface state bands is still under debate [1,2,3,4]. We have performed scanning tunneling spectroscopy measurements at $T = 5.5\,\mathrm{K}$ to investigate the electronic properties of Ni(111) above and below the Fermi level with high energy resolution. Our data allow for the precise determination of band onsets and effective masses of the *sp*-derived surface states and thereby enable us to quantify their magnetic exchange splitting.

[1] M. Donath *et al.*, Phys. Rev. Lett. **70**, 2802 (1993).
[2] J. Braun *et al.*, J. Phys.: Condens. Matter **16**, S2539 (2004).
[3] T. Ohwaki *et al.*, Phys. Rev. B **73**, 235424 (2006).
[4] J. Lobo-Checa *et al.*, Phys. Rev. B **77**, 075415 (2008).

## O 52: Gaede Prize Talk

Time: Wednesday 12:30–13:00 Location: HSZ 02

O 52.1 Wed 12:30 HSZ 02

**Spectroscopy and microscopy of graphene on metals** — •Yuriy Dedkov — SPECS Surface Nano Analysis GmbH, Berlin, Germany

Graphene on metals, which structure can vary from simple lattice matched to commensurate moiré structures, is an ideal system for different kinds of surface science experiments allowing to study many fascinating phenomena. Here we present several examples on the application of electron spectroscopy (NEXAFS, XMCD, XPS, ARPES) and scanning probe methods (STM and AFM) for the investigation of the electronic structure of these systems. These combined approaches allow to understand the bonding mechanism at the graphene-metal interface, the main features of the graphene-derived electronic structure as well as the imaging contrasts in the scanning probe experiments. All experimental data are compared with the state-of-the-art DFT calculations that lead to the deep understanding of the observed phenomena.

## O 53: Invited Talk (Alexandre Tkatchenko)

Time: Wednesday 15:00–15:45 Location: TRE Phy

**Invited Talk** O 53.1 Wed 15:00 TRE Phy

**The Many-Body Path Towards Quantitative Modeling of Complex Adsorption Systems** — •Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Reliable (accurate and efficient) modeling of the structure, stability, and electronic properties of complex adsorption systems remains a daunting task for modern electronic structure calculations. In the context of approximate density-functional theory, two thorny issues prevent us from reaching the goal of quantitative predictions: the (in)famous self-interaction error and the lack of reliable methods for an accurate description of van der Waals (vdW) interactions for hybrid organic/inorganic systems (HIOS). Both issues arise from the complexity posed by many-electron quantum mechanics, thereby demanding effective and novel solutions. Focusing on the role of vdW interactions, our recent developments of approximate many-body methods will be discussed along with a few surprises we found when applying these methods to HIOS: (1) The vdW energy can contribute more to the binding of covalently bonded systems than it does for physisorbed molecules; (2) the physically bound precursor state for aromatics on Pt(111) can be more stable than the corresponding chemisorbed state; (3) many-body vdW interactions lead to a binding energy for a fullerene molecule adsorbed on multi-layered graphene that *decreases* as a function of the number of underlying graphene layers. Finally, we discuss the challenges that lie ahead on the curved path towards fully quantitative many-body modeling of complex adsorption systems.

# O 54: Organic Electronics and Photovoltaics V (CPP jointly with DS, HL, O)

Spectroscopy, OFETs, OLEDs, Photo switches

Time: Wednesday 15:00–18:15 Location: ZEU 260

O 54.1 Wed 15:00 ZEU 260

**Comprehensive efficiency analysis of organic light-emitting diodes featuring horizontal emitter orientation and triplet-to-singlet up-conversion** — •Tobias Schmidt[1], Bert Scholz[1], Christian Mayr[1], Andreas Rausch[2], Thomas Wehlus[2], Dirk Michaelis[3], Norbert Danz[3], Thilo Reusch[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]OSRAM Opto Semiconductors GmbH, Leibnizstrasse 4, 93055 Regensburg, Germany — [3]Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

The external quantum efficiency (EQE) of an organic light-emitting diode can strongly be affected by orientation of the emissive dipole moments, and for fluorescent dyes, by triplet-to-singlet up-conversion leading to an enhanced radiative exciton fraction ($\eta_r$), exceeding the spin-statistical limit of 25 %. By a combination of EQE investigations with time resolved photo- and electroluminescence measurements we are able to quantify the lower limit of the additionally created singlet excitons, e.g. by thermally activated delayed fluorescence, as well as the factors being responsible for light-outcoupling. For the investigated fluorescent system the EQE is boosted by two effects. First, due to horizontal alignment of the transition dipole moments, the outcoupling factor is enhanced by a factor of 1.3. Second, the enhanced $\eta_r$ value of 36 %, results in an additional efficiency increase by a factor of 1.44. As a consequence of the combination of both effects the EQE almost doubles and values up to 5 % are achieved for direct emission in spite of a comparatively low emitter efficiency of 40 % only.

O 54.2 Wed 15:15 ZEU 260

**Multi-analytical investigation of SAM formation in printing relevant timescales III: OFET devices** — •Milan Alt[1,2,6], Janusz Schinke[2,3], Sabina Hillebrandt[2,5], Marc Hänsel[2,4], Kaja Deing[2,6], Uli Lemmer[1,2], and Norman Mechau[1,2] — [1]Karlsruher Institute of Technology — [2]InnovationLab, Heidelberg — [3]TU Braunschweig — [4]TU Darmstadt — [5]Uni Heidelberg — [6]Merck KGaA

Self-assembled monolayers (SAMs) can be used to effectively reduce contact resistances originating from energetic misalignments at metal-semiconductor interfaces. Solution processing of SAMs has been intensively studied and is in principle compatible with high throughput printing techniques. However, most studies on SAMs feature immersion in very dilute solutions for many hours, in some cases up to several days. The objective of this work is to understand SAM accumulation with a focus on short time scales in order to estimate weather the deposition of well performing SAMs can be speeded up sufficiently to be compatible with typical film drying times in printing. We combined analytical characterization of SAM treated metal surfaces via photoelectron- and IR-spectroscopy, as well as Kelvin Probe with measurements of the actual injection barriers in OFET devices. We chose the widely used 1H,1H,2H,2H-Perfluorodecanethiol SAM and investigated its quality and charge injection performance in dependency of the process parameters immersion time and molecular concentration. Additionally, we studied the impact of ambient condition on SAM deposition and the resulting SAM performance, in order to account for a realistic fabrication environment.

O 54.3 Wed 15:30 ZEU 260

**Multi-analytical investigation of SAM formation on printing-relevant time scales I: Kelvin probe and photoelectron spectroscopy** — •Janusz Schinke[1,5], Marc Hänsel[2,5], Milan Alt[3,4,5], Sabina Hillebrandt[2,5], Eric Mankel[6,5], Wolfram Jaegermann[6,5], Wolfgang Kowalsky[1,5], and Robert Lovrincic[1,5] — [1]TUBS, Inst. f. Hochfrequenztechnik — [2]Uni HD, Kirchhoff-Inst. für Physik — [3]Karlsruher Inst. f. Technologie — [4]Merck KGaA — [5]InnovationLab GmbH, Heidelberg — [6]TUD, Materials Science Inst.

In organic electronic devices, charge injection at the contacts is crucial for electrical performance. The devices require electrodes with a sufficiently low contact resistance at the metal-semiconductor interface to inject into or collect charge carriers from the transporting layer. A smart way to align the energetics at the interface is the use of self-assembled monolayers (SAMs). We have studied the properties of 1H,1H,2H,2H-Perfluorodecanethiol using photoelectron spectroscopy (XPS/UPS), infrared spectroscopy (IR), ambient Kelvin probe (KP), and contact angle (CA) measurements and the injection barriers were also measured in actual devices - organic field effect transistors. Using these methods we were able to obtain a very deep understanding of the whole SAM adsorption process, as well as the impact of immersion time, concentration and the influence of ambient conditions on the resulting monolayer and its performance. With this knowledge we estimate optimized parameters to speed up the treatment process, in contrast to most studies where long immersion times are used, to be compatible with typical times used in standard printing methods.

O 54.4 Wed 15:45 ZEU 260

**Multi-analytical investigation of SAM formation on printing-relevant time scales II: infrared-reflection-absorption-spectroscopy** — •Sabina Hillebrandt[1,5], Janusz Schinke[2,5], Milan Alt[3,4,5], Robert Lovrincic[2,5], Tobias Glaser[1,5], and Annemarie Pucci[1,5] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik — [3]Karlsruher Institut für Technologie — [4]Merck KGaA, Darmstadt — [5]Innovationlab GmbH, Heidelberg

In organic semiconductor devices the improvement of charge carrier injection between metal contact and organic semiconductor is a major concern. Self-assembled monolayers (SAMs) built up interface dipoles on metal surfaces that can increase or lower the work function of the material. Therefore SAMs can be used as injection layers. The properties of solution-processed SAMs such as orientation and interface dipole are influenced by various factors like concentration of the molecule in solution, immersion time and purity of the solution or substrate.

Infrared-reflection-absorption-spectroscopy (IRRAS) is very sensitive to changes in the orientation of SAMs on metal surfaces, thus we performed IRRAS measurements on SAMs consisting of 1H,1H,2H,2H-perfluorinated decanethiol on evaporated gold substrates. Orientation, ordering and quality of the SAM were investigated under systematic variation of immersion time and concentration of the molecule in solution. Taking into account realistic printing conditions we also investigated very short immersion times and high concentrations as well as the impact of oxygen in solvent and substrate on the layer formation.

O 54.5 Wed 16:00 ZEU 260

**Towards fully printed organic light-emitting diodes: investigation of solution processed electron injection layers** — •Sebastian Stolz[1,4], Gerardo Hernandez-Sosa[1,4], Michael Scherer[2,4], Eric Mankel[3,4], Robert Lovrinčić[2,4], Janusz Schinke[2,4], Uli Lemmer[1,4], and Norman Mechau[1,4] — [1]Karlsruhe Institute of Technology, Light Technology Institute — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik — [3]Technische Universität Darmstadt, Materials Science Institute, Surface Science Division — [4]InnovationLab GmbH, Heidelberg

The fabrication of organic light-emitting diodes (OLEDs) by high throughput printing techniques requires the development of solution processable electron injection layers. Today, either alkali salts or low work-function alkaline earth metals are used as cathode layers in OLEDs. As these materials are highly reactive, they cannot be easily solution processed. In this work, we present blue fluorescent light-emitting diodes which use silver in combination with Polyethylenimine (PEI) and Polyethylenimine-ethoxylated (PEIE) as cathode layer. We demonstrate that both materials can be effectively used as electron injection layers in OLEDs and correlate the performance of the devices to the characteristics of the PEI(E) layers. Photoelectron spectroscopy is used to estimate the polymer thickness and the corresponding change in cathode work-function while the homogeneity of the layers is evaluated by AFM measurements. We show that OLEDs using PEI/PEIE and silver as cathode layer yield an improved performance and shelf lifetime compared to reference devices that use calcium, instead.

**15 min. break**

O 54.6 Wed 16:30 ZEU 260

**Micro-structured organic field effect transistor on commercial poly(urethane) resin as substrate and gate dielectric** — Jan

Hartel, Derck Schlettwein, and •Christopher Keil — Institute of Applied Physics, Laboratory of Materials Research, Justus-Liebig-University Giessen, Germany.

Dielectric layers of a commercial cross-linked poly (urethane) (PU) were prepared on a conductively coated film and served as gate dielectric and as substrate for the growth of an organic semiconductor film in an alternative approach to all-organic field effect transistors (OFET). A method was developed to process micro-structured electrodes on top of the PU dielectric layer which proved superior to the traditional lift-off-procedure. The influence of the aspect ratio of the electrodes within the organic transistor on a given dielectric layer will be discussed with respect to the calculation of the relative permittivity and the gate capacitance. A method is proposed to compensate short electrode effects which would otherwise lead to an underestimation of the gate capacitance and hence to a miscalculation of the OFET properties.

O 54.7 Wed 16:45 ZEU 260

**Time-resolved potentiometry of organic thin film transistors** — •Jan Murawski, Tobias Mönch, Moritz Philipp Hein, Peter Milde, and Lukas M. Eng — Technische Universität Dresden, Institut für Angewandte Photophysik

High speed application still poses a challenge for organic thin film transistors (OTFTs) due to their low charge carrier mobilities, high driving voltages, and low on/off-current ratios. Few investigations have been reported on the switching dynamics of OTFTs on the nanoscale, even fewer in the relevant temporal operation regime as required for high speed applications. Yet, such investigations are crucial for understanding the bottle-necks in OTFTs dynamic performance.

Here, we introduce time-resolved Kelvin probe force microscopy (tr-KPFM) to track the time evolution of surface potential wave fronts inside the channel of a pentacene-based bottom-gate coplanar OTFT. The relevant dynamical evolution proceeds in the microsecond regime and is easily resolved by our quantitative tr-KPFM method. Comparing our experiment with simulations reveals the presence of Schottky barriers in the real device to be responsible not only for a reduced effective electric field across the transistor channel (and thus a reduced field mobility) but also for inducing a delayed re-injection of charge carriers at the electrode-semiconductor interface. Although the charge-carrier mobility would allow for faster switching, charging the Schottky barrier constitutes the bottle-neck to be overcome for higher working frequencies in OTFTs.

O 54.8 Wed 17:00 ZEU 260

**High-Mobility, Low-Voltage Organic TFTs based on Air-Stable DNTT Derivatives: Time-Dependent Improvement in Contact Resistance and Dynamic Performance** — •Ulrike Kraft[1,3], Ute Zschieschang[1], Kazuo Takimiya[2], Edwin Weber[3], and Hagen Klauk[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]RIKEN Advanced Science Institute, Wako, Japan — [3]Technical University Bergakademie Freiberg, Germany

The organic semiconductor dinaphtothienothiophene and its derivatives C10-DNTT and diphenyl-DNTT provide larger carrier mobilities and better air stability than, e.g., pentacene. We present a detailed comparison of the thin-film morphology, static and dynamic performance and stability of low-voltage (3 V) thin film transistors based on vacuum-deposited films. Freshly fabricated TFTs (channel length: 100 um) have hole mobilities ranging from 3 cm2/Vs (DNTT) to 5 cm2/Vs (diphenyl-DNTT), with on/off ratios of 10ˆ7.

During the first few hours after fabrication, the effective mobility of short-channel TFTs (L=1 um) increases by about 20-30%, due to an improvement in the contact resistance (measured with TLM). The dependence of this effect on the exposure to different gas atmospheres, humidity and to light was investigated. To study the impact on the dynamic performance of the TFTs, we fabricated unipolar ring oscillators on flexible PEN substrates. The stage delay of DNTT TFTs (L=1 um) measured at 3 V drops from 920 to 410 ns during the first 4 days of exposure to ambient air, which is the shortest delay reported for flexible organic TFTs at supply voltages <10 V.

O 54.9 Wed 17:15 ZEU 260

**Continuously tunable organic semiconductor distributed Feedback (DFB) lasers as an example for optical components built from shape-memory polymers** — •Senta Schauer[1], Xin Liu[2], Tobias Meier[1], Marc Schneider[1], Matthias Worgull[1], Uli Lemmer[1,2], and Hendrik Hölscher[1] — [1]Karlsruhe Institute of Technology, Institute of Microstructure Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Karlsruhe Institute of Technology, Light Technology Institute, Engesserstraße 13, 76131 Karlsruhe, Germany

Phase gratings are important tools for many applications in optics and photonics, e.g., they serve as resonators in DFB-lasers. We manufactured Bragg gratings from a shape-memory polymer (SMP) to tune their period over a wide range without any mechanical components. SMPs can remember a predefined shape and recover to it even after strong deformations, if they are triggered by a stimulus. We used the polyurethane Tecoflex(R), which is a thermally triggered SMP, to fabricate nanostructured gratings via hot embossing. After stretching, these gratings feature an increased period which shrinks back to its original length after the activation of the recovery process. In order to demonstrate the practical applicability of these gratings as useful components for photonics, we successfully fabricated continuously tunable DFB-lasers based on SMP grating substrates with Alq3:DCM serving as active material. By changing the grating period via the shape-memory effect, the emitted wavelength of the laser changes likewise. So far we demonstrated shifts of the emission spectrum by 30nm.

O 54.10 Wed 17:30 ZEU 260

**Optical studies of excitonic precursor spin species under magnetic resonance in organic light emitting diodes.** — •Hermann Kraus, Sebastian Bange, and John M. Lupton — Universität Regensburg, 93040 Regensburg, Deutschland

Large magnetoresistance effects e.g. due to spin-dependent recombination rates are well-known for OLEDs [C. Boehme et al., Nat. Nano 8, 612 (2013)], although models are still under debate given that they remain hard to verify from a measurement of integrated current and luminance values[J. M. Lupton et al., Nature Mat. 7, 598 (2008)]. Spin resonance of paramagnetic species enables direct manipulation of carrier and excitonic precursor spins, providing a wealth of new insight into dynamic spin properties. Previous work on electrical or optical detection of spin manipulation [W. J. Baker et al., Nature Comm. 3, 898 (2012); W. J. Baker et al., Phys. Rev. B 84, 165205 (2011)] misses out on the opportunity to directly observe the presence of triplet exciton species that are at the heart of spin-dependent recombination models. A few polymeric and small-molecular compounds are now known to exhibit reasonable triplet emission without modification of the polaron pair and exciton dynamics by strong spin-orbit interaction [D. Chaudhuri et al., Angew. Chem. Int. Ed. DOI 10.1002/anie.201307601(2013); J. M. Lupton et al., Phys. Rev. Lett. 89 167401(2002)]. Those materials are ideal candidates to directly track spin singlet and triplet excitonic species in organic light-emitting diodes under conditions of magnetic resonance, by comparing the fluorescence (singlet) to phosphorescence (triplet) intensity.

O 54.11 Wed 17:45 ZEU 260

***Ab-initio* quantum dynamics simulation of photo-induced molecular switching: Azobenzene on coinage metals** — •Reinhard J. Maurer and Karsten Reuter — Department Chemie, Technische Universität München, Germany

The constant pursuit towards further miniaturization of electronic devices slowly reaches the point where individual molecules may serve as the main functional units. Unfortunately, more often than not, an inherent molecular function is quenched by overly strong coupling to the environment; a permanent danger, specifically in the case of metal surface adsorption. Nevertheless, metal surface adsorption may also introduce new functionality, such as in the case of photo-induced molecular switching of tetra-*tert*-butyl-functionalized Azobenzene (TBA) on Au(111). In this work we attempt a full *ab-initio* description of the explicit nuclear and electronic dynamics to analyze a novel substrate-mediated process that was suggested for this system [1]. The immense system size and a continuum of electronic states demand an effective modelling approach explicitly accounting only for the most important degrees of freedom. Employing an efficient density-functional theory based $\Delta$SCF approach [2] we construct and analyze the involved excited-state potential energy surfaces (PESs), and establish a mixed-quantum classical dynamics simulation. A particular focus is the effect of the image-charge induced changes on the excited-state PESs and the excited-state lifetime- and temperature-dependence of the quantum yield. [1] Wolf, Tegeder, Surf. Sci. **603**, 1506–1517 (2009); [2] Maurer, Reuter, J. Chem. Phys. **139**, 014708 (2013)

O 54.12 Wed 18:00 ZEU 260

**Reversible switching and light-induced structural changes in spin-coated thin films of Azobenzene-polymers** —

•Christopher Weber[1], Tobias Liebig[1], David Bléger[2], Stefan Hecht[2], Jürgen Rabe[1], and Stefan Kowarik[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik — [2]Humboldt-Universität zu Berlin, Institut für Chemie

Functionalized surfaces with molecules whose conformation can be reversibly switched between two isomeric forms by light are relevant for future devices -e.g. for switching adaptive materials, storing two states in memory applications, and switching current in molecular electronics. Here we use grazing incidence x-ray diffraction (GIXD), atomic force microscopy (AFM) and differential reflectance spectroscopy (DRS) to study light-induced structural changes in spin-coated thin films of Azobenzene-polymers with Alkyl side-chains. In solution, the individual Azobenzene-polymer shrinks upon UV-irradiation. Submonolayers of Azobenzene-polymers on Silicon oxide are still switchable with high efficiency, but do not show the same shrinking behavior, as suggested by AFM measurements before and after UV-illumination. Increasing the thickness to multilayers drastically changes the switching behavior, because of strong sterical hindrance. Interestingly, GIXD shows that the in-plane Bragg peaks corresponding to the coherent ordering of the Alkyl side-chains disappear when the sample is illuminated with UV-light and partially reappear after a few minutes in the dark, showing that switching is still possible in the crystalline state albeit with slower kinetics.

## O 55: Focussed Session: Towards a Quantitative Understanding of Complex Adsorption Structures: Surface Science goes Organic I

Substantial effort has been devoted within the past few years to develop new experimental and theoretical techniques capable of quantitatively describing the interface between complex molecules and metal surfaces. This includes the determination of precise adsorption structures at sub-Angstrom level and adsorption energies with chemical accuracy, the detailed investigation of interaction potentials, and the unraveling of atomistic bonding mechanisms. This symposium will highlight corresponding studies and discuss current frontiers.

Organizers: Karsten Reuter (TU München), Stefan Tautz (FZ Jülich)

Time: Wednesday 16:00–19:00 Location: TRE Phy

**Topical Talk** O 55.1 Wed 16:00 TRE Phy

**Trends in the energies and entropies of adsorbates on single-crystal surfaces** — •Charles Campbell — University of Washington, Seattle, WA, USA

Experimental measurements of the enthalpies and entropies of adsorbed molecules, atoms and molecular fragments on well-defined metal and oxide surfaces will be reviewed. Trends are revealed that show how adsorption energies and adsorbate entropies vary with the molecular structure and the nature of the surface. These results will be discussed in light of relevant theoretical predictions.

O 55.2 Wed 16:30 TRE Phy

**Benzene and Its Derivatives Adsorbed on Metal Surfaces: A Bag Full of Surprises** — •Wei Liu, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

The study of molecule/metal interfaces is important for fundamental and applied surface science, and the electronic properties of these interfaces can be tuned by controlling their geometries. In this regard, a particular challenge for electronic structure theory is to reliably model the structure and stability of such hybrid interfaces. Here, we demonstrate that our recently developed DFT+vdW$^{surf}$ method [1] is able to describe 25 systems [*e.g.*, benzene/Au(111), benzene/Pt(111), naphthalene/Pt(111), thiophene/Ag(111), DIP/Ag(111), and PTCDA/Au(111)] with an accuracy of 0.1 Å in adsorption heights and 0.1 eV in binding energies with respect to reliable experimental data. In addition, our DFT+vdW$^{surf}$ calculations lead to a few peculiar findings: (1) The vdW energy can contribute more to the binding of covalently bonded systems than it does in physisorbed interfaces [2,3]; (2) the binding energies of similar molecules can be identical, despite significantly different adsorption heights; (3) the physically bound (precursor) state for aromatics on Pt(111) can be prominently stabilized and long-lived, making it potentially useful in molecular switches [4].

[1] Ruiz, *et al.*, PRL (2012). [2] Liu, *et al.*, PRB (2012). [3] Liu, *et al.*, NJP (2013). [4] Liu, *et al.*, Nat. Commun. (2013).

O 55.3 Wed 16:45 TRE Phy

**Electronic Properties of Surfaces and Interfaces with Self-Consistent van der Waals Density Functional** — •Nicola Ferri[1], Robert A. Distasio Jr.[2], Roberto Car[2], Alexandre Tkatchenko[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Princeton University, Princeton, NJ, USA

The long-range van der Waals (vdW) energy is a tiny part (0.001%) of the total energy, hence it is typically assumed to have a minor influence on the electronic properties. Here, we address this question through a fully self-consistent (SC) implementation of the long-range Tkatchenko-Scheffler (TS) density functional [1]. The effects of TS-vdW$^{SC}$ on electron density *differences* for atomic and molecular dimers are compared with correlated densities obtained from "gold standard" coupled-cluster quantum-chemical calculations finding a qualitatively and quantitatively accordance. In agreement with previous work [2], we find a very small overall contribution from self-consistency in the structure and stability of vdW-bound molecular complexes. However, TS-vdW$^{SC}$ (coupled with PBE functional) significantly affects electronic properties of coinage metal (111) surfaces, leading to an increase of up to 0.3 eV in the workfunction in agreement with experiments. Furthermore, vdW interactions visibly influence workfunctions in hybrid organic/metal interfaces, changing Pauli push-back and charge transfer contributions. [1] A. Tkatchenko and M. Scheffler, PRL (2009). [2] T. Thonhauser *et al.*, PRB (2007).

O 55.4 Wed 17:00 TRE Phy

**XPS and TPD of small molecules adsorbed on metalloporphyrins** — •Matthias Franke, Michael Röckert, Quratulain Tariq, Ole Lytken, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II

We are using a surface science approach to study the binding of small molecules to porphyrin metal centers. These interactions are widely encountered in nature, but also provide the basis for many kinds of chemical sensors [1]. Despite the number of theoretical studies on this topic, the results still remain inconsistent [2] and need further experimental data.

We have been adsorbing O2, CO and NO on multilayers of cobalt(II)-tetraphenylporphyrin. Changes in the chemical environment of the metal center were investigated with X-ray Photoelectron Spectroscopy (XPS), while Temperature Programmed Desorption (TPD) was used to measure the strength of the chemical bond between the metal centers and the adsorbed molecules. NO was found to adsorb strongly, with a desorption peak above room temperature, whereas O2 and CO both adsorb much weaker and desorb already below 150 K.

[1] Di Natale, C; Monti, D.; Paolesse, R.; materials today, 2010, 13, 7-8

[2] Shubina, E. T.; advances in inorganic chemistry, 2010, 62, 279

**Topical Talk** O 55.5 Wed 17:15 TRE Phy

**Surface crystallography of organic layers** — •Georg Held — Department of Chemistry, University of Reading, UK — Diamond Light Source, Harwell, UK

In supramolecular structures of organic molecules on surfaces chemical bonds are formed at different levels, from covalent to Van der

Waals. Their interplay determines, both the surface geometry and the electronic structure of these overlayers and, hence, detailed structural characterisation can reveal important information about the balance of the interactions involved. Many organic layers have been well characterized at the molecular level, mostly using scanning probe microscopy and/or spectroscopic methods, but experimental crystallographic information about inter-atomic bonds (intra-molecular, inter-molecular and molecule-substrate) is rare. LEED-IV structural analysis, despite being one of the most powerful techniques for surface crystallography in general, is still facing a number of problems, when applied to organic layers. Current limitations are imposed by the available computer power for large unit cells but also by the size and quality of the experimental data set. We will discuss strategies for improving the data set and modifications to the standard analysis methods that are necessary to make full use of these improvements. The second part of the talk will concentrate on structures of organic layers, such as amino acids on Cu{110}, which have been determined by LEED, and discuss the implications in terms of chemical bond formation and molecular recognition at surfaces.

O 55.6 Wed 17:45 TRE Phy

**High-precision LEED measurements of organic monolayers** — •Falko Sojka, Julia Peuker, Tobias Huempfner, Matthias Meissner, Roman Forker, and Torsten Fritz — Friedrich Schiller University Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany

Low energy electron diffraction (LEED) on epitaxial layers is a powerful tool to examine long-range ordering at the interface. Due to limitations like distortion of the LEED images, often additional efforts have to be made in order to derive precise epitaxial relations.[1, 2]

Due to our investigations of compensating geometric distortions and other systematic errors in LEED measurements we are able to perform high-precision determination of epitaxial growth and lattice constants. Therefore we analyzed diverse systems of organic monolayers on different substrates using e.g. coronene, hexa-peri-hexabenzocoronene (HBC), and quaterrylene (QT). Our results are partially in contrast to the literature. In our contribution we will also discuss results on organic heterostructures formed from two layers of dissimilar molecules.

In our case we are using two Double-MCP-LEED devices from Omicron and from OCI. These studies are supported by other methods like low temperature scanning tunneling microscopy (LT-STM) and differential reflectance spectroscopy (DRS) [3].

[1] F. Sojka et al., *Rev. Sci. Instrum.* **84**, 015111 (2013).
[2] F. Sojka et al., *Ultramicroscopy* **133**, 35-40 (2013).
[3] R. Forker et al., *Annu. Rep. Prog. Chem., Sect. C: Phys. Chem.* **108**, 34-68 (2012).

O 55.7 Wed 18:00 TRE Phy

**Photoelectron diffraction and the organic / inorganic interface** — •David A Duncan[1], Dagmar Kreikemeyer Lorenzo[2], Werner Unterberger[2], Francesco Allegretti[1], Johannes V Barth[1], and D Phil Woodruff[3] — [1]Technische Universität München — [2]Fritz-Haber Institut, Berlin — [3]University of Warwick, UK

While, there is a growing interest into investigations of biologically-related molecules on surfaces, motivated in part by issues concerned with bio-compatibility and biochemical sensors, very few studies involve quantitative determination of the local adsorption geometries. The technique of scanned-energy mode photoelectron diffraction (PhD) is particularly well-suited to this problem as it allows not only elemental, but chemical state specific local adsorption sites to be determined. Specifically PhD has been utilised to study the building blocks of biological molecules, notably amino acids and nucleobases.

The local adsorption site of the functional groups within these biologically inspired molecules, follows mostly the same pattern as much simpler molecules containing the same groups, retaining mostly the same level of coordination with the substrate, and very similar bond lengths - despite increasing molecular complexity.

O 55.8 Wed 18:15 TRE Phy

**Adsorption height alignment at heteromolecular hybrid interfaces** — •Benjamin Stadtmüller, Sonja Schröder, Francois C. Bocquet, Caroline Henneke, Christoph Kleimann, Serguei Soubatch, Martin Willenbockel, F. Stefan Tautz, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany and Jülich Aachen Research Alliance (JARA-FIT)

The future success of organic electronic devices strongly depends on the ability to control the properties of the active organic materials and their interfaces. In this context the formation of the first organic layer adsorbing on a metal surface plays an important role, which in turn is dominated by the interplay between different interaction mechanisms between the molecules and with the surface.

Here, we report on a systematic investigation of metal-heteromolecular interfaces consisting of two different molecules, both in contact with a metal surface: PTCDA or NTCDA act as the charge accepting, CuPc or SnPc as the charge donating molecular species. We concentrate on structural properties like the adsorption heights, and their interplay with charge donation and acceptance. Most importantly, when comparing homo- and heteromolecular layers of these molecules, we have found a systematic trend of adsorption height adjustment between donor and acceptor molecules. This self alignment goes along with a substrate-mediated charge transfer from the donors to acceptors and a mutual enhancement of the respective characters of the molecules. We propose that this effect is of general validity for $\pi$-conjugated molecules adsorbing on noble metal surfaces.

O 55.9 Wed 18:30 TRE Phy

**Self-metalation of 2HTPP on Cu(111) studied with XSW: Influence of the central metal atom on the bonding distance** — Christoph Bürker[1], •Antoni Franco-Cañellas[1], Katharina Broch[1], Tien-Lin Lee[2], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — [2]Diamond Light Source, UK

Recently, the self-metalation reaction of 2H-tetraphenylporphyrin (2HTPP) on Cu(111) to copper(II)-tetraphenylporphyrin (CuTPP) induced by annealing to 500 K was reported [1]. We present a systematic X-ray standing wave (XSW) study of both molecules, performed at the Diamond Light Source, to investigate the influence of the central metal atom on the adsorption geometry. The measured small bonding distance of both molecules on Cu(111) indicates strong interaction with the substrate [2]. Comparison between the average bonding distance of the carbon atoms and nitrogen atoms reveal a distorted molecule, as the nitrogen atoms adsorb at lower bonding distances. The two chemically equivalent types of nitrogen atoms (iminic and aminic) of 2HTPP exhibit a distorted porphyrin ring. After the chemical reaction to CuTPP no change of the bonding distance of the carbon skeleton is seen, but the entire molecule becomes flattened. The results are compared to a similar scenario for metal-free phthalocyanine $H_2Pc$ and copper-phthalocyanine (CuPc) [3].

[1] J. Xiao et al., J. Phys. Chem C 116 (2012), 12275.
[2] G. Heimel et al., Nature Chem. 5 (2013) 187.
[3] A. Gerlach et al., Phys. Rev. B 71 (2005), 205425.

O 55.10 Wed 18:45 TRE Phy

**The complex polymorphism and thermodynamic behavior of a seemingly simple system: naphthalene on Cu(111)** — •Roman Forker[1], Julia Peuker[1], Matthias Meissner[1], Falko Sojka[1], Takahiro Ueba[2], Takashi Yamada[2], Toshiaki Munakata[2], and Torsten Fritz[1] — [1]Friedrich Schiller University, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan

Naphthalene, $C_{10}H_8$, is the smallest polycyclic aromatic hydrocarbon (PAH). Despite its rather simple, non-chiral chemical structure naphthalene is known to form three different commensurate phases in epitaxial films on Cu(111), including apparently chiral arrangements of molecules in one of them [J. Phys. Chem. C **114**, 13334 (2010)]. In an attempt to understand this polymorphism we performed temperature-dependent and surface coverage-dependent in situ low-energy electron diffraction (LEED) measurements revealing an unexpected and extraordinarily complex structural and thermodynamic behavior. At low coverage the molecules form a disordered gas-like phase which is a consequence of effectively repulsive intermolecular interactions. The chiral structure originates from a precursor that exhibits short-range order at intermediate coverage. This precursor undergoes a steady and reversible orientational shift upon variation of coverage or temperature which ultimately yields a long-range ordered stable epitaxial film, thereby resembling a liquid–solid phase transition. At higher coverage a competing point-on-line structure, which has not been reported before, is preferred to the commensurate chiral structure.

## O 56: Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale V

Time: Wednesday 16:00–19:15 Location: TRE Ma

**Topical Talk** O 56.1 Wed 16:00 TRE Ma

**Theory of nonlinear phononics for coherent light-control of solids** — •Antoine Georges[1,2,3], Alaska Subedi[2], and Andrea Cavalleri[4] — [1]College de France, Paris, France — [2]Ecole Polytechnique - CPHT, Palaiseau, France — [3]University of Geneva, DPMC, Switzerland — [4]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

The use of light to control the structural and electronic properties of solids is an area of great current interest. We present a microscopic theory [arXiv:1311.0544] for ultrafast control of solids with high-intensity Tera-Hertz frequency optical pulses. When resonant with selected infrared-active vibrations, these pulses transiently modify the crystal structure and lead to new collective electronic properties. The theory predicts the dynamical path taken by the crystal lattice using first-principles calculations of the energy surface and classical equations of motion, as well as symmetry considerations. Two classes of dynamics are identified. In the perturbative regime, displacements along the normal mode coordinate of symmetry-preserving Raman-active mode can be achieved by cubic anharmonicities. This validates the mechanism proposed by Först et al. [Nature Physics 7, 854 (2011)] and explains the light-induced insulator-to-metal transition of manganites reported experimentally by Rini et al. [Rini et al. Nature 449, 72 (2007)]. We also predict a new non-perturbative regime in which ultra-fast instabilities that break crystal symmetry can be induced.

O 56.2 Wed 16:30 TRE Ma

**DFT+Frontier Orbital U** — •Emine Kucukbenli and Nicola Marzari — Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH)

Piecewise linearity of the total energy with respect to occupations is not only a fundamental property that should be obeyed by any exact energy functional, but also a starting point to improve approximate functionals that are used in practical applications.

DFT+U enforces piecewise linearity on the Hubbard manifold [1], and it has been shown to greatly improve the accuracy of density-functional theory for transition-metal complexes, thanks to its correction of self-interaction errors [2]. However, it still performs poorly in complexes where significant covalency is present, and intersite corrections (so-called DFT+U+V) have been introduced to improve these challenging cases [3].

Here, we revisit piecewise linearity within the DFT+U and DFT+U+V correction schemes, and explore a novel approach where self-interaction corrections are applied directly to the frontier orbitals. We test this approach on model transition metal complexes, where highly accurate reference results can be established, and on small molecules with varying degrees of covalency.

References: [1] M. Coccoccioni and S. de Gironcoli, Phys. Rev. B 71, 35105 (2005). [2] H. J. Kulik, M. Cococcioni, D. A. Scherlis and N. Marzari, Phys. Rev. Lett. 97, 103001 (2006). [3] V. Leiria Campo Jr and M. Cococcioni, J. Phys. Cond. Matt. 22, 055602 (2010); H. J. Kulik and N. Marzari, J. Chem. Phys. 134, 094103 (2011).

O 56.3 Wed 16:45 TRE Ma

**Quasiparticle self-consistent *GW* method with spin-orbit coupling applied to Bi and HgTe** — •Christoph Friedrich, Irene Aguilera, Markus Betzinger, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present an implementation of the quasiparticle self-consistent (QS) *GW* method where the spin-orbit coupling (SOC) is fully taken into account in each iteration rather than being added *a posteriori.* The implementation is based on the FLAPW method. The SOC gives rise to spin off-diagonal blocks in the Green function $G^{\mathrm{SOC}}$ and the self-energy $\Sigma^{\mathrm{SOC}} = iG^{\mathrm{SOC}}W^{\mathrm{SOC}}$. We applied the QS$G^{\mathrm{SOC}}W^{\mathrm{SOC}}$ method to the semimetal Bi, which presents in experiment small electron and hole pockets and a tiny band gap (11-15 meV) at the L point, all of them largely overestimated by LDA (e.g., the gap is 86 meV). The QS$G^{\mathrm{SOC}}W^{\mathrm{SOC}}$ approach predicts a value of the band gap of 8 meV and electron and hole pockets in very good agreement with experiment. The *a posteriori* treatment of the SOC (QS*GW*+SOC), on the other hand, yields an unphysical result for Bi, predicting it to be a topological insulator with a very large gap at L (260 meV) instead of a trivial semimetal. Similarly, for HgTe, QS*GW*+SOC reorders the bands in a wrong way and opens a gap at the $\Gamma$ point in disagreement with experiment. In contrast, the QS$G^{\mathrm{SOC}}W^{\mathrm{SOC}}$ approach yields a qualitatively and quantitatively correct description of the electronic band structure. We acknowledge support from the Helmholtz Association through the Virtual Institute for Topological Insulators (VITI).

O 56.4 Wed 17:00 TRE Ma

**Studies of semiconducting pyrite and marcasite compounds using many-body perturbation theory in the *GW* approximation** — •Timo Schena, Gustav Bihlmayer, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Germany

FeS$_2$ pyrite and marcasite have recently gained renewed interest as materials for photovoltaic applications, due to their large optical absorption and abundance. Therefore, a reliable description of the fundamental band gap of these compounds within first-principles calculations is desirable. However, common density functional theory (DFT) often suffers from an underestimation of band gaps. This calls for beyond-DFT methods, *e.g.*, the *GW* approximation, which is known to yield gaps in much better agreement with experiment. Although this is widely accepted for “simple” semiconductors, the situation is not well understood for more complicated cases, where the band edges differ in atomic and orbital character. In fact, we observe an uncommon band gap reduction in FeS$_2$ when applying single-shot *GW* on top of DFT, which might be problematic for photovoltaic applications [1]. In this work, we investigate the effects of the *GW* approximation on a couple of pyrite and marcasite compounds, employing the FLAPW code `FLEUR` and the *GW* code `SPEX` (www.flapw.de). In addition to single-shot *GW*, we also compare to the results of the recently implemented quasi-particle self-consistent *GW* approximation. We gratefully acknowledge funding from BMBF of the NADNuM project 03SF0402A.

[1] T. Schena *et al.* Physical Review B (accepted 2013)

**15 min. break**

O 56.5 Wed 17:30 TRE Ma

**Probing d-band Quantum Well States in Palladium Nanofilms** — •Srijan Kumar Saha[1], Sujit Manna[1], Marek Przybylski[1,2], Valeri Stepanyuk[1], and Jurgen Kirschener[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, 30-059 Kraków, Poland — [3]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

We present the results of our new study which probes the d-bands quantum well (QW) states in Pd nanofilms grown on Cu(001) using first-principles density functional theory (DFT) calculations combined with scanning tunneling spectroscopy (STS) experiments. This study reveals that QW states occur in the overlayer films of Pd over a strikingly large film thickness (up to 17 monolayers) and in a large binding energy range (from 0.1 to 3.0 eV below Fermi level), thanks to its distinct and broad 4d-bands. The orbital characters of these states are unambiguously identified by our DFT calculations. Calculations also demonstrate oscillatory multilayer relaxations and d-derived quantum size oscillations in Pd films. The pseudomorphic growth, well-defined interface, and spatially resolved STS allows us to probe individual occupied QW states and extract the accurate dispersion of the ($\Delta_5$-like) d electronic band, as these states are laterally highly localized and give rise to distinct and sharp feature in the tunneling spectra.

O 56.6 Wed 17:45 TRE Ma

**Implementation and analysis of a plane wave and real space pseudopotential method including an efficient spin-orbit coupling treatment tailored to calculate the electronic structure of large-scale semiconductor nanostructures** — •Frank Zirkelbach, Pierre-Yves Prodhomme, Jerome Jackson, and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

The implementation of the *large-scale atomic effective pseudopoten-*

*tial program* to solve the Schrödinger equation of an electronic system is discussed. *Atomic effective pseudopotentials* that are derived from screened local effective crystal potentials of self-consistent density functional theory (DFT) calculations are utilized, which ensure an accurate treatment at reduced computational costs. The capability of describing relevant electronic eigenstates of a quantum dot structure consisting of hundred thousand atoms at an atomistic *ab initio* level comparable to DFT is demonstrated. The possibility to represent the wavefunction and to evaluate parts of the Hamiltonian either in a plane wave or real space basis allows for a coherent analysis of various different approaches. In the fully real space treatment, linear scaling with respect to the system size is achieved. The convergence behavior of the different methods and utilized approximations is shown. Furthermore, an efficient spin-orbit treatment different to previously existing implementations within the pseudopotential formalism is outlined. The accuracy of the method is demonstrated via direct comparison to standard DFT codes.

O 56.7 Wed 18:00 TRE Ma

**Strong Parallelization of Real-Space DFT Calculations** — •Andrea Nobile[1,2], Paul Baumeister[1,2], Daniel Wortmann[1], and Stefan Blügel[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungzentrum Jülich and JARA, 52425 Jülich, Germany — [2]Jülich Supercomputing Center, Forschungzentrum Jülich, 52425 Jülich, Germany

The rapid change in modern supercomputing architectures poses a challenge to well established DFT codes. In particular, the increase in raw floating point power obtained through parallelism at different levels is not easily exploitable by using the traditional direct diagonalization methods. We will present our new real-space Projector Augmented Wave (PAW) implementation. The real-space representation of the wave functions, densities and potentials, enables the usage of very flexible boundary conditions and naturally adapts to massively parallel architectures. Parallelism can be exploited in the form of domain decomposition of the three dimensional grid, k-point sampling and bands. The kinetic energy operator, realized as a finite difference stencil, is localized. As a consequence the real-space representation of the Hamiltonian is sparse. This limits the amount of necessary communications and allows an application of the operator to a trial vector in order(N) operations. We will present results about the efficiency of the most numerical intensive parts of the code and we will compare the accuracy of the calculations for reference systems with other established DFT methods.

O 56.8 Wed 18:15 TRE Ma

**Rare Earth Metals in Density-Functional Theory** — •Marco Casadei[1], Xinguo Ren[2], Patrick Rinke[1], Angel Rubio[1,3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Technology, Hefei, China — [3]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

The presence of $f$ electrons in the rare earths and their interaction with the $s$ and $p$ electrons give rise to several physical phenomena. One prominent example is the isostructural $\alpha$-$\gamma$ phase transition in cerium (Ce). We have shown that density-functional theory (DFT) captures the volume collapse associated with the transition, but only if advanced functionals such as exact exchange plus correlation in the random-phase approximation (EX+cRPA) are used [1]. The volume collapse is understood in terms of a *localization/delocalization* of the $f$ electrons. We then addressed the question: *is the isostructural volume collapse in cerium unique*? By applying DFT, we studied lanthanum (La), praseodymium (Pr) and neodymium (Nd), which undergo several structural changes with pressure. We find that the transitions are already captured at a lower level of DFT (i.e. with (semi)-local functionals) and therefore conclude that $f$-electrons are not the driving force in this case. Within hybrid functionals, we find only one phase in lanthanum, which has no $f$-electrons, and more than one stable solution in the fcc crystal for Pr and Nd, as found for Ce. Unlike in Ce, however, there is always one solution that is the most stable, thus no isostructural volume collapse emerges in agreement with experiments. [1] M. Casadei *et al.*, Phys. Rev. Lett. **109**, 14642 (2012).

O 56.9 Wed 18:30 TRE Ma

**Electronic Structure and van der Waals Interactions in the Stability and Mobility of Point Defects in Semiconductors** — •Wang Gao and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Point defects are abundant in materials, and significantly affect the electronic, optical, and magnetic properties of solids. However, our understanding of the stability and mobility of point defects remains incomplete, despite decades of intensive work on the subject. In the framework of density-functional theory, Perdew-Burke-Ernzerhof functional underestimates formation energies by 0.7 eV due to the electron self-interaction error, while Heyd-Scuseria-Ernzerhof (HSE) functional yields formation energies in better agreement with high-level many-body methods, but often overestimates migration barriers by up to 0.4 eV.

Using HSE coupled with screened long-range vdW interactions [1], we demonstrate that HSE+vdW can simultaneously and accurately describe the formation energies and migration barriers of point defects. The inclusion of vdW interactions significantly changes the transition state geometries, and brings migration barrier into close agreement with experimental values for six different defects. For multiatom vacancies and point defects in heavier semiconductors, vdW interactions play an increasingly larger role [2].

[1] G. X. Zhang, *et al.*, PRL **107**, 245501 (2011); A. Tkatchenko, *et al.*, PRL **108**, 236402 (2012).

[2] W. Gao and A. Tkatchenko, PRL **111**, 045501 (2013).

O 56.10 Wed 18:45 TRE Ma

**Scaling Laws for van der Waals Interactions in Nanostructured Materials** — •Vivekanand Gobre and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Berlin

Accurate description of van der Waals (vdW) interactions is crucial for precise prediction of structure and stability of complex materials. VdW forces originate from interactions between fluctuating multipoles in matter and play a significant role in the self-assembly of nanostructured materials. Many models used to describe vdW interactions in nanomaterials are based on a simple pairwise-additive approximation, neglecting the strong electrodynamic response effects caused by long-range fluctuations in matter. We develop and utilize an efficient microscopic method [1,2] to demonstrate that vdW interactions in nanomaterials act at distances greater than typically assumed, and can be characterized by different scaling laws depending on the dimensionality and size of the system. Specifically, we study the behaviour of vdW interactions in single-layer and multilayer graphene, fullerenes of varying size, single-wall carbon nanotubes and graphene nanoribbons. As a function of nanostructure size, the van der Waals coefficients follow unusual trends for all of the considered systems, and deviate significantly from the conventionally employed pairwise-additive picture. We propose that the peculiar van der Waals interactions in nanostructured materials could be exploited to control their self-assembly. [1] Tkatchenko, DiStasio, Car, and Scheffler, PRL (2012); [2] Gobre, Tkatchenko, Nat. Commun. (2013).

O 56.11 Wed 19:00 TRE Ma

**2D nanopatterns of shape-persistent molecular polygons on HOPG** — •Stefan-S. Jester, Nina Schönfelder, Eva Sigmund, and Sigurd Höger — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Shape-persistent organic molecules with flexible side chains self-assemble at the solution/solid interface to form 2D nanoarchitectures. Scanning tunneling microscopy yields a submolecularly resolved insight into the adsorbate structures. A key issue is how the shape and symmetry of the backbones and their alkyl chain substitution pattern determine the shape and symmetry of the adsorbate patterns. Recently we focused on molecular polygons (triangles, squares, pentagons, and hexagons) with dithiophene corners and phenylene-alkynylene sides.[1] In my talk I will give insight into the relation between Archimedean surface patterns and supramolecular 2D adlayers. [1] S.-S. Jester, E. Sigmund, S. Höger *J. Am. Chem. Soc.* **2011**, *133*, 11062.

# O 57: Plasmonics and Nanooptics II

Time: Wednesday 16:00–19:00 Location: GER 38

O 57.1 Wed 16:00 GER 38

**Controlling the emission and movement of electrons on a nanoscale with few-cycle laser pulses** — •Jan Vogelsang, Björn Piglosiewicz, Slawa Schmidt, Doojae Park, Jörg Robin, Petra Gross, and Christoph Lienau — Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany

Due to their large field enhancement at the apex, metallic nanotapers became a workhorse for studying strong-field effects at solid state surfaces in the last years. Sufficiently high laser electric field strengths exceeding 10 V/nm can be reached without melting the atomic lattice, such that the ocillating laser field becomes comparable or even stronger than the Coulomb field binding the electrons to the nuclei. Since the field enhancement is limited to a volume as small as the taper apex itself, the electrons are influenced by the external electric field only on a potentially nanometersized volume on a time scale given by the laser pulse duration[1].

In this talk, recent results of our group on the direct control of electron emission and acceleration in strong electric fields are discussed[2]. In particular, the influence of the carrier-envelope-phase of the incident laser pulse on the photoelectron spectra will be covered[3].

[1] Herink, G. et al., Nature 483, 190-193 (2012).

[2] Park, D. J. et al., Phys. Rev. Lett. 109, 244803 (2012).

[3] Piglosiewicz, B. et al., Nature Photonics (2013) (doi:10.1038/nphoton.2013.288).

O 57.2 Wed 16:15 GER 38

**Field-driven THz-streaking of Nanotip Photoemission** — •Lara Wimmer, Georg Herink, Katharina E. Echternkamp, Daniel R. Solli, Sergey V Yalunin, and Claus Ropers — 4. Physical Institute - University of Göttingen, Göttingen, Germany

We present an ultrafast, nanoscale streaking scheme for field-driven photoemission control using single-cycle THz transients at the apex of a sharp gold tip [1]. The locally enhanced THz-field allows for a high-contrast enhancement or suppression of the near-infrared photoemission yield and a tuning of the photoelectron kinetic energy distribution, both in spectral position and width. This streaking scheme is unique to nanostructures because of the strong sub-wavelength confinement of the driving field [2]. In particular, the associated electron dynamics are governed by the momentary THz field at the instance of photoemission, rather than by a temporal integral, i.e. the vector potential, as in optical streaking experiments for attosecond spectroscopy [3]. Besides the fundamental interest in the characterization and control of electron trajectories within ultrashort optical near-fields, the approach carries significant potential for pulse compression in ultrafast electron diffraction and microscopy experiments.

[1] Wimmer et al., arXiv: 1307:2581 (2013)

[2] Herink et al., Nature 483, 190-193 (2012)

[3] Corkum, Krausz, Nature Physics 3, 381 - 387 (2007)

O 57.3 Wed 16:30 GER 38

**Reciprocity provides optimal coupling of a single emitter to a plasmonic nanoantenna** — •Thorsten Feichtner[1] and Bert Hecht[2] — [1]Max-Planck-Institute for the Science of Light, Erlangen, Germany — [2]Nano-Optics & Biophotonics Group, Department of Experimental Physics 5, Röntgen Research Center for Complex Material Research (RCCM), University of Würzburg, Germany

The emission rate of a point-like single emitter is defined by the local density of states at its position. The local density of states can be enhanced by means of plasmonic nano antennas. The resulting antenna-enhanced emitters are of major interest for many applications as e.g. near-field microscopy, single molecule detection and quantum optics. In the present work we will use reciprocity to derive a set of rules that affords optimal coupling between a single emitter and an optical antenna. After a validation for the analytically solvable case of a dipole in front of a sphere we apply these rules to a numerical study of the outstanding performance of split-ring-antennas [1]. Finally, based on the rules, we propose an optimal antenna design that optimizes both the coupling between single emitter and antenna as well as the coupling between antenna and far-field. The presented framework will also be useful to study surface enhanced spectroscopies, e.g. SERS.

O 57.4 Wed 16:45 GER 38

**Excitation and decay rate enhancements of purely magnetic dipole transitions in Er$^{3+}$ ions near gold nanoparticles** — •Deepu Kumar[1], Florian Hallermann[1], Alexander Sprafke[2], Dmitry Chigrin[1], and Gero von Plessen[1] — [1]RWTH Aachen University, 52056 Aachen, Germany — [2]$\mu$MD Group, Institute of Physics, Martin-Luther University Halle- Wittenberg, 06120 Halle, Germany

The excitation and emission rates of molecular and ionic emitters placed in the vicinity of metal nanoparticles (MNP), can be enhanced due to near-field effects of the particles. In general, magnetic-dipole (MD) transitions can be neglected as their rates are much lower than those of the electric dipole (ED) transitions. In rare-earth ions however, such as trivalent erbium (Er$^{3+}$), MD transitions contribute to some of the intra-4f transitions. For the overall transition rate enhancement in Er$^{3+}$ ions due to the MNP, the changes in both the ED and MD transition rates have to be taken into account. We calculate the effects of gold MNP on the excitation and decay rates of Er$^{3+}$ ions by using Mie theory and the finite element method (FEM). We compare the MNP-induced decay rate changes for purely electric and purely magnetic dipoles.

O 57.5 Wed 17:00 GER 38

**Probing the Local Density of States in Nano-Photonic Systems: a Numerical Discussion** — •Julia F. M. Werra[1], Andreas W. Schell[2], Philip Engel[2], Christian Wolff[3], Oliver Benson[2], and Kurt Busch[1,3] — [1]Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik & Photonik, D-12489 Berlin, Germany — [2]Humboldt-Universität zu Berlin, Institut für Physik, AG Nanooptik, D-12489 Berlin, Germany — [3]Max-Born-Institut, D-12489 Berlin, Germany

The photonic local density of states (LDOS) of a nano-photonic system quantifies the position dependent coupling between a point emitter and the electromagnetic modes. Thus, it is the key characteristic of such systems in the context of radiation dynamics; especially in the realm of plasmonics with its strong and highly confined field enhancements and in the nano-scale regime.

In this talk, we will present theoretical and numerical foundations to quantitatively calculate the LDOS of an arbitrary geometry within the discontinuous Galerkin time-domain method. As an example, we will focus on nitrogen-vacancy centers taking especially its specific energy level scheme into account and compare our computations to experimental data. This facilitates a detailed quantitative interpretation and understanding of quantum-emitter based fluorescence life-time imaging (see Ref. [1]).

[1] Andreas W. Schell, Philip Engel, Julia F. M. Werra, *et al.* (submitted).

O 57.6 Wed 17:15 GER 38

**Gold nanocone arrays as effective SERS substrates** — •Julia Fulmes, Christian Schäfer, Falk Anger, Dominik A. Gollmer, Andreas Horrer, Frank Schreiber, Dieter P. Kern, and Monika Fleischer — Institute for Applied Physics, University of Tübingen, Tübingen, Germany

Raman spectroscopy is a well-known technique for the detection and characterization of molecules. Spontaneous Raman scattering is typically very weak, but can be increased by many orders of magnitude by using surface enhanced Raman spectroscopy (SERS). We exploit arrays of plasmonic gold nanostructures (cones) with sharp tips of less than 10 nm in diameter [1] over large areas [2] for SERS. Due to the conical shape a strongly localized and enhanced electromagnetic field can be excited close to the cone apex. This allows for employing gold nanocone arrays for the detection of molecules with high sensitivity [3]. The successful application of gold nanocone arrays as SERS substrates for the analysis of different types of molecules, such as pentacene, 4-mercaptobenzoic acid and rubrene will be shown. By purposefully positioning molecules only on defined parts of the plasmonic nanostructures the Raman signal enhancement activity is investigated.

[1] M. Fleischer et al., Nanotechnology 21, 065301 (2010); [2] A. Horrer et al., Small, doi: 10.1002/smll.201300449 (2013); [3] J. Fulmes et al., in preparation.

O 57.7 Wed 17:30 GER 38

**Probing antenna enhanced near-fields with nanometer-scale**

**resolution** — •F. Neubrech[1,2], S. Beck[2,3], T. Glaser[2,3], M. Hentschel[1], H. Giessen[1] und A. Pucci[2,3,4] — [1]4th Physics Institute and Research Center SCoPE, Stuttgart, Germany — [2]Kirchhoff Institute for Physics, Heidelberg, Germany — [3]InnovationLab GmbH, Heidelberg, Germany — [4]Centre for Advanced Materials (CAM), Heidelberg, Germany

Nanoantenna-assisted surface enhanced infrared spectroscopy is a powerful tool to detect minute amounts of analytes. Based on the confined electromagnetic near fields of the resonantly excited metal nanoparticles, the molecular vibrations of the analytes are enhanced by orders of magnitudes. On the other hand, the enhanced vibrational signal strength of well-known probe molecules can also be utilized to obtain information on the near field enhancement with resolution only limited by the size of the probe molecule. Following this approach, we employed 4,4*-bis(N-carbazolyl)-1,1*-biphenyl (CBP) to measure the local near fields of resonantly excited nanoantennas with nanometer-scale resolution. Therefore, we stepwise evaporated CBP molecules under ultra-high vacuum conditions onto the metal nanostructures and acquired infrared spectra after each evaporation step. Besides the decreasing vibrational signal per nanometer, we observed a red-shift of the resonance frequency with increasing thickness. This shift originates from the polarizability change caused by the evaporated material. Furthermore, we performed finite different time domain simulations and found a good qualitative agreement with our experimental data.

O 57.8 Wed 17:45 GER 38

**Hybrid plasmonic oligomer for large-area low-cost nano-size gas sensors** — •Jun Zhao, Nikolai Strohfeldt, Andreas Tittl und Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Plasmonic gas sensing on the single nanoparticle level has drawn a lot of attention over the last years [1, 2]. We demonstrate direct contact gas sensing using hybrid complex plasmonic nanostructures, such as multilayer oligomers, where gold directly touches the palladium. Optimizing the sensing nanogeometry, we obtain spectral shifts of more than 10 nm depending on different H2 concentrations, which show a very high sensitivity of our system. We investigate the optical response of varied sandwich structure geometries, which can be used for different sensing applications. Our samples are fabricated by low-cost hole-mask colloidal nanolithography [3, 4] over areas of 1 cm2, and give very large absorption and scattering signals.

[1] N. Liu et al., Nature Mater. 2011, 10, 631. [2] A. Tittl et al., Nano Lett. 2013, 13, 1816. [3] S. Cataldo, J. Zhao et al., ACS Nano 2012, 6, 979. [4] J. Zhao et al., Adv. Mater. 2012, 24, 247.

O 57.9 Wed 18:00 GER 38

**Plasmonic sensing with functionalized hydrogels** — •Martin Mesch[1], Chunjie Zhang[2], Paul V. Braun[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, USA

Plasmonic structures have shown to be a sensitive and versatile tool for different sensing applications. As they inherently respond to anything that changes their dielectric environment, selectivity has to be added separately. In our approach, we utilize a thin layer of a functionalized hydrogel to embed our gold nanostructures. This layer is about 1 micrometer in thickness and consists of a cross-linked polymer network soaked with water.

One possible functionalization makes the hydrogel swell in the presence of glucose. This effect implies a change in the refractive index, and hence is in turn subject to detection via the plasmon resonance shift.

Experiments demonstrate that this system allows for detection of glucose concentrations in the physiological (low millimolar) range, as the hydrogel additionally amplifies the signal, compared to just the refractive index change introduced by glucose in the solution. Response times depend, besides the thickness of the layer, also on the composition of the polymer, and are currently in the order of a few minutes.

O 57.10 Wed 18:15 GER 38

**Metal plasmonic structures based on anodic aluminum oxide (AAO) and ultrathin alumina membranes (UTAM) for SERS and sensor applications** — •Wenxin Wang, Yan Zheng, Ranjith Vellacheri, Lin Cheng, Chengliang Wang, Huaping Zhao, Ahmed Al-Haddad, and Yong Lei — Ilmenau University of Technology, Institute of Physics & IMN MacroNano* (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau (Germany)

A variety of nano-structures can be fabricated by using anodic aluminum oxide template (AAO) and ultrathin alumina membranes (UTAM) through controlling the anodization voltage, time, and other parameters. With wet chemical etching process, pore size can be further adjusted. Additionally, dual even triple kind of pore sizes in a single template can be obtained if a third even fourth anodization process is applied, Here, we present Au, Ag , and Au-Ag composite nanostructured arrays prepared by the above-mentioned templates for enhanced Raman and Bio-sensing. The results show that these nanostructured arrays exhibit special absorption and senseing response to light, therefore implying the promising potencial of Au, Ag , andAu-Ag composite nanostructured arrays as suitable candidates for the applications of SERS substrate as well as bio-assay.

O 57.11 Wed 18:30 GER 38

**the applications of Au nanostructure arrays to sensors** — •Zhijie Wang, Dawei Cao, Liaoyong Wen, Yan Mi, Ranjith Vellacheri, and Yong Lei — Ilmenau University of Technology, Institute of Physics & IMN MacroNano* (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau

Noble nano-materials, particularly Au nanoparticles and nanowires, show an outstanding localized surface plasmon property associated with the enhanced surface electromagnetic field due to its localization in nano-scale. The surface plasmon resonance peaks and intensities of the Au nano-materials are tunable through the manipulation of the shape, the size and the surface modifications of the Au nanoparticles. In contrast to the conventional sensor applications of Au nanoparticles, just by dispersing them in the analyte solution to collect optical signal, herein, we fabricated Au nanowires and particles arrays on substrates. Through surface modifications by cysteine, the surface plasmon peaks of these Au nanostructures shifted obviously according to the different analytes. Possibility to design Au nano-sensors for collecting electronic signal from the reaction between the surface plasmons and analytes will be discussed.

O 57.12 Wed 18:45 GER 38

**Theoretical investigation of the emission statistics of a spaser** — •Michael Gegg[1,2], T. Sverre Theuerholz[1], Andreas Knorr[1], and Marten Richter[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Freie Universität Berlin, Berlin, Germany

Surface plasmons have recieved considerable attention over the past few years. Surface plasmons bypass the diffraction limit in conventional optics. Moreover they are bosonic quasiparticles, thus exhibiting the same rich quantum statistical phenomenology as photons and phonons.

We present a theoretical model for the interaction of an arbitrary number of identical quantum dots with a metal nanoparticle. The quantum dots act as a gain medium, inducing plasmons on the metal nanoparticle via dipole-dipole coupling [1]. This system was proposed as a candidate for a spaser [2] and it was employed to construct a nanosized laserlike device [3]. We analyse the plasmon statistics and its dependency on the number of quantum dots, dipole coupling and incoherent processes.

We find that the system reaches the spasing regime in all investigated cases for the limit of many quantum dots.

[1]T. Sverre Theuerholz, Alexander Carmele, Marten Richter and Andreas Knorr. *Phys. Rev. B*, 87, 2013 [2]M. I. Stockman. *Nature Photon.*, 2, 2008 [3]M. A. Noginov, G. Zhu, A. M. Belgrave, R. Bakker, V. M. Shalaev, E. E. Narimanov, S. Stout, E. Herz, T. Suteewong and U. Wiesner. *Nature*, 460, 2009

# O 58: Oxide and Insulator Surfaces II

Time: Wednesday 16:00–19:00 Location: PHY C 213

O 58.1 Wed 16:00 PHY C 213

**Oxygen activation on Mo-doped CaO films** — Yi Cui[1], •Niklas Nilius[1,2], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany — [2]Carl von Ossietzky Universität, Institut für Physik, D-26111 Oldenburg, Germany

Already trace amounts of aliovalent dopants can be sufficient to change the physical and chemical properties of oxide materials. Using low temperature STM, we have shown that Mo ions in a crystalline CaO film of 8 eV band gap act as charge donors and may provide up to three extra electrons to suitable adsorbates. The relevant species for charge exchange are Mo2+ ions sitting in Ca substitutional sites in near surface layers of the oxide.(1) Their charge state is probed and manipulated with the STM tip. The results were found to be in agreement with DFT calculations of the Mo 4d states split in the crystal field of the CaO lattice. Charge transfer from the Mo donors is identified both into metallic (Au) and molecular adsorbates (O2) bound to the surface.(2) In the latter case, formation of superoxo-species is revealed, characterized by a large affinity for dissociation. Additional means to modify electronic and optical properties of oxides via doping are envisioned.

1. Cui, Nilius, Freund, Prada, Giordano, Pacchioni, Phys. Rev. B 88 (2013) 205421.
2. Cui, Nilius, Shao, Baldowski, Sauer, Freund, Angew. Chem. Int. Ed. 52 (2013) 11385.

O 58.2 Wed 16:15 PHY C 213

**High chemical activity of a perovskite surface: Reaction of CO with $Sr_3Ru_2O_7$** — •Bernhard Stöger[1], Marcel Hieckel[1], Florian Mittendorfer[1], Zhiming Wang[1], Michael Schmid[1], David Fobes[3], Jin Peng[3], Raimund Podloucky[2], Zhiqiang Mao[3], Josef Redinger[1], and Ulrike Diebold[1] — [1]Institute of Applied Physics, Vienna University of Technology, Vienna, Austria — [2]Institute for Physical Chemistry, University of Vienna, Vienna, Austria — [3]Department of Physics and Engineering Physics, Tulane University, New Orleans, LA, USA

We focus our studies on $Sr_3Ru_2O_7$, which is the two-layer member of the ruthenate Ruddlesden-Popper series $Sr_{n+1}Ru_nO_{3n+1}$. In-situ cleaving of high-quality single crystals opens up the possibility to investigate a very well defined Sr-O surface layer by low-temperature Scanning Tunneling Microscopy. Exposing $Sr_3Ru_2O_7$ to CO at 78 K shows that CO adsorbs at regular surface sites above an apical surface O atom with a binding energy, $E_{\mathrm{ads}}$, of 0.6 eV. Above 100 K this physisorbed CO reacts by pushing out the surface O atom, forming a bent $CO_2$ molecule with its C atom bound to the Ru underneath. The resulting species is best described as chemisorbed metal carboxylate (Ru-COO). The low activation energy (0.29 eV) of the process and the high binding energy ($E_{\mathrm{ads}} = 2.17$ eV) of the resulting adsorbate confirm a strong reaction between CO and regular surface sites of $Sr_3Ru_2O_7$.

This work was supported by the Austrian Science Fund (FWF project F45).

O 58.3 Wed 16:30 PHY C 213

**Adsorption of water on rutile (110) – Ground and excited states** — •Jan Mitschker and Thorsten Klüner — Theoretical Chemistry, Carl von Ossietzky Universität Oldenburg, PO Box 2503, 26111 Oldenburg

The interaction of water with $TiO_2$ is of great importance for a variety of technical applications like self-cleaning surfaces. Water splitting on these surfaces may become a new route to hydrogen used as a fuel in the future. Despite this promising ability of $TiO_2$, a fundamental understanding of the interaction of water with rutile, especially after an electronic excitation with light is still missing.

Here, we present results for the water/$TiO_2$ system. We use the embedded cluster approach in order to calculate potential energy surfaces for this system. The rutile surface is modelled by a $Ti_9O_18Mg_7^{14+}$ cluster embedded in about 4500 point charges to account for the long-ranging Coulomb interaction. This model has been used for the CO photodesorption successfully. [1] The potential energy surfaces are calculated on a post Hartree-Fock level of theory. This important for dissociation and excitation energies. We intend to perform a quantum dynamical treatment of the dissociation process within the framework of a stochastic wave-packet model.

In this contribution, we present results for the potential energy surfaces of the electronic ground and a selected excited state.

[1] M. Mehring, T. Klüner, *Chem. Phys. Lett.* 2011, *513*, 212.

O 58.4 Wed 16:45 PHY C 213

**Three-dimensional study of the photodesorption of CO on rutile(110)** — •Hendrik Spieker and Thorsten Klüner — Theoretical Chemistry, Carl von Ossietzky Universität Oldenburg, PO Box 2503, 26111 Oldenburg

Due to its high photocatalytic activity, titanium dioxide is already of interest for a manifold of applications. However, the fundamental mechanisms of the underlying surface photochemistry are not yet completely understood. In this study, the desorption of CO on rutile(100) is studied in terms of a model system. Making use of an embedded cluster approach to simulate the rutile(110)-surface, BSSE-corrected three-dimensional potential energy surfaces for the ground state and relevant excited states of the CO molecule are calculated on a post Hartree-Fock level of theory. The latter serve as potentials for three-dimensional quantum dynamical studies, which unveil a quantum state resolved and up to this point completely unknown desorption mechanism for the CO molecule in consequence of a vertical laser excitation.

O 58.5 Wed 17:00 PHY C 213

**LEED-I(V) structure analysis of the physisorption system CO p(2×1)/NaCl(100)** — •Jochen Vogt and Birgit Vogt — Chemisches Institut der Uni Magdeburg, Magdeburg, Germany

The system CO/NaCl(100) is one of the model systems of physisorption. Although intensively studied both experimentally and theoretically (see e. g. [1-3]), an experimental structure analysis of its low temperature p(2×1) phase has been missing so far. Using the MCP-LEED technique, we have recorded diffraction peak intensities of the saturated p(2×1) phase as a function of electron energy at a temperature of 21 K. The data were the basis of a full dynamical LEED-I(V) analysis. Our structure model, involving two inequivalent molecules related by the observed glide-plane symmetry, contains only 5 molecular structure parameters, and the rumpling of the substrate surface. According to our results, the carbon end of CO is located 2.58±0.08Å over $Na^+$, laterally shifted 0.4±0.1Å towards the neighbor chlorine. The molecular tilt angle is 28±5 degrees with respect to the surface normal, in satisfactory agreement with infrared spectroscopic results [2]. In a structure model with oxygen pointing towards the surface, the Pendry R-factor worsens from 0.22 to 0.25. [1] D. Schmicker, J. P. Toennies, R. Vollmer, H. Weiss, J. Chem. Phys. 95 (1991), 9412 [2] J. Heidberg, E. Kampshoff, M. Suhren, J. Chem. Phys. 95 (1991), 9408 [3] M.-N. Carre et al., Surf. Sci. 347 (1996), 128

O 58.6 Wed 17:15 PHY C 213

**IRRAS on Metal Oxide Single Crystals: First Experiments on ZnO(10-10)** — Maria Buchholz, •Fabian Bebensee, Peter G. Weidler, Alexei Nefedov, and Christof Wöll — Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany

Due to the low reflectivity in the infrared regime of oxides, Infrared Reflection Absorption Spectroscopy (IRRAS) studies on molecules adsorbed on metal oxide single crystals have remained elusive until recently. Furthermore, the fact that the classic surface selection rule for IRRAS does not apply on dielectrics renders the data analysis in such experiments rather difficult. Here, we present the first experiments on adsorption of molecules on zinc oxide (ZnO) single crystals. We demonstrate the great potential this technique offers for the study of such adsorbate systems emerging from consideration of all three components of the incident polarized light separately [1]. We find that carbon dioxide adsorption results in a tridentate (surface) carbonate [2] oriented along the [0001] direction. Comparing these data recorded on single crystalline ZnO to nanoparticles provides useful insights into the role of defects for the surface chemistry of powder particles.

[1] M. Buchholz, P. G. Weidler, F. Bebensee and C. Wöll, Physical Chemistry Chemical Physics, 2013, DOI:10.1039/C1033CP54643H.

[2] Y. Wang, R. Kováčik, B. Meyer, K. Kotsis, D. Stodt et al., Angewandte Chemie International Edition, 2007, 46, 5624-5627.

O 58.7 Wed 17:30 PHY C 213

**Stability and Metastability of Clusters in a Reactive Atmosphere: Theoretical Evidence for Unexpected Stoichiometries of $\mathbf{Mg}_M\mathbf{O}_x$** — •Saswata Bhattacharya, Sergey V. Levchenko, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

We study the (meta)stability of metal-oxide clusters in a reactive atmosphere at thermodynamic equilibrium, using free metal (Mg) clusters in an oxygen atmosphere as a model system. The low energy minimum structures of a large set of $\mathrm{Mg}_M\mathrm{O}_x$ clusters are generated via a massively parallel cascade genetic algorithm. The term "cascade" means a multi-step procedure with increasing accuracy and each next level uses information obtained at the immediate lower level. It starts with a (reactive) force field and goes up to density-functional theory (DFT) with hybrid functionals. The stable compositions are identified using *ab initio* atomistic thermodynamics. We find[1] that highly oxidised states are more stable at thermodynamic equilibrium when $M \leq 5$, while for bigger sizes ($6 \leq M \leq 15$) there is a competition between stoichiometric ($x = M$) and non-stoichiometric ($x > M$) clusters. The highly oxidised clusters ($x > M$) exhibit peculiar magnetic behaviour, suggesting the possibility of tuning magnetic properties by changing environmental ($T, p_{\mathrm{O}_2}$) conditions. Our studies are validated with the highest level currently achievable within DFT, i.e.; the renormalized second-order perturbation theory (rPT2).

[1] S. Bhattacharya, S. V. Levchenko, L. M. Ghiringhelli, M. Scheffler, *Phys. Rev. Lett.* **111**, 135501 (2013)

O 58.8 Wed 17:45 PHY C 213

**Fe adsorption on the hematite (0001) and magnetite (111) surface** — Tomasz Pabisiak and •Adam Kiejna — Institute of Experimental Physics, University of Wrocław, Wrocław, Poland

A detailed ab initio investigation of the structural, electronic and magnetic properties of Fe-atom adsorption on the hematite (0001) and magnetite (111) surfaces is presented. Spin-polarized density functional theory calculations are applied accounting for strong electron correlation effects by including a Hubbard-type on-site Coulomb repulsion (the DFT+U approach). For each oxide surface, the adsorption on two terminations has been studied: one terminated with iron and the other with oxygen. The binding sites and coordination geometry of Fe adatoms are identified. Different adatom coverages were considered. The Fe atoms bind strongly to the iron-oxide surfaces and induce large changes in their near surface geometry, and the electronic and magnetic properties. The binding of Fe is distinctly stronger at the O- than at the Fe-terminated surfaces of both oxides. The resulting adsorption energetics, structure and bonding are discussed based on the calculated local density of states and electron charge transfer. Comparison with the results for Au and Pd atoms adsorption [1,2] at these surfaces is also made.

This work was supported by the National Science Center (NCN), Poland (Grant No. 2012/07/B/ST3/03009).

[1] A. Kiejna, T. Ossowski, T. Pabisiak, Phys. Rev. B 85, 125414 (2012). [2] A. Kiejna, T. Pabisiak, J. Phys. Condens. Matt. 24, 095003 (2012).

O 58.9 Wed 18:00 PHY C 213

**Tuning the electronic structure of $\mathbf{Fe_3O_4}$ by adsorbates: A DFT+U investigation** — •Narasimham Mulakaluri[1] and Rossitza Pentcheva[2] — [1]Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany — [2]Dept. for Earth and Environmental Sciences, University of Munich,Germany

$\mathrm{Fe_3O_4}$ plays an important role in many technologically relevant catalytic reactions such as HT-WGS (high temperature water gas phase shift reaction). To tune the catalytic activity it is important to understand and selectively modify the surface electronic structure. Using density functional theory together with an on-site Coulomb repulsion term (GGA+$U$), we explore the progressive reduction of the $\mathrm{Fe_3O_4}$(001) surface by additional deposition of Fe [1] or hydrogen [2]. The thermodynamic stability of different terminations reveals that additional Fe atoms switch to surface octahedral sites instead of the bulk structure continuation at tetrahedral sites (A) on top of the B-termination (containing oxygen and octahderal iron). With increasing coverage an antiferromagnetic and strongly buckled FeO layer is formed on top of the $\mathrm{Fe_3O_4}$(001) surface. The deposition of Fe leads to a progressive reduction of Fe in the surface and subsurface layers to Fe2+ and thus allows control of the Fe2+/Fe3+ ratio and the redox activity at the $\mathrm{Fe_3O_4}$(001) surface. The enhancement of Fe2+ in the near surface region is also supported by XPS experiments [1]. Parallels to hydrogen and metal adsorption are also discussed.

[1] Z. Novotny, N. Mulakaluri *et.al*, Phys. Rev. B **87**, 195410 (2013).
[2] N. Mulakaluri, R. Pentcheva, J. Phys. Chem. C **116**, 16447 (2012).

O 58.10 Wed 18:15 PHY C 213

**Thin iron oxides films as support for metal nano-particles: a LEEM/PEEM study** — Francesca Genuzio, Alessandro Sala, •Thomas Schmidt, and Hans-Joachim Freund — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The wide interest in characterizing $\mathrm{Fe_3O_4}$ and $\alpha$-$\mathrm{Fe_2O_3}$, the two most common and stable iron oxide phases, arises from the variety of their technological applications, ranging from magnetic devices to heterogeneous catalysis. Their crystal structure, stoichiometry as well as their surface properties can be tuned by special preparation procedures. Moreover, in thin film systems the interaction with the substrate can strongly influence the chemical and electric properties. As model systems for catalysis, these two oxides are successfully used as supports for noble metal nano-particles. In some particular cases, the strong interaction between the nano-particle and the support (SMSI) can induce their encapsulation, affecting the activity of the system, as observed for Pt nano-particles supported on a $\mathrm{Fe_3O_4}$ film[1]. Here, we report on growth and stability of $\mathrm{Fe_3O_4}$ and $\alpha$-$\mathrm{Fe_2O_3}$ thin films on a Pt(111) substrate, as well as their interaction with Pt nano-particles. The combined LEEM/LEED and XPEEM investigations were carried out with the SMART, the aberration-corrected and energy-filtered LEEM/PEEM installed at BESSY II in Berlin. [1] Z.-H. Qin, M. Lewandowski, Y.-N. Sun, S. Shaikhutdinov, and H.-J. Freund, J. Phys. Chem. C 112, (2008), 10209-10213

O 58.11 Wed 18:30 PHY C 213

**Improving ceramic–polymer interface stability: Ab-initio study of benzoic acid on $\mathbf{TiO_2}$** — •Wolfgang Heckel and Stefan Müller — Hamburg University of Technology, Institute of Advanced Ceramics, Denickestr. 15, D-21073 Hamburg

In order to prepare functional hybrid composites with desired mechanical properties, the control of the interface stability is crucial. For a strong binding, carboxylic acids (CA) as a linker between ceramics and polymer are often used and extensively studied in the past. Current thermal desorption measurements [1] give rise to the assumption, that CA with an aromatic side chain can still improve the binding energy compared to CA with simple aliphatic ones.

We present a DFT analysis of benzoic acid on $\mathrm{TiO_2}$ rutile surfaces. To describe properly the attractive interaction of adsorbing molecules among each other, our results show clearly the requirement of applying an exchange correlation functional with van der Waals correction. The resulting binding energies increase up to about 0.18 eV per molecule compared to CA with aliphatic side chains.

Supported by DFG, SFB 986, project A4.

[1] A. Dreyer and G. Schneider, unpublished

O 58.12 Wed 18:45 PHY C 213

**Directed growth of functionalized triarylamines on KBr(001)** — Christian Steiner[1], Natalie Hammer[2], Ute Meinhardt[2], Bettina Gliemann[2], Milan Kivala[2], and •Sabine Maier[1] — [1]Department of Physics, University of Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Germany

The growth and imaging of well-ordered molecular self-assemblies is often challenging on bulk insulating surfaces owing to the low molecule-surface interaction. However, organic layers on insulating compared to metallic materials are more likely to be relevant for applications, e.g. in electronic devices such as organic field effect transistors. We investigated the self-assembly of triarylamine derivatives on an insulating KBr(001) surface using non-contact atomic force microscopy in ultra high vacuum at low temperature. By carefully balancing the molecule-surface interaction and molecule-molecule interaction using similar triarylamine building blocks but changing the side groups we can direct their self-assembly on KBr from linear structures to flat well-ordered networks. We found that hydrogen-bonding moieties with carboxylic and diaminotriazine side groups prefer to self-assemble in well-ordered films while halogen atoms as side groups support the growth of $\pi - \pi$ stacked linear structures with the molecules standing nearly upright on the surface.

## O 59: Metal Substrates I

Time: Wednesday 16:00–19:15 Location: WIL A317

O 59.1 Wed 16:00 WIL A317

**Growth morphology of thin films on the metallic and oxide surfaces** — •Aleksander Krupski — Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom.

In this work we briefly review recent investigations concerning growth morphology of thin metallic films on the $Mo(110)$ and the $Ni_3Al(111)$ surfaces, and $Fe$ and Copper Phthalocyanine ($C_{32}H_{16}N_8Cu$) on the $Al_2O_3/Ni_3Al(111)$ surface. Comparison of $Ag$, $Au$, $Sn$, and $Pb$ growth on the $Mo(110)$ surface has shown a number of similarities between these adsorption systems except surface alloy formation that has only observed in the case of $Sn$ and $Au$. In the $Pb/Mo(110)$ and $Pb/Ni_3Al(111)$ adsorption systems selective formation of uniform $Pb$ island heights during metal thin film growth has been observed and interpreted in terms of quantum size effects. Furthermore, our studies showed that $Al_2O_3$ on $Ni_3Al(111)$ exhibits a large superstructure in which the unit cell has a commensurate relation to the substrate lattice. In addition, Copper Phthalocyanine chemisorbed weakly onto an ultrathin $Al_2O_3$ film on $Ni_3Al(111)$ and showed a poor template effect of the $Al_2O_3/Ni_3Al(111)$ system. In the case of iron cluster growth on $Al_2O_3/Ni_3Al(111)$ the nucleation sites were independent of deposition temperature, yet cluster shape showed a dependence. In this system, $Fe$ clusters formed a regular hexagonal lattice on the $Al_2O_3/Ni_3Al(111)$.

O 59.2 Wed 16:15 WIL A317

**Annealing of oxidized aluminium alloy surfaces studied by PEEM combined with XPS** — •Lisa Rullik[1], Florian Bertram[1], Jonas Evertsson[1], Anders Mikkelsen[1], Yuran Niu[2], Alexei Zakharov[2], and Edvin Lundgren[1] — [1]Div. of Synchrotron Radiation Research, Lund University, Lund, Sweden — [2]MAX-lab, Lund University, Lund, Sweden

Aluminium alloys are used in a wide range of applications due to their high tensile strength in concomitance with low density. Additionally, aluminium alloys form a native passivating oxide layer, which leads to high corrosion and weathering resistance. In industrial manufacturing, aluminium alloys acquire their desired properties upon heating and welding.

Here, we present how annealing affects the surface layer composition of different aluminium alloys. Using MEM, PEEM and XPS we were able to follow the diffusion process of aluminium and its alloying elements from and towards the surface. For temperatures up to 300°C only slight changes of the surface composition can be observed in PEEM images and XPS spectra. At 400°C a significant diffusion of magnesium to the surface occurs.

O 59.3 Wed 16:30 WIL A317

**Growth of ultrathin Pb layers on the Ni3Al(111) surface studied by AES/LEED/STM/DFT** — •Katarzyna Miśków and Aleksander Krupski — Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom.

The morphology, atomic and electronic structure of ultrathin Pb layers deposited on the $Ni_3Al(111)$ face in ultrahigh vacuum at the substrate temperature, ranging from 200 K to 950 K, were investigated with the use of Auger electron spectroscopy (AES), low-energy electron diffraction (LEED), directional elastic peak electron spectroscopy (DEPES), scanning tunnelling microscopy (STM). Density functional theory calculations (DFT) with the use of CASTEP code were used to describe atomic and electronic structure of the $Pb/Ni_3Al(111)$ system. The analysis of AES and STM measurements indicate that two-dimensional growth of the first Pb monolayer wetting layer takes place. For T = 200 K, lead on the $Ni_3Al(111)$ grows layer-by-layer, while for T = 300 K flat three atomic-layer-high islands seem to grow after the completion of the first lead monolayer. Above 350 K, the Stranski-Krastanov growth mode is observed. The ordered LEED paterns are observed. Above $\theta > 1.0$ ML, a three-dimensional growth of the Pb islands was observed with a strongly preferred atomic-scale magic height (N), hexagonal shape and flat-tops. At coverage $\theta = 3.5$ ML, only islands containing N = 3, 5, 7 and 11 atomic layers of Pb are observed. At the higher coverage $\theta = 5.5$ ML, three types of regular hexagonal islands with side lengths of 25, 30 and 45 nm are observed. Furthermore, three different island adsorption configurations were observed.

O 59.4 Wed 16:45 WIL A317

**Three-dimensional atomic imaging by means of electron diffraction** — •Tobias Lühr[1], Aimo Winkelmann[2], Gert Nolze[3], and Carsten Westphal[1] — [1]TU Dortmund - Experimentelle Physik I, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D 06120 Halle, Germany — [3]Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, D 12205 Berlin, Germany

Diffraction patterns obtained with angle-resolved x-ray photoelectron diffraction (XPD) provide the information of the sample structure on an atomic length scale. Over the last three decades there were many attempts in order to obtain the sample structure applying a holographic reconstruction, due to common properties of XPD-patterns and holograms. However, anisotropic electron scattering, multiple scattering effects, as well as twin image formation generally prevented identifiable reconstructed images of the structure. Here, we demonstrate that all these problems can be circumvented by using electron diffraction patterns at kinetic energies of $E_{kin} \geq 10$ keV. Without adding any structure information, the reconstruction reveals a three-dimensional image displaying up to thousands of atoms located at their correct position. Demonstrating the reconstruction scheme on a bcc-structure we are presenting results on more complex systems as graphite with different emitter types, and polyatomic crystals. In all cases studied up to now, the spatial image reflected the respective crystal structure with all atoms at their correct location.

O 59.5 Wed 17:00 WIL A317

**Thickness-dependent growth study of Pt-Ce alloys on Pt(111)** — •Jeannette Kemmer, Andreas Krönlein, Pin-Jui Hsu, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Recently angle-resolved photoemission spectroscopy has revealed the formation of the coherent low-energy heavy-fermion band near the Fermi level on the $CePt_5$ surface alloy on Pt(111) [1]. We have investigated the coverage-dependent morphology of the various Pt-Ce surface alloys which form upon Ce deposition onto Pt(111) with a home-built low-temperature scanning tunneling microscope. Within the coverage range from $9.6 \times 10^{18}$ atoms/m$^2$ to $34 \times 10^{18}$ atoms/m$^2$ topographic constant-current images show several superstructures similar to those previously reported by Baddeley *et al.* [2]. While the coexistence of different superstructures is observed for low Ce coverages, much higher mounts of Ce lead to the formation of clusters, possibly due to segregation of excess Ce. An optimal surface quality is found for a Ce coverage of $19 \times 10^{18}$ atoms/m$^2$. We will also discuss the electronic properties of the Ce superstructures as observed by scanning tunneling spectroscopy.

[1] M. Klein *et al.*, Phys. Rev. Lett. **106**, 186407 (2011).

[2] C. J. Baddeley *et al.*, Phys. Rev. B **56**, 12 589 (1997).

O 59.6 Wed 17:15 WIL A317

**Comparison of lithium- and magnesium battery anode materials on a microscopic level using DFT** — •Markus Jäckle[1,2] and Axel Gross[1,2] — [1]Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany — [2]Helmholtz Institut Ulm - Elektrochemische Energiespeicherung, 89069 Ulm, Germany

Lithium and magnesium exhibit rather different properties as anode materials with respect to the phenomenon of dendrite formation which can lead to short-cuts in batteries. Diffusion processes are the key to understanding structure forming processes on surfaces. Therefore we have determined adsorption energies and barriers for the self-diffusion on Li and Mg using periodic density functional theory calculations. In addition, the adsorption of sulfur on these electrodes was studied as it represents a common pollutant in catalytical- and electrochemical systems.

According to our calculations, there are characteristic differences between Li and Mg, as far as the self-diffusion is concerned. On Mg, diffusion is much faster than on Li. The structural origins of this difference will be addressed. Furthermore, we will discuss the relevance of our findings for the understanding of the dendrite growth on Li anodes.

O 59.7 Wed 17:30 WIL A317

**Temperature Dependent Electronic Structure of the CuN**

**c(2x2) on Cu(100) Overlayer** — •Ivan Baev, Henrike Hümpel, Michael Martins, and Wilfried Wurth — Institut für Experimentalphysik, Universität Hamburg

CuN c(2x2) on Cu(100) is a promising surface insulator to study nanoparticles. If the size of deposited particles is small, then the coupling of the particles to the surface is often stronger than the size dependent effects within the particles itself. In such a case CuN can be used to decouple the particles from the metallic substrate without the disadvantages of a bulk insulator. Former characterizations of the CuN layer were focused on LEED and STM techniques. Only a few studies involving core level photoemission exist.

We have performed annealing temperature dependent X-Ray photoemission spectroscopy with an energy resolution sufficient to separate various contributions to the resulting core level photoemission lines. Complimentary, we also performed LEED and STM investigations in a so far not investigated temperature and nitrogen-dose range.

The results show that an interpretation of the CuN system involving LEED and STM experiments only, is dangerous. Our stoichiometric evaluation together with core level binding energy shifts shows, that a full monolayer coverage of CuN is formed under rather different conditions than it is generally perceived in the literature. Also, we can show that the usual preparation technique involving low energy sputtering of nitrogen onto Cu(100) is probably not suitable to achieve a large homogeneous CuN coverage density.

O 59.8 Wed 17:45 WIL A317

**Stability of surface adsorption patterns of Se on Mo(110): a first principles study** — •Guido Roma[1], Elaheh Ghorbani[1], Hossein Mirhosseini[1], Janos Kiss[2], and Claudia Felser[2] — [1]Joh. Gutenberg University, Mainz, Germany — [2]MPI for Chemical Physics of Solids, Dresden, Germany

The selenization of molybdenum is technologically relevant for the production of thin film chalcopyrite solar cells. But it could become very important also for the production of nanostructures based on the layered compound $MoSe_2$. However, the control of the process is still very poor, due to the lack of basic knowledge of the surface thermodynamics of the system. We present a theoretical study of the stability of surface adlayers of Se on the Mo(110) surface, predicting surface patterns and their stability range in terms of temperature and selenium partial pressure. Our results, based on density functional theory, show that the attainable Se coverages range from 1/4 to 3/4 of a monolayer for systems in equilibrium with a gas formed of Se molecules. We provide simulated scanning tunneling microscopy images to help the experimental characterization of adsorbed surface patterns.

O 59.9 Wed 18:00 WIL A317

**STM and LEED studies on alloying and oxidation effects at the Mn/Cu(001) interface** — •Jiaming Song[1], Chii-Bin Wu[2], and Wolfgang Kuch[1] — [1]Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin, Germany — [2]Chung Yuan Christian University, Department of Physics, 200 Chung Pei Rd., Chung Li, Taiwan 32023, R.O.C.

Scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) are applied for characterizing the interface properties of Mn/Cu(001) at room temperature. STM reveals a three-dimensional growth mode of Mn on clean Cu(001). When a submonolayer Co is introduced in between, the Mn growth mode is stabilized in a two-dimensional mode. This two-dimensional growth mode can be attributed to the formation of an intermixed alloy of MnCo or even MnCoCu. Growth of Mn on the “missing row” phase of oxidized Cu(001) occurs without the surfactant effect known from the growth of Co, Ni and Fe on that surface. The absence of the surfactant effect of oxygen could be due to a larger binding energy between Mn and oxygen atoms compared to the surface energy. Nevertheless, the Mn growth mode on this oxidized Cu(001) surface is still two-dimensional. This might be due to a reduction of the surface energy of the substrate by the oxygen during the Mn growth, leading to a smoother morphology.

O 59.10 Wed 18:15 WIL A317

**Thermodynamical assessment of stress evolution and jumps during the deposition of polycrystalline films** — •Amirmehdi Saedi and Marcel J. Rost — Kamerlingh Onnes Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands

During Volmer-Weber thin film growth at conditions with sufficiently high atom mobility, the intrinsic film stress becomes compressive in the later stages. Moreover, upon deposition interruptions, the film reacts with a huge tensile jump, that surprisingly, is fully restored back to the original stress values before the interruption, if the deposition is switched on again.

Several mechanisms have been proposed to explain these phenomena, but none of them were able to explain all the details of the experimental results and they remain as mere hypotheses waiting for their proof to come. One suggestion is that the diffusion of adatoms into/out of the grain boundaries (GB) during the deposition/interruption would be responsible for the observed effects. There are some models, based on kinetic arguments, attempting to show that this mechanism is capable of reproducing the experimental observations. However all of these models suffer from a critical shortcoming as they do not take into account the thermodynamical aspects. These include e.g. relationships between the flux, adatom densities, chemical potentials of the surface and grain boundaries, and the elastic energy of the bulk. Here our aim is to check for the first time whether the adatom-GB theory can really survive the test of a rigorous thermodynamical analysis.

O 59.11 Wed 18:30 WIL A317

**Role of stacking, bonding and interaction with substrate in formation of bilayer silicene** — •Paul Pflugradt, Lars Matthes, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität and European Theoretical Spectroscopy Facility (ETSF), Max-Wien-Platz 1, 07743 Jena, Germany

The properties of the two-dimensional systems of group-IV materials are of increasing interest. Unlike graphene, the corresponding silicon-based honeycomb crystal, silicene, is claimed to be experimentally realized as monolayer on silver substrate. However, such conclusions are controversially debated in literature, because of the strong adsorbate-substrate interaction. Very recently promising bilayer silicene has been prepared, whose geometry and properties are widely unknown.

We predict an atomic geometry for this bilayer system, in contrast to the suggestions of experimentalists. Based on ab-initio density functional theory including van der Waals interaction, we make a comprehensive analysis of this new structure. We find a suprising silicene configuration, not stable as monolayer. The translational symmetry, the resulting lattice spacing, and the height of the topmost monolayer are in agreement with the STM findings. The band structure of the complete adsorbate system but also of the peeled-off silicene do not show conical linear bands near the Fermi level, as expected for free-standing 2D crystal.

O 59.12 Wed 18:45 WIL A317

**Lateral Segregation in $Pt_{50}Rh_{50}$(111) induced by a *h*-BN nanomesh** — •Roland Stania[1], Irakli Kalichava[1], Bernd Schönfeld[2], Jürg Osterwalder[1], Wolfgang Heckel[3], Tobias C. Kerscher[3], Stefan Müller[3], Philip R. Willmott[1], and Thomas Greber[1] — [1]Universität Zürich, Physik-Institut — [2]ETH Zürich, LMPT — [3]Hamburg University of Technology, Institute of Advanced Ceramics

Epitaxially grown hexagonal boron nitride (*h*-BN) on Rh(111) forms a corrugated monolayer with a 13 on 12 super-honeycomb-structure known as the *h*-BN nanomesh [1]. In contrast *h*-BN on Pt(111) forms a flat layer with an approximate 10 on 9 superstructure being weaker bonded than the nanomesh [2]. The investigation of *h*-BN/$Pt_{50}Rh_{50}$(111) reveals a corrugated nanomesh-like 11 on 10 superstructure with a periodicity of 2.8 nm. Lateral segregation occurs in the topmost layer of the substrate during growth of *h*-BN, where Rh atoms form islands under the pores of the nanomesh which are surrounded by Pt atoms under the wires. The unit cell size is obtained by surface X-ray diffraction, while angular resolved photoemission indicates the nanomesh structure and the lateral segregation. The picture of lateral segregation at the nanometer scale is perfectly confirmed by density functional theory within a cluster expansion approach.

[1] Corso et al. Science **303** (2004) 217.

[2] Ćavar et al. Surface Science **602** (2008) 1722.

O 59.13 Wed 19:00 WIL A317

**Physisorbed molecular networks as surfactants for the growth of Ag on Ag(100)** — •Claudius Morchutt[2,3], Gustavo Ruano[2,3], Klaus Kern[1,2,3], and Magali Lingenfelder[1,2,3] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne — [3]Max Planck-EPFL Center for Molecular Nanoscience, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne

Homoepitaxial growth of Ag on Ag(100) proceeds by a quasi layer-by-layer fashion at room temperature (RT). This means that higher-layer islands nucleate before the completion of lower layers and it leads to kinetic roughening of the multilayer film. Previous studies have shown that deposition of metal atoms such as Sb can act as surfactants improving the smoothness of the films. However, these surfactants are difficult to remove from the surface after growth. Here we show by Scanning Tunneling Microscopy (STM) in ultra-high vacuum (UHV) that the growth mode of Ag on Ag(100) at RT is significantly modified by the presence of physisorbed molecular networks. The islands consisting of terephtalic acid (TPA, benzene-1,4-dicarboxylic acid) are stabilized via hydrogen bonds. Upon Ag deposition the Ag atoms penetrate the molecular islands without disrupting their supramolecular network that in turn enhances the coarsing of the Ag islands underneath. Furthermore, the organic molecules can easily be removed by post-annealing at moderate temperature.

## O 60: Graphene: Electronic Properties (O jointly with DS, HL, MA, TT)

Time: Wednesday 16:00–19:15 Location: WIL C107

O 60.1 Wed 16:00 WIL C107

**Monomer Doping of Self-Assembled Graphene Nanoribbons for Band Gap Alignment** — •Christopher Bronner[1,3], Stephan Stremlau[1,3], Marie Gille[2], Felix Brausse[2], Anton Haase[1], Stefan Hecht[2], and Petra Tegeder[1,3] — [1]Freie Universität Berlin — [2]Humboldt-Universität zu Berlin — [3]Ruprecht-Karls-Universität Heidelberg

In order to exploit the technologically interesting electronic properties of graphene, several concepts have been discussed which would lead to the opening of a band gap. One approach is spatial confinement of the charge carriers in quasi-one-dimensional graphene nanoribbons (GNRs). The band gap of a GNR scales inversely with its width and particularly nanometer-scale widths are desirable for application e.g. in transistor devices. Since the electronic properties of GNRs depend critically on their structure, precise synthesis is necessary but challenging for conventional methods such as lithography. In contrast, self-assembly from molecular precursors is an intriguing approach which has been employed to fabricate defect-free GNRs with well-defined widths and edge structures. Only this high level of structural precision allows introduction of dopant atoms at specific doping sites and concentrations in the graphene lattice. Nitrogen doping has been known to shift the band structure of GNRs with respect to the Fermi level which is interesting for GNRs in contact with electrodes and other device materials. Using surface-sensitive electron spectroscopies we demonstrate a continuous down-shift of the band structure with increased nitrogen doping of the monomers.

O 60.2 Wed 16:15 WIL C107

**Transport in chemically gated graphene p-n junctions** — •Jens Baringhaus[1], Alexander Stöhr[2], Ulrich Starke[2], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Max-Planck Institut für Festkörperforschung, 70569 Stuttgart, Germany

The chirality of charge carriers in graphene allows them to get through potential barriers without any reflection (known as Klein tunneling). To study this effect the fabrication of well-defined p-n junctions is necessary. We use the intercalation of Ge to convert the buffer layer on the SiC(0001) surface into graphene with local p-type or n-type doping depending on the local Ge coverage. The buffer layer is initially patterned using optical lithography, to fabricate isolated n-p, n-p-n and p-n-p structures. The n- and p-type doping (340 meV, -290 meV) is confirmed by STS which also reveals very narrow p-n junctions with a length below 5 nm. The corresponding electric fields are as high as $10^6$ V/cm and therefore significantly higher than those induced by field effects, providing a perfect environment to study Klein tunneling. Transport experiments are carried out by means of a 4-tip STM system, on n-p-n as well as p-n-p structures. Their resistance was found to be strongly dependent on temperature and the inner barrier length. While short barriers ($<$ 200 nm) appear almost transparent, the resistance increases rapidly for barrier widths exceeding the coherence length ($>$ 600 nm). The resistance of a single p-n junction fits to the theoretically predicted value for a Klein tunneling junction.

O 60.3 Wed 16:30 WIL C107

**Exceptional ballistic transport in epitaxial graphene nanoribbons** — Jens Baringhaus[1], Frederik Edler[1], Claire Berger[2], Walter A. de Heer[2], and •Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Georgia Institute of Technology, Atlanta, Georgia 30332-0430, USA

The patterning of graphene into graphene nanoribbons is an essential task for the development of graphene based devices. For such ribbons with a well-ordered edge geometry the presence of one-dimensional edge states has been predicted. We use a selective graphitization process on SiC-mesa structures to produce graphene nanoribbons with a width of 40 nm. The local electronic properties of the ribbons are investigated by means of a 4-tip STM. In combination with a SEM, the precise positioning of all four tips on the nanometer range is possible to perform local transport measurements. Additionally, local tunneling spectroscopy reveals characteristic features of ferromagnetic zig-zag graphene nanoribbons. Transport experiments carried out on the very same ribbon show a conductance close to $e^2/h$ for a wide temperature range from 30 K up to room temperature and probe spacings between 1 $\mu$m and 10 $\mu$m. Description within the Landauer formalism is possible assuming ballistic transport dominated by a single channel. Transport in the second zeroth subband is only detectable for probe spacings smaller than 1 $\mu$m due to the short localization length of carriers in this subband manifesting in the increase of the conductance to 2 $e^2/h$ at probe spacings below 200 nm.

O 60.4 Wed 16:45 WIL C107

**Electrical Transport in Freestanding Epitaxial Graphene: Evidence of an AB-Stacked Bilayer** — •Johannes Jobst[1,2], Shriram Shivaraman[3], Michael G. Spencer[3], and Heiko B. Weber[2] — [1]Leiden University, Kamerlingh Onnes Laboratorium, P.O. Box 9504, NL-2300 RA Leiden, Netherlands — [2]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [3]School of Electrical and Computer Engineering, Cornell University, Ithaca, NY 14853, USA

We investigate the properties of freestanding epitaxial graphene devices, which are created using a photo-electrochemical etching technique. This technique allows to selectively remove the silicon carbide (SiC) substrate on which the graphene was grown by thermal decomposition of SiC. We focus on completely freestanding devices of various geometries and devoid of any graphene-substrate interactions. We prepare freestanding Hall bars in order to study the low-temperature transport and Shubnikov-de Haas oscillations. We find evidence that the buffer layer is transformed to an additional graphene layer upon the etching process, and that the formed bilayer is AB stacked. Inhomogeneities in the buffer layer or introduced during the etching process are discussed.

O 60.5 Wed 17:00 WIL C107

**Scattering mechanisms in Tl-doped epitaxial graphene** — •Carola Strasser[1], Bart Ludbrook[2], Andrea Damascelli[2], Christian R. Ast[1], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Quantum Matter Institute, UBC, Vancouver, BC V6T 1Z4, Canada — [3]Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Since the charge carrier density in graphene can very easily be tuned by means of chemical doping this approach counts as a promising way to design graphene-based future electronic devices. It was shown [1] that the Fermi level can be shifted over a wide range in either direction. But one has to consider that the dopants do not just donate or take the electrons but they have an impact on the electronic structure: they act as scattering centres and change the charge carrier mobility.

We investigated small amounts of Thallium atoms on a monolayer of epitaxial graphene by angular resolved photoemission spectroscopy and did a careful analysis of the line width. Although Tl is very weakly bound and at first sight a paradigm long-range scatterer, we found that it introduces a sizeable short-range contribution. Only by using a model which combines both, long-range and short-range scattering we were able to describe our observations. This allowed us to put an upper limit on the dielectric constant for Tl-doped epitaxial graphene.

[1] H. Liu et al., *J. Mater. Chem.* **21**, 3335 (2011)

### O 60.6 Wed 17:15 WIL C107

**Excited electron dynamics in spatially aligned 7a-graphene nanoribbons on Au(788)** — •Nils Fabian Kleimeier[1], Alexander Timmer[1], Harry Mönig[1], Xinliang Feng[2], Klaus Müllen[2], Harald Fuchs[1], and Helmut Zacharias[1] — [1]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Max-Planck-Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Photoelectron spectroscopy of spatially aligned straight 7-armchair graphene nanoribbons (7-aGNRs) on Au(788) was carried out under ultra high vacuum conditions utilizing a time-of-flight spectrometer and a multi-anode detector. We found two unoccupied states at energies of $E_1$=3.6 eV and $E_2$=3.9 eV above the Fermi energy by exciting the sample with different photon energies (3.94 eV to 4.35 eV) from a femtosecond OPA. When exciting the sample with ultrashort pules (20 fs) at $\lambda$=390 nm ($h\nu$=3.15 eV) by frequency- doubling the output of a femtosecond Ti:sapphire laser amplifier, these states can further be investigated by 3-photon photoemission using a third state at an energy of $E_3$-$E_F$=0.6 eV as intermediate. All three states are in agreement with IPE measurements we performed previously on this system [1]. Thus the electronic dynamics of the state can be measured by time-resolved 3-photon photoemission spectroscopy with cross-polarized laser pulses. Preliminary evaluation of these measurements indicates electronic lifetimes of the unoccupied states of $\tau \sim$110 fs and 85 fs for the states at E-$E_F$ 3.9 eV and 3.6 eV, respectively.

References: [1] S. Linden et al., Phys. Rev. Lett. 108 (2012) 216801

### O 60.7 Wed 17:30 WIL C107

**Optical characterization of atomically precise graphene nanoribbons** — •Richard Denk[1], Michael Hohage[1], Jinming Cai[2], Pascal Ruffieux[2], Roman Fasel[2], and Peter Zeppenfeld[1] — [1]Experimental Physics, JKU Linz, Altenbergerstrasse 69, 4040 Linz, Austria — [2]nanotech@surfaces, EMPA, Überlandstasse 129, 6800 Dübendorf, Switzerland

Graphene nanoribbons (GNRs) promise high potential for future nanoscale electronic devices. While 2-dimensional graphene is semimetallic, electron confinement and edge effects in narrow (<10nm) GNRs can result in the opening of a band gap. The electronic and optical properties, however, strongly depend on the structural details of the GNRs. Only recent advances in the bottom-up fabrication of atomically precise GNRs [1] have enabled reliable experimental investigations of well-defined GNRs.

We have studied the fabrication process and the optical properties of GNRs on Au(788) using reflectance difference spectroscopy (RDS), taking advantage of the optical anisotropy due to the uniaxial alignment of the GNRs parallel to the step edges of the vicinal Au(788) surface. We find that the optical properties of the GNRs are highly anisotropic and dominated by three excitonic transitions, in excellent agreement with theoretical calculations.

[1] J. Cai at el, Nature, 466 (2010) 470.

### O 60.8 Wed 17:45 WIL C107

**Electronic and transport properties of BNC heterostructures, a first-principles investigation.** — •Simon Dubois and Jean-Christophe Charlier — Institute of Condensed Matter and Nanosciences, UCL, Louvain-La-Neuve, Belgium

Two dimensional hexagonal BN (h-BN), an isomorph of graphene with a lattice mismatch of only 1 .7%, is a wide gap insulator as its bulk counterpart. Advances in the synthesis of hybrid BNC heterostructures offer new opportunities to engineer the electronic properties of low-dimensional systems. Recently, it has been shown that the introduction of h-BN nanodomains into graphene enables to induce a tunable band gap in the honeycomb lattice. Lateral junctions between electrically conductive graphene and insulating h-BN provide new ways to embed electrically isolated elements within single atomic layers. Not only the two-dimensional BNC heterostructures hold promises for new applications but also the corresponding quasi-1D nanoribbons as well as the few layers structures obtained by plane stacking.

We report on the properties of low energy carriers in various kind of BNC heterostructures investigated by means of first-principles calculations: quasi one dimensional junctions made of h-BN and graphene ribbons, two-dimensional atomic layers made of hybridized domains, as well as few-layers stacks.

### O 60.9 Wed 18:00 WIL C107

**Time- and Angle-Resolved Photoemission Studies of Epitaxial Graphene** — •Søren Ulstrup[1], Jens C. Johannsen[2], Federico Cilento[3], Alberto Crepaldi[3], Michele Zacchigna[3], Jill A. Miwa[1], Philip D. C. King[4], Cephise Cacho[5], Edmond Turcu[5], Emma Springate[5], Felix Fromm[6], Christian Raidel[6], Thomas Seyller[6], Fulvio Parmigiani[3], Marco Grioni[2], and Philip Hofmann[1] — [1]Aarhus University, Aarhus, Denmark — [2]EPFL, Lausanne, Switzerland — [3]Sincrotrone Trieste, Trieste, Italy — [4]University of St. Andrews, St. Andrews, United Kingdom — [5]STFC Rutherford Appleton Laboratory, Didcot, United Kingdom — [6]Technical University of Chemnitz, Chemnitz, Germany

Understanding of the ultrafast carrier dynamics in graphene is of central importance for many electronic and optoelectronic applications. With the advent of high harmonic laser-based time- and angle-resolved photoemission (TR-ARPES) it is possible to gain a direct view of the non-equilibrium electronic structure around the Dirac point in graphene with femtosecond time resolution. Here, we characterize the dynamic processes around the Dirac point in epitaxial graphene using TR-ARPES measurements. In particular, we study the time-scales and significance of hot electron thermalization processes and electron-phonon coupling, and address the possibility of carrier multiplication.

### O 60.10 Wed 18:15 WIL C107

**Electronic and Transport Properties of Epitaxial Graphene on the Atomic Scale** — •Philip Willke[1], Thomas Druga[1], Alexander Schneider[2], Rainer Ulbrich[1], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Lehrstuhl für Festkörperphysik, FAU Erlangen, D-91058, Germany

The application of graphene in future devices requires a thorough understanding of its transport properties on the nanometer scale. We present a scanning tunneling potentiometry study at 6 K of electron scattering in mono- and bilayer graphene on n-doped SiC. Using STP we combine the imaging of local transport fields and sample topography. By probing simultaneously the thermovoltage signal [1] created due to slightly different temperatures of sample and tip, we can moreover obtain sensitive information on the electronic structure at the Fermi energy. We demonstrate how both transport and electronic information can be disentangled from STP measurements. We identify substrate steps and monolayer-bilayer junctions as local scattering centers which impede the electronic current and create local voltage drops that we compare to recent measurements at 72 K. [2] Moreover, wrinkles and substrate inhomogeinities have been identified as further sources of scattering. We acknowledge the financial support by the SPP 1459 "Graphene".

[1] K. J. Engel, M. Wenderoth, N. Quaas, T. Reusch, K. Sauthoff and R.Ulbrich, Phys. Rev. B 63, 165402 (2001)

[2] S. H. Ji et al., Nature Materials 11, 114-119 (2012)

### O 60.11 Wed 18:30 WIL C107

**Exchange coupling between $3d$-transition metal adatoms and Ni(111) mediated by graphene** — •Simon Fichtner, Paolo Ferriani, and Stefan Heinze — Institut für Theoretische Physik und Astrophysik, Christian-Albrecht-Universität zu Kiel, D-24098 Kiel, Germany

Recently, $3d$-transition metal (TM) adatoms on graphene have been intensively studied both experimentally (e.g. [1]) and theoretically (e.g. [2]). However, the possibility to stabilize their magnetic moment by exchange coupling to an underlying magnetic substrate has received little attention so far. Graphene on Ni(111) is a very good candidate in this respect as it has been experimentally shown to grow pseudomorphically. Here, we determine the electronic and magnetic properties of $3d$-TM adatoms adsorbed on graphene on Ni(111) based on density functional theory as implemented in the VASP code. We perform a systematic study on the dependence of the exchange interaction across the $3d$-TM series and take local correlations into account using the DFT+U formalism. We demonstrate the essential influence of the alignment of the adatoms 3d-states with the spin-polarized graphene states on the magnetic coupling with the Ni surface.

[1] Eelbo et al., Phys. Rev. Lett. **110**, 136804, 2013

[2] Wehling et al., Phys. Rev. B **84**, 235110, 2011

### O 60.12 Wed 18:45 WIL C107

**Highly spin-polarized Dirac fermions at the graphene-Co interface** — •Dmitry Marchenko[1,2], Andrei Varykhalov[1], Jaime Sánchez- Barriga[1], and Oliver Rader[1] — [1]Helmholtz-Zentrum

Berlin für Materialien und Energie, Berlin, Germany — [2]Physikalische und Theoretische Chemie, Freie Universität Berlin, Berlin, Germany

The interface of graphene with ferromagnets is very interesting for spintronics due to possible use of peculiar graphene electronic structure in transport and spin-filter applications when graphene is used together with nickel or cobalt as ferromagnetic contacts for spin injection and detection [1]. Despite a strong hybridization between graphene and ferromagnetic substrate states the graphene Dirac cone was observed by angle-resolved photoemission without gap between pi and pi* parts [2]. Here we report strong spin polarization of the Dirac cone measured by spin- and angle-resolved photoemission. Wave-vector dependent measurements exclude a Rashba-type spin-orbit contribution to the spin polarization; ferromagnetic origin is verified by reversal of the remanent magnetization. The importance of the spin polarization at the interface for spin filtering is pointed out.

[1] V. M. Karpan et al., Phys. Rev. Lett. 99, 176602 (2007) [2] A. Varykhalov et al., Phys. Rev. X 2, 041017 (2012)

O 60.13 Wed 19:00 WIL C107

**Controlling and understanding the non-linear photoluminescence in graphene on a femtosecond time scale** — •Richard Ciesielski[1], Alberto Comin[1], Matthias Handloser[1], Kevin Donkers[1], Torben Winzer[2], Ermin Malic[2], and Achim Hartschuh[1] — [1]Ludwig Maximilians Universität München & CeNS — [2]TU Berlin

Upon excitation, graphene exhibits nonlinear photoluminescence [1-3] that reflects the charge-carrier population and relaxation around the K-point. We present microscopic measurements on high quality exfoliated graphene samples with a pulsed laser system of ca. 18fs and a broad spectrum centred at 800nm.

Using a pulse shaping setup we can measure and manipulate the incident pulse in amplitude and phase. We find that the PL intensity depends sensitively on the temporal shape of the laser pulse, which we use to study and control the charge-carrier relaxation processes of graphene. Our findings are compared to numerical calculations.

[1] Stöhr, Wachtrup, Phys. Rev. B 82, 121408(R) (2010)

[2] Malic, Winzer, Bobkin, Knorr, Phys. Rev. B 84, 205404 (2011)

[3] Malic, Knorr, John Wiley & Sons (2013)

## O 61: Nanostructures at Surfaces III

Time: Wednesday 16:00–19:00 Location: WIL B321

O 61.1 Wed 16:00 WIL B321

**XANES and UV-Vis measurements on Ag clusters deposited into ionic liquid** — •David Engemann[1], Stefanie Roese[1], Stefanie Duffe[1], Kristina Kvashnina[2], Pieter Glatzel[2], and Heinz Hövel[1] — [1]Fakultät Physik / Delta, Technische Universität Dortmund, 44227 Dortmund — [2]European Synchrotron Radiation Facility (ESRF), 6 Rue Jules Horowitz, BP220, 38043 Grenoble

The properties of silver clusters can differ widely from that of bulk material. These differences correspond to the size of the clusters, their chemical environment and, if deposited, the supporting or embedding material. For applications of clusters for example in medicine their properties must be tuned in or for the presence of liquid environments. Deposition experiments were performed with Room Temperature Ionic Liquids (RTIL) as embedding material for clusters due to their applicability in high vacuum techniques.

Silver was vaporised by a thermal cluster source and cluster were formed by atom collisions in a super sonic expansion nozzle while expanding into a vacuum. The cluster than were deposited into 1-butyl-3-methylimidazolium hexafluorophosphat (BMIM-$PF_6$). This RTIL, an organic salt in liquid state, consists of a big organic cation (BMIM) and a small inorganic anion ($PF_6$). The asymmetry between the cation and the anion prevents the liquid from condensation at room temperature. These systems were investigated with UV-Vis measurements of the cluster plasmon extinction. Also first X-ray Absorption Near Edge Structure (XANES) spectroscopy measurements at the Ag-$L_2$ absorption edge were performed and will be presented.

O 61.2 Wed 16:15 WIL B321

**Mass selected copper clusters on xenon and argon investigated with ultraviolet photoelectron spectroscopy (UPS)** — •Christoph Schröder[1], Natalie Miroslawski[1], Paul Salmen[1], Dominik Wolter[1], Bernd von Issendorff[2], and Heinz Hövel[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Albert-Ludwigs-Universität Freiburg, Physikalisches Institut, D-79104 Freiburg

We deposit mass selected copper clusters on Cu(111), Au(111) and HOPG. To minimize the cluster surface interaction the substrates are covered with rare gas layers before softlanding the nanoparticles. These samples are measured with ultraviolet photoelectron spectroscopy (UPS) using a photon energy of h$\nu$=11.6 eV. We obtain signal in the sp-band region of the clusters which should be comparable to free beam cluster spectra [1,2] of the same clustersize, because of the low cluster surface interaction. This gives us hints about what happens to the electronic structure of clusters when they have contact to a surface. Furthermore we investigate the shift of the spectra caused by changing the substrate.

[1] O. Kostko, PhD-thesis, Albert-Ludwig-Universität Freiburg (2007).

[2] H. Häkkinen, M. Moseler, O. Kostko, N. Morgner, M. A. Hoffmann and B. v. Issendorff, Phys. Rev. Lett. **93**, 093401 (2004).

O 61.3 Wed 16:30 WIL B321

**Metal and metal oxide nanoparticles generated in gas phase by pulsed DC sputtering in a reactive gas admixture** — •Oleksandr Polonskyi, Amir Mohammad Ahadi, Alexander Hinz, Egle Vasiliauskaite, Thomas Strunskus, and Franz Faupel — Institute for Materials Science, Chair for Multicomponent Materials, CAU at Kiel, Kaiserstr. 2, 24143 Kiel, Germany

Metal nanoparticles have been of high scientific interest in the last decades due to their unique chemical, physical, mechanical, electrical, magnetic and optical properties. Gas aggregation cluster sources (GAS) based on the magnetron sputtering (Haberland concept) are widely utilized for fabrication of various metal nanoparticles. This work is focused on deposition of metal and metal oxide nanoparticles (Ag, TiOx, AlxOy, SiOx) by means of GAS with continuous or pulsed DC magnetron sputtering. Usually argon was used as a working gas, but in case of reactive metals (Ti, Al) a low concentration of oxygen or nitrogen was admixed, which is necessary for the cluster formation process. It was also observed that a gas aggregation cluster source based on pulsed reactive DC magnetron sputtering gives rise to a huge increase in deposition rate of nanoparticles by more than one order of magnitude compared to continuous operation (e.g., TiOx nanoparticles) [1]. The influence of the sputtering parameters and reactive gas admixing on the nanoparticles formation process was investigated. The prepared nanoparticles were characterized with regard to chemical composition, morphology and optical properties.

[1] Polonskyi et al., Appl. Phys. Lett. 103, 033118 (2013)

O 61.4 Wed 16:45 WIL B321

**Utilizing Dog-Boning to fabricate High-Aspect-Ratio Nanofences** — •Vera Hoffmann[1], Gunther Scheunert[2], René Kullock[3], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Centre for Nanostructured Media, School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, United Kingdom — [3]Department of Experimental Physics 5, University of Würzburg, 97074 Würzburg, Germany

By combining electroplating, as the first thin-film technique ever in use [1], and anodized aluminum oxide (AAO), to create nanoscale templates, one can fabricate macroscopically large areas of uniform nanorod arrays [2]. In order to better exploit these arrays for sophisticated applications, e.g. catalysis or dielectric-index sensing, an additional structuring would be desirable. Previous approaches with additional top layers on the AAO prior to electroplating or the subsequent removal of nanorods with laser ablation led to fringed rims and thus limit the applicability of the resulting structures.

Here, we present a new way of structuring by utilitizing the dogboning effect of electroplating and structured ground electrodes to deliberately fabricate nanofences – lines of free-standing high-aspect ratio nanorods [3]. We will show and explain the mechanisms behind this fabrication as well as outline future applications.

[1] L. B. Hunt, Gold Bulletin, 6, 16 (1973). [2] R. Atkinson et al. Phys. Rev. B 73, 2354021 (2006). [3] G. Scheunert, V. Hoffmann et al. J. El. Chem. Soc., 161 D26-D30 (2014), DOI:10.1149/2.024401jes

O 61.5 Wed 17:00 WIL B321

**Truly monodisperse clusters on boron nitride films and self-assembled monolayers** — •Fabian Knoller, Sarah Wieghold, Michael König, Friedrich Esch, and Ulrich Heiz — Technische Universität München, Catalysis Research Center, Chair of Physical Chemistry, Lichtenbergstr. 4, 85748 Garching, Germany

Matter in the non-scalable size regime displays unique, size-dependent chemical and physical properties. We study truly monodisperse supported clusters for catalytic applications, by characterizing their behavior under harsh conditions by Scanning Tunneling Microscopy (STM).

For this purpose, we soft-land size-selected PdN clusters first on epitaxial boron nitride films on Rh(111) for the study at elevated temperatures and under controlled dosage of reaction gases. It can be shown that the clusters are located at specific sites of the Moiré-structure and that these adsorption sites change upon ripening.

Second, we soft-land the clusters on self-assembled monolayers of n-dodecylthiole on Au(111) for studies in liquid ambients. Heating of the SAM sample under UHV conditions leads to long-range ordering of the film on which the PdN clusters are deposited. Their structure is conserved upon transfer into aqueous ambient (0.1M $KClO_4$) and imaging by electrochemical STM.

O 61.6 Wed 17:15 WIL B321

**Structure of graphene/Ir(111) supported metal clusters** — •Dirk Franz[1,2], Timm Gerber[3], Carsten Busse[3], Thomas Michely[3], Nils Blanc[4,5], Johann Coraux[4], Uta Hejral[1,2], Roman Shayduk[1], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, D-22603 Hamburg, Germany — [2]Fachbereich Physik, Universität Hamburg, D-20355 Hamburg, Germany — [3]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [4]Institut NEEL, CNRS and Universite Joseph Fourier, BP166, F-38042 Grenoble Cedex 9, France — [5]CEA-UJF, INAC, SP2M, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France

It was previously shown that different 2d metal cluster arrays can been grown using the moire of graphene/Ir(111) as a template [1].

We have employed several surface sensitive techniques (SXRD, XRR, GISAXS, HEXRD, STM) to investigate the structure of the particles (shape, epitaxy, strain) and the coherence of the 2d lattice. SXRD and GISAXS analysis benefits substantial from the regular arrangement of the particles and has the potential to be a possible standard technique to solve the atomic structure of ordered cluster arrays.

In particular we investigated the structure of Ir clusters in ultra high vacuum [2], Pt cluster in CO environment and alloy clusters with sequential deposition and co-deposition of Pt/Rh. A shape change of Pt/Rh clusters in an oxidizing environment has been observed.

[1] N'Diaye et al. in: Phys. Rev. Lett. 97, 215501 (2006)

[2] Franz et al. in: Phys. Rev. Lett. 110, 065503 (2013)

O 61.7 Wed 17:30 WIL B321

**Ripening of truly monodisperse clusters under the STM** — •Friedrich Esch[1], Yves Fukamori[1], Michael König[1], Bokwon Yoon[2], Bo Wang[1], Uzi Landman[2], and Ulrich Heiz[1] — [1]Technische Universität München, Catalysis Research Center, Chair of Physical Chemistry, Lichtenbergstr. 4, 85748 Garching, Germany — [2]School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332, USA

Matter in the non-scalable size regime displays unique, size-dependent chemical and physical properties. We study truly monodisperse supported clusters, i.e. with every cluster of same size and adsorption site and thus chemical environment. To this purpose, we soft-land size-selected $Pd_N$ clusters on epitaxial, Moiré-structured graphene and boron nitride films.

The well-defined samples allow for studying ripening mechanisms at the atomic scale by Scanning Tunneling Microscopy (STM), by following the dynamics of individual clusters as well as the particle size distributions of ensembles of hundreds of clusters [1]. The cluster-substrate interaction determines which ripening mechanism holds, Ostwald or Smoluchowski ripening. It is shown periodically wettable substrates can be used to optimize cluster stability at elevated temperatures. Periodic wettability leads to apparent adsorption site crossovers at the ripening transition from clusters to nanoparticles.

[1] Y. Fukamori, M. König, B. Yoon, B. Wang, F. Esch, U. Heiz and U. Landman, *Fundamental Insight into the Substrate-Dependent Ripening of Monodisperse Clusters*, Chem. Cat. Chem. 5 (2013) 3330-3341

O 61.8 Wed 17:45 WIL B321

**Molecule substrate registry on h-BN supported by Rh(111)** — •Marcella Iannuzzi — Universität Zürich, Schweiz

Modern nano-templates based on hexagonal boron nitride or graphene grown on transition metals show potential for future applications, due to their outstanding mechanical, thermal, and electronic properties. The mismatch between the lattice constant of the sp2 overlayer and the substrate produces modulated structures, which act as nano-templates for self-assembly, electron confinement, or intercalation. We apply scanning tunneling microscopy and density functional theory to investigate the adsorption of molecules and the formation and dynamics of defects. This work focus on the site-selectivity of h-BN/Rh(111) (nanomesh) for the adsorption of hexaiodo-cyclo-hexaphenylene (I6-CHP) and H2-phthalocyanine. In both cases we observe the preferential absorption within the pore of the nanomesh and the preferential orientation with respect to the substrate. Furthermore, the significant effects on the molecular electronic properties due t the interaction with the substrate are discussed. Advanced sampling techniques and tuned analysis tools for the characterization lead to a better understanding of the interaction between the precursor molecule and the substrate, which could be exploited in the development of new structure and process, as the production of graphene derivatives on metal supported insulators.

O 61.9 Wed 18:00 WIL B321

**Tracking of cluster island diffusion on HOPG using non-contact AFM** — Mumin Koç, Gauthier Torricelli, and •Klaus von Haeften — Department of Physics and Astronomy, University of Leicester, UK

Silicon oxide nanoparticles produced by co-deposition of silicon clusters and water vapour show very weak interaction in solution [1,2]. To elucidate the microscopic origins of the weak interaction, we deposited these clusters on highly oriented pyrolytic graphite (HOPG) surfaces and investigated their dynamics using non-contact AFM. The AFM images showed that practically all clusters were agglomerated into islands of different sizes. Larger islands were predominantly immobile, whereas a number of smaller islands were found to perform random walks in a Brownian-motion type fashion. The diffusion constant was determined from the time dependence of the mean square displacement. Detailed inspection of the island dynamics revealed correlated motion of 'dimer-islands', dissociation, and independent random walks of the dimer fragments. The role of the equipartition of energy between surface, islands, clusters and the AFM tip are discussed.

[1] A. Brewer and K. von Haeften, Appl. Phys. Lett. 94, 261102 (2009). [2] G. Torricelli, A. Akraiam, and K. von Haeften, Nanotechnology 22, 315711 (2011).

O 61.10 Wed 18:15 WIL B321

**Magnetic anisotropy of monolayer Co/Ir(111) and graphene/Co/Ir(111)** — •Alexander B. Shick[1], Frantisek Maca[1], and Alexander I. Lichtenstein[2] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [2]Institute of Theoretical Physics, University of Hamburg, Hamburg, Germany

The positive magnetic anisotropy in cobalt-intercalated graphene on Ir(111) attracts interest due to spintronics applications [1]. The magnetism, and the magnetic anisotropy energy (MAE) of monolayer Co/Ir(111) and graphene/Co/Ir(111) are studied making use of the first-principles FP-LAPW, and the magnetic torque methods, including the element-specific contributions to the MAE. We found reasonable agreement for the MAE with previous KKR-ASA calculations of monolayer Co on Ir(111) for unrelaxed structure [2]. The structure relaxation provides a substantial positive MAE enhancement, and the MAE of 0.45 meV per Co is consistent with experiment [3]. The magnetic moments and the MAE are strongly affected by presence of graphene. For the placement with one of the C atoms on the top of Co ("top" position) the MAE becomes negative. For different arrangement, with graphene in the hexagonal hollow positions over the monolayer Co ("hex"), the effect of graphene is weaker, and the MAE stays positive. The role of Coulomb correlations beyond DFT will be discussed. [1] N. Rougemaille *et al.,* Appl. Phys. Lett., **101**, 142403 (2012); [2] S. Bornemann *et al.,* Phys. Rev **B86**, 104436 (2012); [3] J.E. Bickel *et al.,* Phys. Rev **B84**, 054454 (2011).

O 61.11 Wed 18:30 WIL B321

**Nanojunctions on Epitaxial Graphene** — •Konrad Ullmann and Heiko B. Weber — Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg, Germany

We will report on the fabrication and characterization of graphene nanojunctions, created on epitaxial graphene (0001). Micrometer-sized constrictions are fabricated by electron-beam lithography. By a current driven process similar to electromigration, nanojunctions can reproducible be fabricated. The nanojunctions give access to the formation of single-molecule junctions with graphene electrodes.

O 61.12 Wed 18:45 WIL B321

**Observation of 4 nm Pitch Stripe Domains Formed by Exposing Graphene to Ambient Air** — •Daniel Sebastian Wastl[1], Florian Speck[2], Elisabeth Wutscher[1], Markus Ostler[3], Thomas Seyller[2,3], and Franz Josef Giessibl[1] — [1]Institut für experimentelle und angewandte Physik, Universität Regensburg, 93053 Regensburg, Germany — [2]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [3]Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

We study epitaxial graphene on the 6H-SiC(0001) surface under ambient conditions using frequency-modulation atomic force microscopy. We observe large terraces with a self assembled stripe structure within a highly adsorbate covered surface on top of the graphene[1]. To identify the origin of the structure, we compare the experimental data on graphene with calculations and experiments on graphite that predict the formation of a solid-gas monolayer in the solid-liquid interface of hydrophobic surfaces.

[1] Wastl et al. ACS Nano, 2013, doi: 10.1021/nn403988y

## O 62: Posters: Surface Reactions and Dynamics, Nanostructures

Time: Wednesday 17:30–21:00 Location: P1

O 62.1 Wed 17:30 P1

**Formation of superhydrogenated PAHs through interaction with atomic hydrogen and hydrogenated carbonaceous grains** — •John Thrower[1,2], Emil Friis[1], Anders Skov[1], Bjarke Jørgensen[1], Louis Nilsson[1], Saoud Baouche[1], Richard Balog[1], and Liv Hornekaer[1] — [1]Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark — [2]Present Address: Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany

Processes occurring on dust grain surfaces play a crucial role in interstellar chemical evolution. In particular, $H_2$, the most abundant molecule, is only formed efficiently through surface reactions. Polycyclic aromatic hydrocarbon (PAH) molecules account for up to 10% of the total carbon budget. It has been suggested that in warmer environments, *e.g.* photodissociation regions (PDRs), PAHs are involved in $H_2$ formation [1]. Building on previous DFT calculations [2], we present mass spectrometric investigations of the formation of superhydrogenated PAH molecules through H-atom addition to coronene ($C_{24}H_{12}$) which reveal abstraction reactions that release $H_2$ [3]. Furthermore, we demonstrate that hydrogenated graphitic surfaces can act as an addition source of H-atoms that can react with physisorbed PAH molecules, potentially releasing H and $H_2$ from the grain surface.

[1] E. Habart, F. Boulanger, L. Verstraete, *et al.*, *Astron. Astrophys.*, **414**, 531 (2004).

[2] E. Rauls and L. Hornekær, *Astrophys. J.*, **679**, 531 (2008).

[3] J. D. Thrower, B. Jørgensen, E. E. Friis, *et al.*, *Astrophys. J.*, **752**, 3 (2012).

O 62.2 Wed 17:30 P1

**Thermal desorption spectroscopy of astrophysically relevant molecules on olivine and single crystal forsterite** — •Tushar Suhasaria[1,2], Nadine Heming[1], Robert Frigge[1], Björn Siemer[1], and Helmut Zacharias[1,2] — [1]Physikalisches Institut, University of Münster, Germany — [2]Graduate School of Chemistry, University of Münster, Germany

Chemical surface reactions on dust grains are a possible way of molecule formation in the Interstellar Medium (ISM). These grains typically consist of graphitic and silicate materials. At low temperatures in molecular clouds ($T < 20$ K) atoms and molecules freeze out and form ices around the dust grains [1].Temperature programmed desorption (TPD) spectroscopy is an established method to define the binding energies between molecules and surfaces of astronomical interest. We have performed TPD measurements on several molecules like $D_2$, CO, $CH_4$, $CO_2$ and $NH_3$ adsorbed on single crystal forsterite ($MgSiO_4$) and olivine ($Mg_x$ $Fe_{1-x}$ $SiO_4$) surfaces. We determine the average binding energies, order and pre-exponential factors for such molecules on silicate surfaces and present a comparison of such properties on two silicate surfaces.

1] Tielens A. G. G. M., 2005, the physics and chemistry of the interstellar medium, Cambridge University Press.

O 62.3 Wed 17:30 P1

**Carbon Dioxide Adsorption in Charged and Uncharged Carbon Nanotube Arrays** — •Mahshid Rahimi[1], Jayant K. Singh[2], and Florian Müller-Plathe[1] — [1]Technische Universität Darmstadt, Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Alarich-Weiss-Str. 4, D-64287 Darmstadt, Germany — [2]Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur-208016, India

Grand-canonical Monte Carlo simulations is carried out to understand the adsorption of CO2, onto bundles of 3D aligned double-walled charged and uncharged carbon nanotubes of diameter 5 nm at 303 K. The simulation of partial adsorption isotherms, i.e. only inner tube volume, only interstices between tubes, and unrestricted, allow a breakdown of the experimental adsorption isotherms into contributions of different regions. The results for uncharged carbon nanotubes are compatible with microscopic observations of the majority of the inner tube volumes being accessible for CO2. Further, the unrestricted adsorption isotherm is quantitatively equivalent to the sum of inner and outer adsorption for the pressure range considered in this work, $p<$ 40 bar, indicating no significant interference between inner and outer regions. The intertube distance, which is varied from 0 to 15 nm, dramatically affects the isosteric heat of adsorption and adsorption capacity. Excess adsorption is found to display a non-linear behavior with d, for unrestricted and outer cases.

O 62.4 Wed 17:30 P1

**Near ambient pressure XPS investigation of the oxidation and the CO oxidation on Pt(111)** — •Mathias Grabau[1], Sandra Krick Calderón[1], László Óvári[2], Hans-Peter Steinrück[1], and Christian Papp[1] — [1]Physikalische Chemie II, University of Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany — [2]MTA-SZTE Reaction Kinetics and Surface Chemistry Research Group, H-6720 Szeged, Rerrich Béla tér 1, Hungary

The oxidation of Pt(111) at oxygen pressures up to 1 mbar was followed *in situ* using (NAP)-XPS at temperatures between 300 and 700 K. The oxidation was found to proceed remarkably at temperatures of 300 and 500 K (oxygen coverage of 1.6 ML after 6 h at 300 K). The analysis of the data revealed varying saturation coverages found *in situ*, indicating a sensitive pressure- and temperature-dependent system. As a follow-up, the oxidation of CO by molecular oxygen on Pt(111) was investigated in the temperature range between 500 and 900 K using different reactant mixtures in continuous flow mode. Considerable reaction was observed at temperatures above 650 K under oxidizing conditions. Reaction onset at lower oxygen ratios was found for higher temperatures. Oxide formation under reaction conditions ($T \geq 650$ K) was observed to lead to a lower catalyst activity up to complete inhibition of the CO oxidation reaction.

O 62.5 Wed 17:30 P1

**Microcalorimetric study of the hydrogen-to-water oxidation on solid-state** $Pt/TiO_2/Ti$ **emf cells** — •Ömer Cakabay, Mhamed El Achhab, and Klaus Schierbaum — Department of Materials Science, Institute for Experimental Condensed Matter Physics, Heinrich-Heine-University Düsseldorf

We study the hydrogen-to-water oxidation on $Pt/TiO_2/Ti$ layer structures in which the oxide is grown by a high-voltage electrochemical anodization. By means of microcalorimetry, we determine various kinetic parameters including the film and pore diffusion rates, the turn-over numbers, the activation energies and the reaction orders of hydrogen-to-water oxidation on platinum coated anodized titanium foils. By identifying these parameters, the experimental determination of the mass transport limitations as well as the temperature dependence of the activity of the catalyst are achieved.

O 62.6 Wed 17:30 P1

**CO oxidation at nanoporous gold: TPD, XPS, and DFT study** — Sarah Röhe, Lyudmila Moskaleva, Andreas Schaefer, Arne Wittstock, •Volkmar Zielasek, and Marcus Bäumer — Institut für Angewandte und Physikalische Chemie, Universität Bremen

Nanoporous gold (np-Au) is an efficient catalyst for CO oxidation, even below RT. To gain insight into relevant mechanisms and surface species, we employed TPD and XPS in UHV directly at np-Au catalyst samples which were produced by leaching of silver from AgAu alloy and then activated for CO oxidation in a continuous-flow reactor. Supported by DFT calculations, the experiments indicate that the catalytic activity is based on a complex interplay of gold, silver, CO, and several oxygen species on and within the np-Au surface.

Residual silver is crucial for the ability of np-Au to chemisorb molecular oxygen, resulting in presumably atomic oxygen (Oact) at the surface available for CO oxidation. TPD after exposing np-Au to CO at 105 K shows pronounced CO and CO2 desorption at temperatures above 200 K, indicating an additional, more stable type of CO binding sites on np-Au as compared to pure gold. Only CO at these binding sites is oxidized by Oact. DFT calculations demonstrate that the strong binding of CO to np-Au cannot be explained by the presence of silver residues. It can be conceived, however, that it is induced by the formation of O-Au-CO complexes at low-coordinated surface sites. In fact, besides silver and Oact, we find various resident oxygen species on and within the np-Au surface. Their presence may be as crucial for the catalytic activity of np-Au as residual silver.

O 62.7 Wed 17:30 P1

**Electron dynamics of the topological insulator $Sb_2Te_2S$** — •Sophia Ketterl[1], Thomas Kunze[1,2], Thorsten U. Kampen[2], Evgeny Chulkov[3], and Martin Weinelt[1] — [1]FU Berlin, Germany — [2]SPECS GmbH, Germany — [3]UPV/EHU San Sebastian, Spain

The strength of the electron-phonon coupling in topological insulators is currently debated. Both strong and weak coupling constants have been reported [1,2].

We investigate the electron dynamics of the p-doped $Sb_2Te_2S$ via time-resolved two-photon photoemission measurements with an angle-resolving time-of-flight spectrometer. p-doped $Sb_2Te_2S$ exhibits a Dirac cone above the Fermi energy. In our experiment, the Dirac cone is populated by an infrared pump-pulse via direct absorption and interband scattering from the conduction band. In the Dirac cone we observe lifetimes on the picosecond timescale. The spectra hint at a stepwise relaxation via small-energy transfer processes. Cooling of the system leads to faster electron dynamics. This dynamics will be discussed in light of electron-electron and electron-phonon scattering.

[1] R. C. Hatch *et. al.*, *Phys. Rev. B* **83**, 241303 (2011).
[2] Z.-H. Pan *et. al.*, *Phys. Rev. Lett.* **108**, 187001 (2012).

O 62.8 Wed 17:30 P1

**Laser-triggered miniaturized electron gun for ultrafast low-energy electron diffraction** — •Gero Storeck, Simon Schweda, Max Gulde, Sascha Schäfer, and Claus Ropers — IV. Physical Institute, University of Göttingen, 37077 Göttingen, Germany

The time-resolved analysis of structural dynamics at surfaces will yield insight into a rich class of previously inaccessible effects, which are unique to quasi-two-dimensional systems. A main experimental challenge in the realization of optical pump/ electron probe schemes is the generation of short electron pulses at low energies and their undispersed propagation to the sample. Nanometric photocathodes were recently suggested to minimize spatial and temporal broadening and have been successfully implemented in a time-resolved diffraction experiment in a transmission geometry [1].

Here, we present the development of a compact pulsed electron gun for time-resolved low-energy electron experiments in backscattering diffraction. This will provide for a novel and versatile tool in ultrafast surface science.

[1] M. Gulde et al. (submitted).

O 62.9 Wed 17:30 P1

**Electronic surface structure of Au/Ge(001) and comparison with the pure Ge(001) substrate studied by 2PPE** — Kristof Zielke, •Kamil Bobowski, Cornelius Gahl, and Martin Weinelt — Fachbereich Physik der Freien Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

For submonolayer gold coverage Au/Ge(001) has been shown to form nanowires which exhibit properties typical for a one-dimensional Luttinger liquid [1]. We have investigated the electronic structure of the Au/Ge(001) surface in dependency of gold coverage and annealing temperature by two-photon photoemission spectroscopy (2PPE). While the surface states $D_{\mathbf{up}}$ and $D_{\mathbf{down}}$ of the clean Ge(001) surface are suppressed upon gold adsorption, a new unoccupied state appears about 800 meV above $E_F$ at normal emission. Additionally, time resolved investigations show a significant decrease in excited state lifetimes.

[1] C. Blumenstein *et. al.*, *J. Phys.: Condens. Matter* **25**, 014015 (2013).

O 62.10 Wed 17:30 P1

**Exploring hot electron dynamics in the layered semiconductor $2H$-MoS$_2$ by time- and angle-resolved photoelectron spectroscopy** — •Petra Hein, Kerstin Hanff, Gerald Rohde, Ankatrin Stange, Michael Bauer, Lutz Kipp, and Kai Rossnagel — Institute of Experimental and Applied Physics, University of Kiel, Germany

Pump-probe experiments with ultrashort pulses delivered by femtosecond laser systems provide important insights into the dynamics of condensed matter on fundamental time scales. In particular, high-harmonic extreme ultraviolet pulses can be used to investigate the temporal evolution of the electronic structure after excitation with an optical pump pulse. Previous time-resolved photoemission studies on layered transition-metal dichalcogenides (TMDCs) have focused on the dynamics of charge-density-wave and Mott insulating phases [1]. Here, we concentrate on the photo-induced electron dynamics in semiconducting TMDCs, with the indirect bandgap semiconductor $2H$-MoS$_2$ serving as a model system. Specifically, we study the relaxation processes of the photo-excited electrons in dependence of the pump fluence, energy, and polarization. We also report the effects of alkali metal intercalation on the band structure and electron dynamics. Possible similarities of surface-intercalated $2H$-MoS$_2$ and monolayer $2H$-MoS$_2$ are discussed.

[1] S. Hellmann *et al.*, Nat. Commun. **3**, 1069 (2012).

O 62.11 Wed 17:30 P1

**Attosecond time resolved photoemission on solid surfaces** — •Sergej Neb, Fabian Merschjohann, Peter Bartz, Matthias Hensen, Christian Strüber, Norbert Müller, Walter Pfeiffer, and Ulrich Heinzmann — Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld

The availability of single attosecond (as) XUV pulses allows investigating ultrafast electron dynamics on the as time scale. For a (110) tungsten surface Cavalieri et al. reported that the photoemission from tungsten 4f states is delayed by about 100 as with respect to the electron emission from the valence band [1]. The physical origin of this delay is not yet understood and controversial theoretical models coexist. Further as-time-resolved photoemission studies using other surfaces help to resolve this controversy.

Here we report on as-time-resolved photoemission from a van-der-Waals crystal that exhibits a completely different electronic structure. XUV pulses with about 300 as duration are generated by high harmonic generation in a Ne target using 5 fs IR laser pulses with stable carrier-envelope phase. The layered structure of the investigated solid yields element specific photoelectrons emitted from different depth and thus helps resolving the physical origin of temporal delays in photoemission.

[1] A.L.Cavalieri et al., Nature 449, 1029 (2007)

O 62.12 Wed 17:30 P1

**Time- and angle-resolved XUV ARPES at sub-15 fs temporal resolution** — •Gerald Rohde, Arne Hendel, Lexian Yang, Ankatrin Stange, Kerstin Hanff, Christian Sohrt, Lutz Kipp, Kai Rossnagel, and Michael Bauer — Institut für Experimentelle und Angewandte Physik der Christian-Albrechts-Universität zu Kiel

Time- and angle-resolved photoelectron spectroscopy (trARPES) provides a most direct access to ultrafast electronic processes in condensed matter systems. Application of XUV photon pulses generated in High-

Harmonic Generation (HHG) light sources allows probing transient electronic structure within the entire Brillouin zone and beyond [1]. Typically, it is the pump pulse that limits the time-resolution of such experiments to values of $\geq 30$ fs so that extremely fast phenomena such as characteristic melting times of electronic phases [2] or the thermalization of a nascent electron distribution [3] may remain unresolved.

Here we present a HHG-based trARPES setup exhibiting a substantially improved time-resolution. The optical pump-line of the experiment is operated using sub-6 fs pulses at a center wavelength of about 800 nm as generated in an amplifier-driven hollow-fiber chirped-mirror compressor. In the contribution, details of the compressor optimization procedure and its integration into the existing trARPES setup are described. First trARPES measurements on $1T$-TiSe$_2$ are shown providing direct experimental evidence for a sub-15 fs time-resolution.
[1] T. Rohwer et al., Nature **471**, 490 (2011)
[2] S. Hellmann et al., Nature Communications **3**, 1069 (2012)
[3] G. Rohde et al., Eur. Phys. J.-Spec. Top. **222**, 997 (2013)

O 62.13 Wed 17:30 P1

**Investigating Very Low Energy Electron Transmission through Thin Metallic Films** — •Daniel Panzer and Gerd Schönhense — Institut für Physik, Johannes-Gutenberg Universität, 55128 Mainz

The inelastic mean free path of electrons in matter is strongly energy dependent (it increases steeply at low energies <20eV [1]), and spin sensitive [2,3]. In the present work we use an imaging system that projects an electron optical image from a thermal or photoemitter onto an ultrathin metallic film and then watch the transmitted electrons using a standard Photo Emission Electron Microscope (PEEM) column. This allows for a wide range of combinations of different emitters and thin films. Thermionic emitters like BaO and $Y_2O_3$ provide high intensity to rate transmission for thicker sample films or multi-layer systems. Threshold photoemission provides a smaller emission energy width to better evaluate transmission of samples like Au, Pt and Pd at different kinetic energies. A pulsed photoemitter in combination with a delay line detector facilitates time-of-flight measurements to distinguish between different scattering processes. A uniformly magnetized ferromagnetic film should eventually enable spin-filtering an electronic image coming from a spin-polarized photoemitter.

References:
[1] M.P. Seah, W.A. Dench, Surf. a. Interface Analysis (1979), 1(1):2.
[2] W. Weber, S. Riesen, H.C. Siegmann, Science 291 (2001), 1015
[3] P. Dey, W. Weber, J. Phys.: Condens. Matter 23 (2011), 473201

O 62.14 Wed 17:30 P1

**Dynamical Study of Electron Transfer in Alkanethiolate Self-Assembled Monolayers Adsorbed at the Au(111) Surface** — •Veronika Prucker[1], Pedro B. Coto[1], Óscar Rubio-Pons[1], Michel Bockstedte[1], Haobin Wang[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Interdisziplinäres Zentrum für Molekulare Materialien (ICMM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]Department of Chemistry and Biochemistry, MSC 3C, New Mexico State University, Las Cruces, New Mexico 88003, USA

In this contribution, we present a dynamical ab-initio study of electron transfer (ET) in a series of self-assembled monolayers consisting of nitrile substituted short-chain alcanethiolate molecules on gold substrates. Employing a model Hamiltonian, which is parametrised by first principles electronic structure calculations [1], and dynamical simulations, we analyse the main factors underlying the ET process. In accordance to experiments [2,3], we demonstrate the dependence of the ET process on the molecular chain length and on the symmetry of the donor state, which allows to control the electron injection times even in the case of nearly degenerate donor states [4]. Additionally, we discuss the influence of electronic-vibrational coupling on the ET process.
[1] I. Kondov *et al.*, J. Phys. Chem. C 111, 11970 (2007).
[2] F. Blobner *et al.*, J. Phys. Chem. Lett. 3, 436 (2012).
[3] P. Kao *et al.*, J. Phys. Chem. C 114, 13766 (2010).
[4] V. Prucker *et al.*, J. Phys. Chem. C, accepted (2013).

O 62.15 Wed 17:30 P1

**Femtosecond time-resolved two-photon photoemission spectroscopy of $C_6H_5F$/Cu(111)** — •Ishita Agarwal, Isabella Avigo, Manuel Ligges, Ping Zhou, and Uwe Bovensiepen — Faculty of Physics, University of Duisburg-Essen, Duisburg

The electron dynamics at a metal-organic interface is studied with two-photon photoemission (2PPE) spectroscopy. We report here binding energies, band dispersion, and lifetimes of unoccupied metal-molecular interface states for up to 3 monolayers (ML) of mono-fluorobenzene ($C_6H_5F$) adsorbed on Cu(111). For all coverages, an unoccupied electronic state with a binding energy of $3.67 \pm 0.05$ eV above the Fermi level ($E_F$) was found. In addition, between 1 and 2 ML, a second unoccupied feature with a binding energy of $3.54 \pm 0.05$ eV above $E_F$ was observed. Using angle-resolved spectroscopy the band dispersion of these unoccupied states was studied and an effective mass of $(0.76 \pm 0.20) \times m_e$ and $(0.8 \pm 0.2) \times m_e$ was found, respectively. Time-resolved 2PPE measurements indicate an ultrashort lifetime of about 10 fs. Overall, the observations resemble previous coverage dependent 2PPE studies of $C_6F_6$/Cu(111)[1] and $C_6H_6$/Cu(111)[2] which suggest a structural influence on the unoccupied electronic structure at the interface. Funding by the DFG through BO1823/5-1 is gratefully acknowledged.
[1] D.Velic, et al., *J. Chem. Phys.*, **109**, 9155, (1998)
[2] C.Gahl, et al., *Faraday Discuss.*, **117**, 191, (2001)

O 62.16 Wed 17:30 P1

**Spin Effects in Ultrafast Charge Transfer Measurements on Ar/Co Interfaces using a TOF-Mott-Polarimeter** — •Tobias Sundermann[1], Norbert Müller[1], Ulrich Heinzmann[1], Johannes Bauer[2], Runyuan Han[2], Peter Feulner[2], and Wilfried Wurth[3] — [1]Molecular and Surface Physics, Bielefeld University — [2]Physik-Department E20, TU München — [3]Physik-Department, University of Hamburg

Using the principle of the core hole clock method [1] the spin dependent charge transfer is studied from resonantly excited physisorbed Ar atoms into an in plane magnetized Co adlayer on W(110). For exciting the $Ar2p_{3/2} \to 4s$ resonance circularly as well as linearly polarized synchrotron radiation of energy $h\nu = 244.55 eV$ is used (BESSY beamline UE56/II PGM2, single bunch mode). Emitted electrons are energy and spin analyzed by means of a TOF spectrometer followed by a spherical Mott polarimeter [2] operated in retarding mode at 45 keV scattering energy. Excitation by circularly polarized radiation results in a spin polarization up to 35% ± 5% of the Auger electrons following the decay of the excited oriented Ar $2p_{3/2}$ holes. With excitation by linearly polarized radiation smaller spin polarization effects appear for autoionization emission channels. These effects result from a spin dependent charge transfer from excited unpolarized Ar 4s states to empty Co conduction band states with minority spin preferred.
[1] D. Menzel, Chem. Soc. Rev., 37 (2008)
[2] G. Snell et al., Phys. Rev. Lett. 76, 3923 (1996)

O 62.17 Wed 17:30 P1

**Circular dichroism of the unoccupied topological surface state of $SnSb_2Te_4$** — •Sebastian Otto and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Time- and angle-resolved two-photon photoemission is used to study the electronic structure and dynamics at the surface of $SnSb_2Te_4$. Circular dichroism is used to map the spin structure of the topological surface state. Due to the intrinsic p-doping the topological surface state is centered at $0.32 \pm 0.03$ eV above the Fermi level with a group velocity of 3.4 eVÅ. The circular dichroism pattern of the Dirac cone shows a strong dependence on the polarization of the probe pulse while the polarization of the pump pulse has no significant effect. This stands in good agreement with time-resolved measurements showing a transient population of the topological surface state dominated by refilling from the conduction band minimum.

O 62.18 Wed 17:30 P1

**Structured hetero-material nanorod arrays** — •Eric Jehnes, Vera Hoffmann, Fabian Patrovsky, Matthias Böhm, and Lukas M. Eng — Institute of Applied Photophysics, TU Dresden, D-01062 Dresden, Germany

Metal nanorod arrays grown in anodic aluminium oxide (AAO) show distinct plasmonic resonances [1] that cover a wide range of future applications - for instance in optical sensors, biosensors, nanoantennas, waveguides, etc.. In order to improve their applicability addional structuring is needed both laterally, horizontally and radially.

We show such an approach by laser interference lithography, electrochemical deposition and multiple etching steps. Our processing results in core-shell and segmented nanorods composed of gold, silver, cobalt and/or nickel. The lateral structuring creates nanorod arrangements of dense lines covering a large area.

[1] R. Kullock et al., J. Opt. Soc. Am. B, 27, 1819

O 62.19 Wed 17:30 P1

**Tunable Silicon Nanowire Arrays Based on A New Method to Transfer Large Area of Ultra-Thin Alumina Membranes** — •Ahmed Al-Haddad[1,2], Ranjith Vellacheri[1], Samar Tarish[1,2], Yan Zheng[1], Liaoyong Wen[1], Yang Xu[1], and Yong Lei[1] — [1]Institute for Physics and IMN MacroNano (ZIK), Ilmenau University of Technology, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany. — [2]Department of Physics, College of Science, The University of Mustansiryah, Baghdad, Iraq.

A new effective method was developed to transfer large area ultra-thin alumina membrane (UTAM) with Au thin film as supporting layer to Si wafer. UTAM was prepared by a two-step anodization of aluminum foil with controllable thicknesses (100-400nm), followed by the transportation to Si wafer using a special cell and the removal of the backside Al and barrier Al2O3 layer. Several drops of DI water were added on Si before placing the UTAM to increase the adhesion between UTAM and Si surface. Furthermore, ordered Au nanodots arrays on Si surface were obtained by physical vapor deposition of Au with a thickness of 20 nm, which could be further used for. Moreover, the obtained Au grid from supporting UTAM was used for metal-assisted chemical etching to fabricate Si nanowires arrays. Furthermore, the structure and surface morphology were examined by Raman spectroscopy and scanning electron microscopy, respectively.

O 62.20 Wed 17:30 P1

**Structuring of nanorods for sensing applications** — •Rico Eissmann, Andreas Hille, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

Metal nanorod arrays are elegant for various sensing applications. The fabrication of nanorod arrays is an established technique. [1] In this study graded nanorod arrays, having a variably tuned rod diameter, are investigated. In combination with integrating such graded nanorod arrays on CCD/CMOS chips it allows for very small sensor applications.

The optical and plasmonic properties of those graded nanorod arrays are calculated with the multiple multipole method [2]. The distinct plasmonic behavior of nanorods with different geometric parameters (volume, rod length and distance) allows to use them as an optical filter on light-sensitive electronic devices, and moreover to record spectrally selected wavelengths.

[1] P. Evans et al. Growth and properties of gold and nickel nanorods in thin film alumina. doi:10.1088/0957-4484/17/23/006

[2] C. Hafner. Post-modern Electromagnetics: Using Intelligent MaXwell Solvers. John Wiley & Sons, New York, 1999

O 62.21 Wed 17:30 P1

**$C_{60}$ fullerenes on noble gas layers (Ar/Xe): Photoelectron spectroscopy with ultraviolet light** — •Dominik Wolter, Christoph Schröder, Natalie Miroslawski, and Heinz Hövel — Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany

We have investigated $C_{60}$ clusters deposited and measured at temperatures between 10 K and 13 K on 60 monolayers of xenon (Xe) with 10 monolayers of argon (Ar) on top using ultraviolet photoelectron spectroscopy. The noble gas layers were adsorbed at 45 K (Xe) and 10 K (Ar) on copper(111), silver(111) and gold(111) substrates. To get a well ordered surface the first layer of each gas was adsorbed at slightly higher temperatures (75 K for Xe and 25 K for Ar). We used an Ar-gas discharge lamp ($h\nu = 11.6\,\mathrm{eV}$) with a heatable LiF-window to suppress the satellite lines [1]. To extract the signal of the fullerenes we measured the spectra for the rare gas covered substrate before deposition and subtracted them from measurements after the deposition. The observed shift of the $C_{60}$ spectra depending on substrate and the noble gas layers is of importance for the interpretation of UPS on mass selected metal clusters on similar surfaces.

[1] M.Budke and M.Donath, Appl. Phys. Lett. **92**, 231918 (2008); S.Suga, et al., Rev. Sci. Instruments **81**, 105111 (2010)

O 62.22 Wed 17:30 P1

**Simulations with FEFF of XANES spectra on Ag clusters deposited in PDMS and silica aerogel** — •Stefanie Roese, David Engemann, and Heinz Hövel — Fakultät Physik / DELTA,Technische Universität Dortmund, 44227 Dortmund

For many applications of clusters such as catalysis the knowledge of geometrical structure, size and electronic properties is essential.

Depositing Ag clusters produced in a supersonic expansion into silica aerogel or PDMS can prevent the clusters from coalescence. Silica aerogel is a very porous compound of $SiO_2$ nanoparticles containing up to 99 % empty space. PDMS is a polymer in which the clusters are dispersed by deposition.

The $L_2$ and $L_3$ edge of the Ag clusters is investigated with XANES carried out at the synchrotron radiation sources ESRF (ID 26) and DELTA (BL 8).

The experimental data are compared to ab initio multiple scattering calculations [1] for different cluster sizes and structures. The calculations include information about the geometric and electronic structure of the deposited clusters and also about their chemical environment. We examine cluster structures modeled with a Gupta potential [2] and compare the calculated XANES spectra to the measured ones.

The focus is here on the number of next neighbors and the next-neighbor distances to investigate the geometrical structure of the Ag clusters.

[1] J. J. Rehr et al., Phys. Chem. Chem.Phys., 12, 5503-5513 (2010)

[2] W. Huang et al., Chem. Phys. Lett., 507:199-202 (2011)

O 62.23 Wed 17:30 P1

**Optical measurements and simulations for cluster plasmons in various environments** — •David Odenthal, David Engemann, and Heinz Hövel — Fakultät Physik/DELTA, Technische Universität Dortmund, 44227 Dortmund

The research on clusters, consisting from a few up to some hundreds silver atoms, shall shed light on their behaviour compared to a solid-state body or a single atom. Depositioning clusters into various environments is necessary to apply their special properties, for instance their reactivity in catalysis.

To investigate the properties of clusters on surfaces, various amounts of clusters were deposited into silica aerogel (chem. $SiO_2$). Aerogel is a highly porous compound which contains mainly air (up to 99 vol.-%) and it is highly transparent for the wavelengths used in the experiments. The samples were irradiated with light ranging from ultraviolet to visible, so that cluster plasmons[1] were excited and the extinction spectrum was recorded. The results were then compared with theoretical models, so that physical variables like the thickness of a surrounding shell could be determined.

[1] U. Kreibig and M. Vollmer. *Optical Properties of Metal Clusters.* Springer-Verlag Berlin Heidelberg, 1995.

O 62.24 Wed 17:30 P1

**Two-photon photoemission spectroscopy: The effect of cluster superlattices on the electronic structure of Ir(111)/graphene** — •Kira Jochmann, Florian Knall, and Thorsten M. Bernhardt — University of Ulm, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany

A single graphite layer - namely graphene - supported by a metal crystal surface provides an ideal template for the ordered growth of regular cluster nanostructures with equally spaced and sized clusters. The ability to synthesize such ideal model systems opens completely new opportunities for fundamental research.

Two-photon photoemission (2PPE) spectroscopy is a method to experimentally gain an insight into the unoccupied electronic structure of these systems. The rather high work function of an iridium single crystal surface decreases with increasing graphene coverage, which enables the possibility to detect image potential state electrons by 2PPE at a laser wavelength of 266 nm [1].

In this contribution we report the influence of an Ir cluster superlattice on the overall workfunction and the image potential states, observed on the Ir(111)/graphene system as a function of Iridium coverage. Furthermore the influence of these nanostructures on the lifetime of the image potential states can be monitored by the means of time-resolved 2PPE.

[1] D. Niesner, Th. Fauster, J. I. Dadap, N. Zaki, K. R. Knox, P.-C. Yeh, R. Bhandari, R. M. Osgood, M. Petrović, M. Kralj, Phys. Rev. B 85, 081402 (2012).

O 62.25 Wed 17:30 P1

**Initial growth of heteromolecular layers studied by LEEM** — •Caroline Henneke, Daniel Schwarz, Jonas van Bebber, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and Jülich Aachen Reseach Al-

liance (JARA)-Fundamentals of Future Information Technology

One crucial issue for the performance of organic materials in electronic devices is the ability to specifically design the interfaces between different active layers according to their functional purpose. Heteromolecular films are of highest interest in this context, in particular their initial growth and the structure formation of the first molecular layer since this layer acts as a template for further growth.

We have investigated a prototypical donor-acceptor system containing copper-II-phthalocyanine (CuPc) and 3,4,9,10-perylentetracarboxylic-acid dianhydride (PTCDA) molecules adsorbed in mixed films on low-index noble metal surfaces. Kinetic processes like thin film growth, the formation of the organic mixed layer, and the transitions between different phases were studied in real time with LEEM. The lateral structure of the different phases was investigated with LEED.

O 62.26 Wed 17:30 P1

**Simulation of angle-resolved photoemission cross-sections for organic/metal interfaces** — •Dario Knebl, Daniel Lüftner, Bernd Kollmann, and Peter Puschnig — Karl-Franzens-Universität Graz, Institut für Physik

Several combined experimental / theoretical investigations have demonstrated a close relation between the angle-resolved photoemission (ARPES) intensity of oriented organic molecular films and the Fourier transform of the molecular orbital. So far, experimental ARPES data has been accounted for by neglecting the interaction of molecule with the underlying metal substrates. The remaining small differences have been tentatively attributed to modifications of the molecular states due to molecule-substrate hybridization, though alternative explanations, e.g., light polarization effects or the failure of the simple plane-wave final state approximation could not be excluded. Here we calculate ARPES intensity maps for the prototypical PTCDA/Ag(110) interface by explicitly considering molecule-substrate interactions within ab-inito density functional calculations. In order to take into account the free mean path of photo-emitted electrons, we modify the final state plane wave by introducing an exponential decay term of the final state. We perform careful convergence studies with respect to the number of metallic layers and the number of k-points, and compare our results to ARPES measurements. Thereby, we shed light on the molecule-metal hybridization and reveal limitations of the plane-wave final state approximation for such molecular films.

O 62.27 Wed 17:30 P1

**STM investigations of functional platform adlayers on Au(111) surfaces** — •Andreas Bloedorn[1], Sonja Kuhn[1], Frauke Claussen[1], Ulrich Jung[1], Sandra Ulrich[2], Rainer Herges[2], and Olaf Magnussen[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany — [2]Otto Diels-Institut für Organische Chemie, Universität Kiel, 24098 Kiel, Germany

Functionalized adsorbate layers are of great interest for advanced nanosystems containing molecular switches, motors, or light harvesting systems. We employ triazatriangulenium (TATA) [1,2,3] or trioxatriangulenium (TOTA) [4] ions for attaching functional molecules to a metal surface. These molecular platforms can be functionalized at the central carbon atom as well as by alkyl side chains. Using this versatile concept, it is possible to control the orientation and distance of the functional group with respect to the surface and the intermolecular distance.

Here, detailed STM investigations of TATA adlayers with alkyl side chains from propyl to dodecyl on Au(111) surfaces are presented, showing that the favoured hexagonal superstructure varies with the alkyl chain length. Furthermore, results on functionalized TATA derivatives containing azobenzene derivatives or porphyrins are shown.

This work was supported by the Deutsche Forschungsgemeinschaft via SFB 677.

[1] Baisch et al., J. Am. Chem. Soc. (2009), 131, 442. [2] Kuhn et al., PCCP (2010), 12, 4481. [3] Kubitschke et al., Eur. J. Org. Chem. (2010), 5041. [4] Kuhn et al., Chem. Commun., (2011), 47, 8880-8882.

O 62.28 Wed 17:30 P1

**Self-assembled molecular triangles with a central pillar unit pointing towards the third dimension** — •Stefan-Sven Jester, Anna Jochemich, Eva Sigmund, and Sigurd Höger — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Shape-persistent molecular triangles with an intraannular unit pointing towards the third dimension are designed, synthesized and investigated. The molecules self-assemble at the solution/solid interface on HOPG to form highly ordered patterns. *In situ* scanning tunneling microscopy gives an insight into the driving forces for supramolecular self-assembly. The molecular design and substitution pattern is consistent with our previously published set of molecular triangles, squares, pentagons, and hexagons.[1] Consequent with our expectation, the intraannular substituted triangular molecules mix with the hexagons to form periodic cocrystals. [1] S.-S. Jester, E. Sigmund, S. Höger *J. Am. Chem. Soc.* **2011**, *133*, 11062.

O 62.29 Wed 17:30 P1

**IV-Analysis of organic adsorbates investigated by MCP-LEED** — •Ina Krieger[1], Oliver Bauer[1], Georg Held[2], and Moritz Sokolowski[1] — [1]Institute for Physical and Theoretical Chemistry, University of Bonn, Wegelerstraße 12, 53115 Bonn, Germany — [2]University of Reading, Department of Chemistry, Whiteknights, Reading, RG6 6AD, UK

OVER the last years, the adsorption geometries of some large aromatic molecules on metal surfaces could be determined by the normal incidence wave technique (NIXSW). However, NIXSW is rather elaborate and requires synchrotron radiation. In addition, any substrate reconstruction is difficult to access by NIXSW. Hence we investigate whether LEED-IV analysis, the conventional method for the determination of adsorption sites of adsorbates, is suitable for this purpose. We have chosen PTCDA on Ag(100) as a test systems, because this adsorption geometry had been determined in detail by NIXSW and DFT before [1]. We find reasonable agreement of experimental and theoretical IV curves and support for the surface buckling predicted by DFT. In addition, we discuss current problems of the experiment and the theoretical evaluation. Supported by the DFG.

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[1] O. Bauer, G. Mercurio, M. Willenbockel, et al., Physical Review B 86 (2012) 235431.

O 62.30 Wed 17:30 P1

**First Steps Towards Anchoring Large Functional Organic Molecules on MgO(100)** — •Quratulain Tariq, Michael Röckert, Matthias Franke, Hans-Peter Steinrück, and Ole Lytken — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen, Egerlandstraße 3, Germany

The emerging field of organic/oxide interfaces has a huge scientific and technological potential in molecular electronics, solar energy conversion, catalysis or sensor development. At the microscopic level, however, oxide bonding sites, interaction mechanisms, bonding geometries and structure formation processes at organic/oxide interfaces are among the most poorly understood and least controlled aspects of such systems. Controlled growth of nanostructured films requires selective bonding between particular linker groups and specific surface sites. Such linkers may also generate a defined molecular contact to larger functional molecular entities such as porphyrins or fullerenes. By an appropriate choice of the linker groups, the bonding sites, orientation, density and ordering of such systems could in principle be controlled. In present study, we will be investigating the surface interactions, thermal stability and transformations of the benzonitrile (C6H5-CN) and catechol (C6H4(OH)2) on MgO(100) thin films on Ag(100) as a function of temperature and coverage, by means of x-ray photoemission spectroscopy (XPS) and temperature programmed desorption (TPD).

O 62.31 Wed 17:30 P1

**Highly strained bicyclophanes on HOPG** — Gabi Ohlendorf[1], Christian W. Mahler[1], •Stefan-S. Jester[1], Gregor Schnakenburg[2], Stefan Grimme[3], and Sigurd Höger[1] — [1]Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany — [2]Universität Bonn, Institut für Anorganische Chemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany — [3]Universität Bonn, Mulliken Center for Theoretical Chemistry, Institut für Physikalische und Theoretische Chemie, Beringstrasse 4, 53115 Bonn, Germany

Architectures with aromatic units aligned perpendicularly to the graphite surface are rarely observed but may become of interest when functionalization towards the volume phase is desired. Recently, our group reported on a convenient synthesis of complex phenyl substituted *p*-phenylene oligomers without the need of common transition metal catalyzed cross-coupling reactions requiring complex protective group strategies. Based on these oligophenylenes, bicyclic components are obtained in very good yields. As confirmed by state-of-the-art DFT calculations, the molecules have a planar bicyclic unit with a perpendicular center which seems to be a promising structural unit to reach the purpose of three-dimensional growth on surfaces. Self-assembled monolayers of the bicyclophanes at the solid/liquid interface of 1-phenyloctane and HOPG are visualized by scanning tunneling microscopy (STM). [1] G. Ohlendorf, C. W. Mahler, S.-S. Jester, G. Schnakenburg, S. Grimme, S. Höger *Angew. Chem. Int. Ed.* **2013**, *125*, 12308.

O 62.32 Wed 17:30 P1

**Adsorption Dynamics of Tetrahydrofuran on Si(001)** — •Marcus Lipponer[1], Michael Dürr[1,2], and Ulrich Höfer[1] — [1]Fachbereich Physik, Philipps-Universität Marburg — [2]Institut für Angewandte Physik, Justus-Liebig-Universität Giessen

The functionalization of semiconductor surfaces by means of organic molecules is of great interest due to possible applications in the field of nanoelectronics. However, only little information is available on the reaction dynamics of organic molecules on semiconductor surfaces. Recent STM/XPS experiments from our group have shown that tetrahydrofuran (THF), which is a cyclic ether molecule and is used as a typical organic solvent, shows a complex surface chemistry on Si(001). These experiments suggest that initial reaction with the silicon surface occurs via an electron lone pair of the oxygen atom by forming a dative bond with the lower atom of the Si dimer.

On this poster, we show results from molecular beam experiments of THF on Si(001): With increasing kinetic energy of the impinging molecules, we find a decrease of the initial sticking coefficient as it is typical for a non-activated reaction channel. However, the decrease is much less pronounced than e.g. in the case of $C_2H_4$/Si(001), pointing towards a more efficient energy dissipation in the case of THF/Si(001). With increasing surface temperature a decrease of the initial sticking coefficient is observed, which gives information on the energetics of the datively bound intermediate state.

## O 63: Posters: Scanning Probe Methods

Time: Wednesday 17:30–21:00 Location: P2

O 63.1 Wed 17:30 P2

**Toward a multiprobe- high frequency- spin-polarized scanning tunneling microscope** — •Johannes Friedlein, Andreas Sonntag, Jonas Harm, Stefan Krause, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg

Controlling the dynamics of domain walls in nanowires by spin-polarized currents and magnetic fields is essential for the development of new spintronic devices [1,2]. Recently, the determination of spin-relaxation times in the nanosecond regime by means of pump-probe methods using a spin-polarized scanning tunneling microscope (SP-STM) has been reported [3].

We propose a multiprobe SP-STM that is optimized for picosecond time resolution in an external magnetic field and at temperatures below 2 K. This setup will enable us to investigate ultrafast spin transport dynamics in magnetic systems down to the atomic scale using pump-probe methods, e.g. measuring the domain wall propagation velocity along an atomic chain. Applying voltage pulses shorter than 100 ps to the tunnel junction requires a high bandwidth of at least 10 GHz and a short cabling length. This is in direct contrast to the low temperature concept of minimizing thermal flux input. We will present design considerations for simultaneously achieving the desired high frequency, low temperature and multiprobe properties.

[1] D. A. Allwood *et al.*, Science **309**, 1688 (2005)
[2] S. S. P. Parkin *et al.*, Science **320**, 190 (2008)
[3] S. Loth *et al.*, Science **329**, 1628 (2010)

O 63.2 Wed 17:30 P2

**Manipulating the magnetic properties of a single atom by controlled hydrogenation** — Alexander Ako Khajetoorians[1], Tobias Schlenk[1], Manuel Steinbrecher[1], Maria Valentyuk[2], Benedikt Schweflinghaus[3], Manuel dos Santos Dias[3], Mohammed Bouhassoune[3], Samir Lounis[3], Alexander Lichtenstein[2], •Jens Wiebe[1], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, Hamburg University — [2]I. Theoretical Institute of Physics, Hamburg University — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA

Utilizing a combination of inelastic scanning tunneling spectroscopy and first-principles calculations within density functional theory, we describe how the magnetic properties of a single Fe atom on Pt(111) is modified by the adsorption of hydrogen. The most prominent effect of hydrogen adsorption onto a clean Fe atom is to modify the magnetic anisotropy and thereby the excitation energy. Binding site dependent studies as a function of the number of adsorbed hydrogen atoms shows that hydrogenation favors out of plane magnetic anisotropy. For the case of the hcp adatom, where the clean adatom has an easy plane anisotropy, full hydrogenation leads to significant Kondo screening. Magnetic field and temperature dependent studies of the Kondo resonance confirm a Kondo temperature of a few Kelvin. We further illustrate, by tip induced desorption, that we can controllably reverse the magnetic properties of these Fe hydrogen complexes. These conclusions are corroborated by calculations of hydrogenation-induced modifications in the relaxation and band structure.

O 63.3 Wed 17:30 P2

**Electronic and magnetic properties of $\mathrm{Gd_3N@C_{80}}$ on Cu(100)** — •Gelavizh Ahmadi[1], Christian F Hermanns[1], Matthias Bernien[1], Alex Krüger[1], Christian Schmidt[1], Sören T Wasserroth[1], Benjamin W Heinrich[1], Martin Schneider[2], Piet W Brouwer[2], Katharina J Franke[1], Eugen Weschke[3], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut für Theoretische Physik and Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Straße 15, 12489 Berlin, Germany

Rare earth elements with large magnetic moments have attracted enormous attention in spintronic studies. One promising way to gain a better control of their magnetic properties is using a carbon cage to encapsulate them. We use scanning tunneling microscopy (STM) and spectroscopy (STS) combined with angle-dependent X-ray magnetic circular dichroism (XMCD) to investigate $\mathrm{Gd_3N@C_{80}}$ endohedral fullerenes adsorbed on Cu (100). STM topographs reveal that the molecules adsorb with different orientation with respect to the substrate. Spectra of the differential conductance show resonances which are linked to the molecular orbital of the carbon cage. Depending on the orientation of the fullerene cage the energy position of the molecular orbitals varies. Furthermore XMCD spectra evidence ferromagnetic coupling of the magnetic moments of the gadolinium atoms within one cage.

O 63.4 Wed 17:30 P2

**Tunneling anisotropic magnetoresistance at the single atom limit** — •Johannes Schöneberg[1], Nicolas Néel[2], Silke Schröder[3], Paolo Ferriani[3], Jörg Kröger[2], Richard Berndt[1], and Stefan Heinze[3] — [1]IEAP der Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [3]ITAP der Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

The spin orbit coupling (SOC) links the magnetic moment of electrons to the crystal lattice. In a scanning tunneling microscope, this enables the study of magnetic characteristics without the need for spin polarized tips. A prominent example is the second monolayer Fe/W(110) where nonmagnetic tips served to observe the domain walls at low bias in maps of the differential conductance. The observed contrast is due to different mixing of the states dominating the tunneling current caused by the changing orientation of the spin quantization axis. We use this surface to examine the SOC induced change in the differential conductance at the single atom limit. To this end atoms adsorbed on domains as well as domain walls are investigated. The different magnetic environments lead to variations in the conductance. This difference is quantified by means of the tunneling anisotropic magnetoresistance (TAMR).

O 63.5 Wed 17:30 P2

**Spin-dependent scanning probe images of antiferromagnetic NiO(001) surfaces: A first-principles approach** — •Mihail Granovskij, Andreas Schrön, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

We present an accurate *ab-initio* description of the magnetic exchange force microscopy (MExFM). As a prototypical system the antiferromagnetic NiO(001) surface probed with a Fe tip is investigated.[1]

The tip-surface interaction is described on two levels. Short-range chemical and exchange forces between the tip apex and surface atoms are described in the framework of spin-polarized density functional theory (DFT) while long-range van-der-Waals forces are considered within a mesoscopic tip model. Exchange and correlation (XC) are treated within the local density approximation (LDA). For the Ni atoms in the NiO surface and the Fe atoms of the tip apex, an additional on-site Coulomb interaction $U$ acting on the transition-metal $3d$ shells is included (LDA+$U$).

In order to understand the tip-surface interaction, we investigate the changes in the electronic structure of tip and surface versus distance. The resulting frequency shifts and MExFM images are presented and compared with recent experimental data.

[1] M. Granovskij *et al.*, Phys. Rev. B 88, 184416 (2013)

O 63.6 Wed 17:30 P2

**Ab-initio Calculation of the Vibrational Spectra of Single Molecules** — •Felix Schwarz[1,2], Yongfeng Wang[3,4], Richard Berndt[3], Erich Runge[1], Werner A. Hofer[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau — [2]Stephenson Institute for Renewable Energy, University of Liverpool, Liverpool L69 3BX, United Kingdom — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel — [4]Department of Electronics, Peking University, Beijing 100871, China

Inelastic electron tunnelling spectroscopy with a scanning tunnelling microscope is an important tool for the chemical analysis of single molecules on surfaces. However, the amplitude of vibrational signatures in spectra of the differential conductance (dI/dV) is difficult to predict. Here, an ab-initio method to quantify contributions of molecular vibrations to dI/dV spectra following Lorente [1] is presented. The applicability of the method for fairly large molecules is demonstrated for tin-phthalocyanine on Ag(111). Calculated and experimental data are in good agreement. The experimentally observed satellite peaks around the lowest unoccupied molecular orbital are assigned to vibrational resonances. In addition, non-local effects of the electron-vibration coupling are presented.

[1] N. Lorente, Appl. Phys. A 78, 799 (2004)

O 63.7 Wed 17:30 P2

**Proposal for tracing the local ionization dynamics of adsorbed molecules by photo-assisted scanning tunneling microscopy** — •Michael Schüler and Jamal Berakdar — Martin-Luther University Halle-Wittenberg, Institute for Physics, Karl-Heinrich-von-Fritsch-Straße 3, 06120 Halle, Germany

For tracing the spatiotemporal evolution of electronic systems we suggest and analyze theoretically a setup that exploits the excellent spatial resolution based on scanning tunneling microscopy techniques combined with the temporal resolution of femtosecond pump-probe photoelectron spectroscopy. As an example we consider the laser-induced, local vibrational dynamics of a surface-adsorbed molecule. The photoelectrons released by a laser pulse can be collected by the scanning tip and utilized to access the spatio-temporal dynamics. Our proof-of-principle calculations are based on the solution of the time-dependent Schrödinger equation supported by the ab initio computation of the matrix elements determining the dynamics.

O 63.8 Wed 17:30 P2

**Capacitively guided tip-to-tip positioning for multiprobe spin-polarized scanning tunneling microscopy** — •Jonas Harm, Johannes Friedlein, Andreas Sonntag, Stefan Krause, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Hamburg, Germany

To investigate magnetic transport properties on the atomic scale, we currently set up a multiprobe spin-polarized scanning tunneling microscope (SP-STM), that is designed for high-frequency applications in a magnetic field of 3 T at temperatures below 2 K in ultra-high vacuum. One of the challenges in such a system is the positioning of two tunneling tips at a distance of only a few nanometers. The external magnetic field excludes the use of a scanning electron microscope for positioning the tips within a common scan frame [1]. We present a novel tip-to-tip approach, extending known tip-to-tip tunneling methods [2,3] by utilizing distance dependence of the capacitance between two tips, allowing a fast and safe approach. Since the minimum distance between the tips is limited by their tip radii and opening angles, we adapted tip preparation techniques [4], thereby enabling future transport measurements at tip-to-tip distances in the range of $10 - 20$ nm.

[1] T. Nakayama *et al.*, Adv. Mater. **24**, 1675 (2012)
[2] A. Matsui *et al.*, Rev. Sci. Instrum. **78**, 106107 (2007)
[3] H. Grube *et al.*, Rev. Sci. Instrum. **72**, 4388 (2001)
[4] Y. Khan *et al.*, Rev. Sci. Instrum. **83**, 063708 (2012)

O 63.9 Wed 17:30 P2

**Application of Bardeen's tunneling formula for the calculation of STM data** — •Steffen Seiler[1], Roman Kováčik[2], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich

The tunneling current in scanning tunneling microscopy (STM) is determined by a convolution of the electronic structure of the tip and the substrate. However, in the most commonly used method for calculating STM data, the Tersoff-Hamann approximation [1], all specific details of the tip electronic structure are neglected. One step beyond this simplification is Bardeen's perturbation approach [2], in which the tip electronic structure is explicitly taken into account.

Both methods have been implemented in our STM simulation program [3]. The code was recently largely extended and modified, most importantly by including multiple k-points and fractional occupation numbers for a proper treatment of metallic systems. The program was tested for various oxidized Cu surface structures and tip models. Different benchmark tests were carried out, all confirming the correct functionality of the program and giving some interesting insights into the electronic structure of CuO$_x$ monolayers on a Cu(111) substrate.

[1] J. Tersoff, D. Hamann, *Phys. Rev. B* **31**, 805 (1985).
[2] J. Bardeen, *Phys. Rev. Lett.* **6**, 57 (1961).
[3] R. Kováčik, B. Meyer, D. Marx, *Angew. Chem. IE*, **46**, 4894 (2007).

O 63.10 Wed 17:30 P2

**Detecting the topographic, chemical and magnetic contrast at surfaces with nanometer spatial resolution** — •Danilo Andrea Zanin, Mehmet Erbudak, Lorenzo G. De Pietro, Hugo Cabrera, Andreas Fognini, Thomas Michlmayr, Yves M. Acremann, Alessandro Vindigni, Danilo Pescia, and Urs Ramsperger — ETH Zurich, Switzerland

For many decades the development and investigation of magnetic nanostructured materials has been motivated by the quest for novel paradigms for magnetostorage and spintronics. The possibility of resolving magnetic-textures in real space with increasing spatial resolution has, indeed, always opened novel applicative and fundamental perspectives. Scanning-Electron-Microscopy with Polarization Analysis (SEMPA), e.g., made it possible to directly observe the re-entrant transitions of magnetic-domain patterns in thin films of Fe on Cu(001). Inspired by the Russel Young topografiner we redesigned the SEMPA setup, by replacing the primary electron beam source and the probing method. We dubbed this new technique Near Field-Emission Scanning Electron Microscopy (NFESEM). Currently, NFESEM technique is capable to resolve the topography of metals and semiconductors with nanometer lateral resolution and detect the entire spectrum of SE induced by a low-energy primary electron beam. We report on promising results of single-energy surface imaging, which confirm the technical feasibility of electron spectroscopy and magnetic-domain mapping with a nanometer spatial resolution.

O 63.11 Wed 17:30 P2

**Construction of a multiscale and multitype scanning probe microscope** — •Boris Gross, Hanna Fedderwitz, Hendrik Sträter, and Niklas Nilius — Carl-von-Ossietzky Universität, Oldenburg, Deutschland

Little is known about the optical and electronic phenomena that control the functionality of thin-film solar cells on a mesoscopic length scale ranging from tens of $nm$ up to a few $\mu m$. In fact, conventional techniques to characterize dielectric surfaces average over macroscopic sample areas and are therefore unsuitable to probe local effects. In contrast, SPM approaches capable of atomic resolution are still too complex and challenging to use them for a quick sample characterization. The gap between both techniques might still hold important information on the functionality of electronic and photovoltaic devices, in particular if not only morphological but also spectroscopic techniques are available for characterization. In this poster, we present the design for a versatile scanning probe microscope that combines the capabilities of AFM and STM with local photo-luminescence spectroscopy. The microscope's key parameters are: Multi-scaling capabilities with image sizes from $10\,nm$ to $500\,\mu m$, various feedback modes to enable AFM and STM operation, use of different probe tips as nearfield sensor for local reflection and transmission studies and variable pressure and temperature ranges between $10^3 - 10^{-6}\,mbar$ and $77 - 300\,K$.

O 63.12 Wed 17:30 P2

**Construction of a low-temperature STM for luminescence spectroscopy** — •Hanna Fedderwitz, Boris Gross, Hendrik Sträter, and Niklas Nilius — Carl von Ossietzky Universität Oldenburg

Luminescence spectroscopy stimulated by electrons of an STM tip has recently been used to analyze the nature of point defects in ZnO films (1). The approach enabled a spectral identification of O and Zn vacancies with 100nm spatial resolution. These limits were given by the need to produce a finite number of electron-hole-pairs in the oxide band gap via impact of energetic tip-electrons. The required electron energy was determined to be 100eV, too high to map the optical response with true nm resolution and without damaging the oxide surface.

To overcome these limitations, we have developed a new scanning tunneling microscope suitable for low-temperature luminescence measurements. The setup is based on the beetle design, but uses a tapered and metal-coated optical fiber as sensor tip. The microscope is surrounded by a parabolic mirror for efficient photon collection. Our setup enables an all-optical characterization of sample surfaces, in which photons are either injected into or collected from the tip-sample junction via the fiber tip. The tip-sample distance is controlled by the STM-feedback loop, which also allows us to probe the sample topography with atomic resolution. The target application for our new setup is photoluminescence spectroscopy on thin dielectric films as used in photocatalysis.

(1) Stavale, Nilius, Freund, J. Phys. Chem. Lett. 4, 3972 (2013)

O 63.13 Wed 17:30 P2

**Fabrication of gold nanocone near-field scanning optical microscopy probes** — •Omar Tanirah, Dieter P. Kern, and Monika Fleischer — Institute for Applied Physics, Eberhard Karls University Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Near-field scanning optical microscopy (NSOM) is an excellent method in its ability to probe the morphology of samples at the same time as their local optical properties, and can be integrated with tip-enhanced Raman spectroscopy. Hence, simultaneous investigatons of the morphology, physical and chemical properties on the nanometer scale can be obtained. The NSOM probe has an important role in enhancing the performance of the NSOM measurements. One such approach is the fabrication of probes based on plasmonic nanostructures. They exhibit localized surface plasmon resonances, and enable a resolution far beyond the diffraction limit. Gold nanocones are interesting plasmonic nanostructures for this purpose, since the near-field of the plasmons is strongly localized around the nanocone tip of radius smaller than 10 nm. We report here the fabrication process of gold nanocones as novel NSOM probes on both cantilevers and optical fibres [1, 2]. The fabrication process is achieved by wet etching, focused gallium ion beam, sputtering, electron beam evaporation, and electron beam induced deposition. Finally, a gold nanocone is formed after etching the samples in an argon-ion milling machine. The samples are characterized using scanning electron microscopy. The fabrication process and resulting probes will be shown. [1] M. Fleischer, Nanotechnol. Rev.1 (2012) 313. [2] M. Fleischer et al., ACS Nano 5 (2011) 2570.

O 63.14 Wed 17:30 P2

**Wavelet analysis of inelastic electron tunneling spectra** — •Matthias Stocker and Berndt Koslowski — Universität Ulm, 89081 Ulm, Germany

Experiments of inelastic electron tunneling spectroscopy (IETS) are carried out typically at the absolute noise limit. Furthermore, the interpretation of such spectra - being just the second derivative of the tunneling current - is greatly hampered by contributions which do not originate from vibrational transitions. As a consequence, data evaluation occupies a central point in IETS. We developed an analysis tool which employs continuous wavelet transform on the basis of the Mexican hat mother function. The Mexican hat function is essentially the second derivative of a Gaussian peak and thus a peak function similar to the Gaussian peaks expected for vibrational transitions in IETS. This wavelet analysis helps very much in localizing and judging vibrational transitions. We introduce the new analysis and compare it to formerly developed techniques.

O 63.15 Wed 17:30 P2

**Dynamic Friction Force Microscopy on antimony nanoparticles** — •Thomas Göddenhenrich, Felix Mertens, and André Schirmeisen — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, D-35392 Gießen

Dynamic Friction Force Microscopy is a valuable scanning probe technique for detection of friction properties. The nonlinear interaction between tip and sample induces a sensitive signal containing the friction information for different tip-sample contacts. The third harmonic lock-in detection on antimony nanoparticles clearly reveals the signal contrast dependence on the modulation amplitude and frequency. Therefore the detection of frictional information of the sample system requires a modulation frequency spectrum to receive the basic information of the damped system between tip and sample, namely the qualitiy factor Q and optimal excitation frequency.

O 63.16 Wed 17:30 P2

**Measuring near field mediated absolute heat fluxes with the Near Field Scanning Thermal Microscope (NSThM)** — •Konstantin Kloppstech, Nils Könne, Achim Kittel, Ludwig Worbes, and David Hellmann — EHF, Fak. V, Inst. f. Physik, CvO Universität Oldenburg

Experimental analysis of near-field heat transfer on the nanoscale by means of absolute fluxes is based on accurate knowledge of our thermocouple sensors thermal resistance. This sensor combines a standard scanning tunneling microscope tip with a coaxial thermocouple, consisting of a thin Pt-wire coated with a 200 nm layer of Au. We present measurements and a wide analysis for our in situ method for measuring the sensors thermal features. Therefore one needs a defined and metrological accessible heat reservoir. That for our sample is held in UHV conditions and consists of a 5 $\mu m$ thin and 3-10 mm long tungsten wire which is glued to an electrically insolated copper block. The thin wire is heated with high frequency AC currents and can be described with the 1D heat diffusion equation. The wire is cooled additionally by approaching the thermocouple tip to its middle. From the decrease in heating we determine the heat flux through the thermocouple tip which then can be attributed to the additionally measured thermopower of the tip sensor. To achieve highest precision we have analyzed our system and present besides measurements the major metrological aspects that must be considered. This enables us to locally probe the near field mediated heat fluxes on the nanoscale by means of absolute values.

O 63.17 Wed 17:30 P2

**Single molecule heat transport** — •Nils Könne, Konstantin Kloppstech, Ludwig Worbes, David Hellmann, and Achim Kittel — EHF, Fak. V, Physik, Carl von Ossietzky Universität Oldenburg

The heat transport and dissipation in molecular junctions is a topic of high interest [1] and scientific value. To overcome the experimental challenges of contacting a single molecule and detecting the heat transport we are using our self-developed near field scanning thermal microscope (NSThM) which consists of a STM with a nanoscale build in thermocouple in the tip. This allows us, to measure simultaneously the electrical $I(t)$ and heat $\dot{Q}(t)$ current as a function of time and temperature under ultra high vacuum conditions. Analogous to the determination of the electrical transport through a molecule we are using the so called $I(t)$-Method, introduced by W. Haiss et al [2] which reveals the spontaneous formation of metal - molecule - metal junctions leading to an on-and-off switching process of a single molecule. This will be used to identify the heat transport through a single molecule. First results are presented for octanedithiol as a typical linear switching molecule. [1] Woochul Lee et al, Nature 498, 209 (2013). [2] Wolfgang Haiss et al, Phys. Chem. Chem. Phys. 6, 4330-4337 (2004)

O 63.18 Wed 17:30 P2

**Electronic pump-probe experiments in STM using THz-pulses** — •Steffen Rolf-Pissarczyk[1,2], Jacob Burgess[1,2], Deung-Jang Choi[1,2], Shichao Yan[1,2], and Sebastian Loth[1,2] — [1]Max-Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg — [2]Max-Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Fast dynamics at picosecond timescales are full of interesting phenomena such as depinning of charge density waves, molecular vibrations or spin precession on surfaces. The challenge is to observe those effects on this timescale with atomic or nanometer spatial resolution. For this propose we combine a scanning tunneling microscope (STM) with ps THz-laser pulses. This technique couples directly to the STM tip with THz radiation instead of exciting the sample with optical pulses. This technique enables control of the electric field at the tunnel junction with the THz pulses independent to the nature of the sample. This generality allows exciting and probing a various number of systems. The experimental setup is similar to all-electronic pump-probe methods but without limitations imposed by the electrical bandwidth of wires. Progress on the new instrument is described and first measurements will be presented.

O 63.19 Wed 17:30 P2

**Laser induced Time Resolved Scanning Tunneling Microscopy** — •Philipp Kloth, Christian Werner, Karen Teichmann, and Martin Wenderoth — IV. physik. Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We present a detailed description of a combined setup of a pulsed laser source and a Scanning Tunneling Microscope (STM) in Ultra High Vacuum. The most demanding issue of light excitation in STM is the handling of thermal effects. For time resolved operation this challenge results in a transformation of standard pump-probe pulses into complex laser pulse patterns. Triggered by the groundbreaking results of Shigekawa [1] our intention was to develop a setup with a stronger focus on the flexibility.

We generate pulsed laser light in a pure electronic way. A diode laser in combination with a high-bandwidth electro-optical modulator produces light excitation from continuous-wave mode to single nanosecond pulses. The voltage pulses are supplied by a commercial function generator. This allows to adapt the pulse pattern exactly to the timescale needed in the experiment.

Results on the GaAs(110) surface show a huge impact on the spectroscopic properties due to the light excitation. Electron-hole pair generation is not only affecting the always present charge region in the sample but also opens new tunnel channels resulting in extra current. Time resolved studies allow to probe these processes individually revealing characteristic decay constants in the nanosecond regime.

[1]Terada et al., Nature Photonics, 4(12), 12 2010.

O 63.20 Wed 17:30 P2

**Design of a variable temperature scanning tunneling microscope** — •Sebastian Schimmel[1,2], Christian Salazar[1], Martha Scheffler[1], Ronny Schlegel[1], Danny Baumann[1], Torben Hänke[1], Bernd Büchner[1,3], and Christian Hess[1,3] — [1]IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany — [2]Westsächsische Hochschule Zwickau — [3]Center for Transport and Devices of Emergent Materials, TU Dresden, 01069 Dresden, Germany

We present the design of a variable-temperature scanning tunneling microscope (STM) in ultra-high vacuum (UHV) conditions and operating temperatures between room temperature and 15 K. Our UHV system comprises a separated STM and preparation chamber which is equipped with all required devices for organic molecular beam epitaxy and spin-polarized scanning tunneling microscopy.

O 63.21 Wed 17:30 P2

**A combined LT-STM/FIM for tip specific tunnelling experiments** — •Ben Wortmann, Matthias Müller, and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

We present details on a homebuilt, compact, low temperature scanning tunnelling microscope that allows in situ field ion microscopy of a cooled tunnelling tip inside the STM. The tip can be characterised without transfer to a different position in the UHV system, so that the probability for the modification of the tip can be strongly reduced. Ideally the tip remains unchanged. The geometry of the microscope resembles a cylinder with a height of 13 cm and a diameter of 4 cm. The STM is screwed directly onto a commercially available continuous flow cryostat which allows cooling to about 5-7 K. The very compact design minimises helium consumption to about 1 litre/hour. Insulation from vibration is provided by a combination of springs and eddy current damping. Shutters at the bottom of the microscope can be opened to expose the tip to a channel plate or closed to assure lower temperatures and minimal thermal drift while tunnelling. A combination of two piezos is used to move a magnetically attached slider holding the tip. The slider can be easily exchanged in vacuum. The performance of the STM setup has already been shown for an almost identical system [1]. [1] (H. Karacuban, M. Lange, J. Schaffert, O. Weingart, Th. Wagner and R. Möller, Surf. Sci. Lett., 603, Issue 5, L39 (2009).

O 63.22 Wed 17:30 P2

**z-resolution of 5 nm in a scanning electron microscope using a nanofinger** — •Martin Grob[1], Eva Maynicke[2], Ivo Burkart[2], Marcus Liebmann[1], Volker Klocke[2], and Markus Morgenstern[1] — [1]II. Inst. Phys. B, RWTH Aachen University, 52074 Aachen — [2]Klocke Nanotechnik, 52076 Aachen

Scanning electron microscopy (SEM) is a common technique for investigating surfaces on the nanometer scale. One main disadvantage is the low vertical resolution compared to the lateral resolution which can only be achieved by proper focussing. To overcome this limitation we implemented a small scanhead which operates the same way as an atomic force microscope (AFM) in the dynamic mode. With this additional sensor in the SEM we can reach a vertical resolution better than 5 nm. With this tool, a direct in-situ control mechanism is given, e.g. structures grown by electron beam induced deposition (EBID) can be characterized under vacuum conditions. In addition, this scanner can provide coordinates on a surface for the navigation of other tools such as contacting tips.

O 63.23 Wed 17:30 P2

**STM investigations of iron thin films on W(110)** — •christian salazar[1], martha scheffler[1], tim kühne[1], danny baumann[1], bernd büchner[1,2], and christian hess[1,2] — [1]Institute for Solid State Research, IFW Dresden, Germany — [2]Center for Transport and Devices of Emergent Materials, TU Dresden, 01069 Dresden, Germany

We have investigated the growth and the magnetic structure of iron thin films on a W(110) single crystal by scanning tunneling microscopy. We found that the growing conditions such as temperature and evaporation rate influence the growth of the nanostructures, so that, we observe the formation of islands, large patches with and without dislocation lines and nanowires. The magnetic properties were studied via spin-polarized scanning tunneling microscopy using different magnetic probes: iron coated tungsten tips, chromium coated tungsten tips and chromium bulk tips. Our data reveal in some cases magnetic domains in the first atomic layer of iron, indicative of in-plane magnetization and in other cases magnetic domains in the second atomic layer of iron, indicative of out-of-plane magnetization.

O 63.24 Wed 17:30 P2

**Kelvin Probe Force Microscopy on the submolecular scale** — •Florian Albrecht[1], Martin Fleischmann[2], Manfred Scheer[2], and Jascha Repp[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Inorganic Chemistry, University of Regensburg, 93053 Regensburg, Germany

Kelvin Probe Force Microscopy (KPFM) has been shown to be a powerful tool to detect the distribution of charges within a single molecule [1].

We performed KPFM measurements on two derivates of cyclic trimeric ortho-phenylene mercury (TPM) molecules in a low temperatures combined scanning tunneling and atomic force microscope with functionalized tips.

Whereas one of the derivates has hydrogen atoms bonded to the phenyl rings the other molecule is perfluorinated. For the latter the KPFM signal shows clear signatures of the polar fluorine carbon bonds. In addition, the fluorine influences the electron density also at the center of the molecule. The charge redistribution within the molecule was made responsible for the weak attraction of electron rich ligands at its center [2]. This charge redistribution is visualized in KPFM maps.

[1] F. Mohn, L. Gross, N. Moll, and G. Meyer, Nature Nanotechnology, 7, 227, (2012)

[2] M. R. Haneline, and F. P. Gabbai, Inorg. Chem., 44, 6248, (2005)

O 63.25 Wed 17:30 P2

**Investigation of 1,6,7,12-tetraazaperylene molecules on an insulating film by means of LT-STM** — •Nemanja Kocić[1], Peter Weiderer[1], Stephan Keller[2], Shi-Xia Liu[2], Silvio Decurtins[2], and Jascha Repp[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Departement für Chemie und Biochemie, Universität Bern, Switzerland

In recent years, metal-organic hybrid structures have received considerable attention because of their tunable electronic and magnetic properties. A promising strategy to obtain thermally and chemically stable structures through covalent bonding of suitable precursors directly on the substrate is the concept of on-surface synthesis. So far, successful demonstrations of on-surface synthesis have been limited to metallic substrates, however, a useful molecular electronic device would require its construction on an insulating surface. To this end, we performed low temperature scanning tunneling microscopy (LT-STM) on the 1,6,7,12-tetraazaperylene molecule (TAPE), which is a highly symmetric, planar, bi-facial bridging ligand with a large extended $\pi$-system. As such, TAPE is an attractive bridging ligand for the formation of new multimetallic systems of regularly spaced spin centers. Molecular self-assembly is investigated on an ultrathin insulating film that provides efficient electronic decoupling from the metal substrate, allowing detailed characterization of the molecular orbitals. When thermally activated at 300 K, individual metal atoms and TAPE molecules form metal-molecular complexes.

O 63.26 Wed 17:30 P2

**Versatile and compact UHV-System for Scanning Tunneling, Scanning Force and Transport Measurements exhibiting an operation time of 10 days below $T = 400$ mK and at $B = \pm 14$ T** — •Jan Raphael Bindel, Mike Pezzotta, Stefan Becker, Marcus Liebmann, and Markus Morgenstern — II. Institute of Physics B, RWTH Aachen, Germany

We use a UHV cryostat which hosts a fully UHV compatible $He_3$ cryostat with charcoal pump. The $He_3$ is condensed in mechanical contact with a 1 K pot, but decoupled afterwards providing low mechanical noise. The base temperature is 380 mK with a hold time greater than 10 days. Optical access enables *in-situ* tip and sample exchange and evaporation into the cooled microscope at 4.2 K. The home-built microscope allows conventional scanning tunneling microscopy and spectroscopy, non-contact atomic force microscopy via a qPlus sensor and magnetotransport measurements of the samples using five contacts at the same sample position, where scanning tunneling microscopy is performed. An *xy* table allows positioning of the tip with respect to the sample over 2x2 mm$^2$. For sample preparation and analysis, a three chamber ultrahigh vacuum system with a base pressure of $10^{-8}$ Pa has been built including low-energy electron diffraction (LEED), Auger electron spectroscopy, sputtering, annealing and evaporation. The whole system has a total height of only 2.60 m. STM images are presented with noise level in z-direction below 2 pm, lateral drift below 40 pm/h obtained at currents down to 500 fA.

O 63.27 Wed 17:30 P2

**Shot noise measurements at atomic contacts** — •Andreas Burtzlaff, Alexander Weismann, and Richard Berndt — IEAP, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Transport in atomic contacts is commonly characterized by measuring the conductance, which is the sum of the contributions of a set of quantum states, the so called transport channels. From the conductance alone, those contributions cannot be disentangled. By measuring the current dependent noise of an atomic contact it is possible to gain information on the number of channels contributing to the transport process and their transmission probabilities. Previously this approach has been successfully applied to semiconductor heterostructures as well as molecules and atomic contacts in MCBJ experiments. We perform such noise measurements using an STM at 4K and under UHV conditions. Preliminary results for single atom contacts will be shown.

O 63.28 Wed 17:30 P2

**Solid State Sample Environment at the European XFEL** — •Carsten Deiter, Oleksiy Drachenko, and Joachim Schulz — European X-Ray Free-Electron Laser Facility GmbH, Notkestr. 85, 22607 Hamburg, Germany

Free-electron lasers offer a variety of unique properties for spectroscopy and imaging. The combination of high peak brilliance and a high repetition rate opens a window to experiments that have not been feasible so far but also introduces challenges in sample preparation and refreshment, especially for solid state samples.

We present a concept and first prototype of a 10Hz sample changer opening the opportunity to expose every bunch train of the XFEL with its 2700 pulses to a new and virgin sample location, combined with temperature control, magnetic fields and optical pump lasers.

O 63.29 Wed 17:30 P2

**A quantum yield measurement setup for the charge compensation for the LISA Pathfinder space mission** — •Indro Biswas[1], Mathias Schulze[1], Gerald Hechenblaikner[2], Tobias Ziegler[2], Nico Brandt[2], Patrick Bergner[2], Felix Erfurth[3], and Markus Pfeil[3] — [1]Deutsches Luft- und Raumfahrtzentrum e.V., Pfaffenwaldring 38-40, 70569 Stuttgart — [2]Astrium Satellites GmbH, 88039 Friedrichshafen — [3]TWT GmbH Science & Innovation, Ernsthaldenstraße 17, 70569 Stuttgart

The evolved Laser Interferometry Space Antenna (eLISA) is an international fundamental research project with the aim of the detection of gravitational waves by monitoring the distance between two test bodies in space. The LISA pathfinder mission will perform experiments in a small scale with lower precision and identify upcoming challenges for the future mission. A contactless minimally invasive discharge system based on the photoemission process is necessary in order to avoid electrostatic forces on the test bodies. For the development the photoemission quantum yields of possible coatings were determined and uprising methodical issues were evaluated. An experimental setup was designed in a high vacuum chamber for the recording of the energy distribution of electrons emitted by UV radiation. The differences between the ideal spherical and a cylindrical setup with a possibility for quick sample exchange are explained.

O 63.30 Wed 17:30 P2

**The new multipurpose ARPES end-station on the SGM3 beamline at ASTRID2** — •Marco Bianchi[1], John E. Vad Andersen[1], Henrik Kjeldsen[1,2], Nykola Jones[1,2], Søren V. Hoffmann[1,2], and Philip Hofmann[1,3] — [1]Department of Physics and Astronomy, Aarhus University, Denmark. — [2]Center for Storage Ring Facilities, Aarhus University, Danmark. — [3]Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Denmark.

A new multipurpose end-station for electronic, geometrical and chemical characterisation has been built on the renewed SGM3 beamline at the synchrotron radiation source ASTRID2 in Aarhus (DK). The beamline covers photon energies from 14 to 150 eV. The system is particularly well suited for electronic structure studies along arbitrary direction in $k_{\|}$, Fermi surface mapping, bulk bands mapping and temperature dependent measurements.

The end-station allows ARPES multichannel detection with a combined energy resolution better than 7 meV and angular resolution better than $0.1^\circ$ with a 4 degree of freedom manipulator at 200-1300 K, or 5 degree of freedom manipulator at 70-800 K, or 6 degree of freedom manipulator at 25-500 K; sample preparation (sputtering, annealing 180-2300 K, chemical treatment, cleaving); STM measurement; Auger spectroscopy and epitaxial/MBE growth of thin films followed by RHEED. The poster describes the light source and the many opportunities of the end-station.

O 63.31 Wed 17:30 P2

**New PEEM and NEXAFS/EXAFS experiments at the synchrotron source DELTA: Ready for user** — •Christoph Keutner, Ulf Berges, Dominique Handschak, and Carsten Westphal — DELTA/Experimentelle Physik I, TU Dortmund, Maria-Goeppert-Mayer-Straße 2, 44221 Dortmund, Germany

We report on the setups of two new experiments at the PGM undulator beamline 11 (30 eV - 1000 eV) of Dortmund's synchrotron source DELTA.

The first experiment is a photoemission electron microscope (PEEM), which uses electrons emitted from an illuminated sample to generate a spatially resolved image of its surface. PEEM can be used for spatially resolved x-ray absorption spectroscopy (XAS) by scanning the photon energy and recording individual images within the sequence. Here, a Staib PEEM 350-20 with a spatial resolution of up to 220 nm is used. In combination with our self-developed S.P.A.M.M. software it enables a fully automatized data acquisition (image-squences and beamline flux) for XAS. The experimenter just has to specify basic parameters - e.g. energy range and step width.

The second setup is an extension to the existing XPS/XPD-machine.

By using our NEMeSUS software it is now possible to preform near-edge x-ray absorption fine structure (NEXAFS) and extended X-ray absorption fine structure (EXAFS) by using the total electron yield (TEY). Hence, a combination of highly surface sensitive XPS/XPD with deeper reaching NEXAFS/EXAFS-techniques in the identical geometric setup can be realized.

O 63.32 Wed 17:30 P2

**Spin-resolved core-level photoemission spectroscopy of W and TaS$_2$** — •Tim Haase, Arndt Quer, Erik Kröger, Lars Oloff, Matthias Kalläne, Lutz Kipp, and Kai Rossnagel — Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany

Electron spin polarization shows up in a number of effects at solid surfaces, most prominently via the spin-momentum locking in Rashba systems and topological insulators, but also of course via the exchange splitting in itinerant ferromagnets. All these effects may be used to validate spin detection schemes in photoemission spectroscopy. Here, however, to characterize a commercial 3D Mott detector, we have used an effect first described by Cherepkov [1,2], i.e., the spin specific photoemission from the core levels of nonmagnetic materials due to excitation with circularly polarized light. Employing the variable polarization soft X-ray beamline P04 of PETRA III (DESY), we have performed electron-spin- and photon-polarization-dependent $4f$ core-level photoemission spectroscopy of W and TaS$_2$. The results are interpreted in the context of free atom theory and possible deviations from the theory are discussed. The results are finally used to determine the Sherman function of the detector.

[1] N. A. Cherepkov, Phys. Lett. 40A, 119 (1972).

[2] N. A. Cherepkov, Soviet Physics JETP 38, 463 (1974).

O 63.33 Wed 17:30 P2

**3D nanofabrication of subsurface structures inside photosensitive glass with fs laser** — •Tobias Milde[1], Ulrike Brokmann[2], Edda Rädlein[2], and Klaus Liefeith[1] — [1]Department of Biomaterials, Institute for Bioprocessing and Analytical Measurement Techniques Heiligenstadt — [2]Group of Inorganic-Nonmetallic Materials, Department of Mechanical Engineering, Technische Universität Ilmenau

The development of miniaturized structures on or below the surface of glass is an issue of present research. Femtosecond-laser-radiation combined with the two photon process is a promising approach to push the written structures towards the nanometer scale. Here we used the photosensitive glass FS21 with its three step photoform process (irradiation, annealing, HF-etching). For the irradiation we used a TiSa oscillator only. These structures and steps are developed to realize a distinct miniaturization of glass components and to improve biocompatibility for specific cells. These structured glass are interesting for microfluidic and lab-on-a-chip devices.

## O 64: Poster: Surfaces, Interfaces and Heterostructures (HL jointly with O)

Time: Wednesday 17:00–20:00 Location: P1

O 64.1 Wed 17:00 P1

**Waveguide Quantum Electrodynamics - Nonlinear Physics at the Few-Photon Level** — Tobias Sproll[1], Christoph Martens[1], •Michael Schneider[1], Peter Schmitteckert[2], and Kurt Busch[1,3] — [1]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany — [2]Institut für Nanotechnologie, Karlsruher Institut für Technologie (KIT), 76344 Eggenstein-Leopoldshafen, Germany — [3]Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik und Photonik, Newtonstr. 15, 12489 Berlin, Germany

The transport of few photons in 1D structures coupled to a fermionic impurity gives rise to a set of non-linear effects, induced by an effective interaction due to Pauli blocking such as photon bunching and the formation of atom-photon bound states.

We analyze a specific example of such systems, namely a 1-D waveguide coupled to a 2-level system, for the case of one and two-photon transport. Therefore we have developed a general theoretical framework, which contains analytic approaches originating in methods of qutantum field theory, like path integrals and Feynman diagrams as well as powerful numerical tools based on solving the time-dependent Schrödinger equation.

Owing its generality, our approach is also applicable to more involved setups, including disorder and dissipation as well as more complicated impurities such as driven and undriven 3-level systems.

O 64.2 Wed 17:00 P1

**Defect states and band bending effects at c-Si(111)/a-SiN:H interfaces** — •Leif Eric Hintzsche[1], Changming Fang[1], Gerald Jordan[1], Martijn Marsman[1], Machteld Lamers[2], Arthur Weeber[2], and Georg Kresse[1] — [1]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — [2]ECN Solar Energy, P.O. Box 1, 1755 ZG Petten, Netherlands

High performance solar cells based on crystalline silicon (c-Si) still play a major role in the photovoltaic market, and amorphous silicon nitride (a-SiN:H) often serves as anti-reflection coating (ARC) and passivation layer on top of those cells. The passivation properties are, thereby, strongly influenced by electronic defect states at the interface. In present study, these defects have been investigated by using ab intio molecular dynamics. We prepared 900 different c-Si/a-SiN:H structures and classified the most important defect types at the interface. Afterwards, we examined their energetic and spacial localization, and their band structure. We generally find higher defect concentrations at the interface, which are dominated by occupied, localized states in the a-SiN part and unoccupied, delocalized states in the c-Si part. While the former are mainly localized at under-coordinated Si atoms, the latter have rather inherited the character of the c-Si conduction band. We argue that this difference is a strong evidence for the band bending effect at the c-Si/a-SiN:H heterojunction.

O 64.3 Wed 17:00 P1

**Influence of surface treatment on NV centers in diamond** — •Stefan Borgsdorf[1], Lina Elbers[1], Aniela Scheffzyk[1], Daniel Laumann[1], Christian Klump[1], Andreas Kaivas[1], Ulrich Köhler[1], Dieter Suter[2], and Frederico D. Brandao[2] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum — [2]Experimentelle Physik IIIA, TU Dortmund

Color centers in diamond, especially NV centers, are practical single photon emitters due to RT operation and candidates for applications in quantum computing. We present a setup for low energy implantation of NV centers near the surface possibly allowing electrical addressing. Furthermore, we survey the influence of different surface and bulk treatments on the diamond and its NV centers. To purify the diamonds we reduced the amount of natural NV centers in optical grade diamonds by heating up to 1500 °C in hydrogen. The luminous intensity could be reduced down to 1/8. The optical grade diamonds were used for first implantations with N15 in discrete lines. Further, electronic grade diamonds will be applied. To control the charge state of the NV centers, the surface was terminated by Hydrogen or Fluorine via a H2- and a CF4-Plasma, respectively. HREELS and AFM measurements were executed to study the surface after plasma treatment. Likewise, the influence of optical transparent passivation layers on the intensity and charge state are object of interest. Finally a UHV chamber is modified to implant directly under UHV conditions and to allow in situ spectroscopic access to the diamond samples.

O 64.4 Wed 17:00 P1

**Investigation of Charge Transport across GaN-Pt Interfaces by Conductive Atomic Force Microscopy** — •Sebnem Tuncay, Andrea Winnerl, Rui Nuno Pereira, and Martin Stutzmann — Walter Schottky Institut, Technische Universität München, Germany

GaN-based semiconductors have attracted great attention for applications including optoelectronics, high-power, high-frequency electronics and biosensing. Besides that, GaN-Pt systems have a considerable potential for future applications in photocatalysis and photoelectrochemical processing. For the latter applications charge transport across interfaces between GaN and metals or electrolytes are of central importance.

In this context, we investigate the charge transport across GaN-Pt interfaces. For sample preparation we use spin-coating in order to deposit Pt nanoparticles on n-type or p-type GaN layers. Using atomic force microscopy and scanning electron microscopy, we image the surface morphology of GaN layers grown on sapphire substrates and characterize the spatial distribution of Pt nanoparticles on such GaN surfaces. Conductive atomic force microscopy enables us to measure and map currents between the Pt nanoparticles and the GaN surface. The current-voltage characteristics of Pt nanoparticles on GaN show Schottky behaviour. Comparing the current-voltage characteristics measured on Pt nanoparticles and directly on the GaN surface is used to understand details of the charge transport across GaN-Pt interfaces.

O 64.5 Wed 17:00 P1

**Impact of high temperature annealing on Pd/GaN(0001) contact morphology** — •Justyna Pers[1], Miłosz Grodzicki[2], Piotr Mazur[3], Stefan Zuber[4], and Antoni Ciszewski[5] — [1]Institute of Experimental Physics, University of Wrocław, pl. Maksa Borna 9, 50-204 Wrocław, Poland — [2]Institute of Experimental Physics, University of Wrocław, pl. Maksa Borna 9, 50-204 Wrocław, Poland — [3]Institute of Experimental Physics, University of Wrocław, pl. Maksa Borna 9, 50-204 Wrocław, Poland — [4]Institute of Experimental Physics, University of Wrocław, pl. Maksa Borna 9, 50-204 Wrocław, Poland — [5]Institute of Experimental Physics, University of Wrocław, pl. Maksa Borna 9, 50-204 Wrocław, Poland

Metal/GaN junction is the necessary part of each modern electronic and optoelectronic devices based on GaN; on the one hand as the ohmic contact for communication, and on the other as Schottky contacts in active devices or diodes. This report concerns Pd layers deposited under ultrahigh vacuum conditions onto n-type GaN(0001) crystals kept at room temperature. Combined surface techniques as XPS, UPS, STM and LEED were used to investigate physicochemical properties of the Pd/GaN(0001) contacts. The obtained Pd films have a grainy morphology beginning from the earliest stage of growth. Electron affinity of the clean n-GaN surface amounts to 3.1 eV. The work function of the Pd film of mean thickness of 1 nm is equal to 5.3 eV. The Schottky's barrier height of the Pd/GaN(0001) junction has the value to 1.60 eV. After heating at 800°C of the Pd/GaN interface, the formation of Pd-Ga alloy is observed.

## O 65: Poster: Graphene (HL jointly with MA, O)

Time: Wednesday 17:00–20:00 Location: P1

O 65.1 Wed 17:00 P1

**Semi-empirical phonon calculations for graphene on different substrates** — •Henrique Miranda, Alejandro Molina-Sanchez, and Ludger Wirtz — Physics and Materials Science Research Unit, UNIVERSITÉ DU LUXEMBOURG, Luxembourg

We investigate the graphene-substrate interaction via changes in the phonon dispersion of graphene. Ab-initio calculations on these systems are of high computational cost due to the non-commensurability of the unit cells of graphene and the substrate. This leads to the formation of Moiré patterns with accordingly large supercell sizes. We use a semi-empirical force constant model for the calculation of phonons of graphene on different metallic and insulating substrates. The interaction of graphene with the substrate is described via suitably chosen spring constants. The phonon dispersion in the primitive unit cell of graphene is obtained via an "unfolding procedure" similar to the ones used for the discussion of ARPES (angular resolved photo-emission spectroscopy) of graphene on incommensurate substrates.

O 65.2 Wed 17:00 P1

**Bilayer graphene: topological phases and entanglement spectrum** — •Sonja Predin and John Schliemann — Institute for Theoretical Physics,University of Regensburg, D-93040 Regensburg, Germany

We present a calculation of the entanglement spectrum of fermions in bilayer graphene. In particular, a non-trivial topological order of the Abelian phase of the time-reversal symmetry breaking d-wave state is studied. We show that the entanglement spectrum is gapped, additionally we show that edge excitations in the entanglement spectrum form doublet Dirac fields around every K point.

O 65.3 Wed 17:00 P1

**Ultrafast dynamics and photoluminescence of hot carriers in graphene** — •Thomas Danz, Andreas Neff, Reiner Bormann, Sascha Schäfer, and Claus Ropers — IV. Physical Institute, University of Göttingen, 37077 Göttingen, Germany

The ultrafast dynamics of optically excited carriers in graphene can be monitored by pump-probe spectroscopy [1,2]. Furthermore, it was recently shown that the thermalization of hot carriers leads to photoluminescence at wavelengths far away from the exciting pump [3,4]. Here, we present the implementation of an experimental setup which combines transient spectroscopy with sub-15-fs temporal resolution with hot carrier photoluminescence detection under the same excitation conditions. With this approach, we aim at a comprehensive picture of the ultrafast carrier response and the disentanglement of the timescales underlying different relaxation pathways. First experimental results will be presented.

[1] J. M. Dawlaty *et al.*, Appl. Phys. Lett. **92**, 042116 (2008)
[2] M. Breusing *et al.*, Phys. Rev. B. **83**, 153410 (2011)
[3] C. H. Lui *et al.*, Phys. Rev. Lett. **105**, 127404 (2010)
[4] W. Liu *et al.*, Phys. Rev. B. **82**, 081408 (2010)

O 65.4 Wed 17:00 P1

**Electron spin resonance of ion-irradiation induced single vacancies on monolayer graphene characterized by scanning tunneling spectroscopy** — •Sven Just[1], Stephan Zimmermann[2], Vladislav Kataev[2], Marco Pratzer[1], Bernd Büchner[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden

Single vacancies with densities of $0.003/\text{nm}^2 - 3/\text{nm}^2$ are prepared on HOPG and on single layer graphene on $SiO_2$ produced by chemical vapour deposition using Ar ions with 50 eV kinetic energy. The vacancies exhibit a peak at $E_F$ in scanning tunneling spectroscopy, which survives 3 h of air exposure, afterwards a small broadening of the peak is observed. Electron spin resonance shows a peak corresponding to g = 2.0022, if the defect density is above $0.3/\text{nm}^2$, and a peak width of 10 G with an anisotropy below 0.5 G between in-plane and out-of-plane magnetic field. The peak width hardly depends on temperature, while the peak intensity decreases with increasing temperature in the range of 4 K - 20 K.

O 65.5 Wed 17:00 P1

**Enhancing the Raman signal of graphene on SiC(0001) by using a solid immersion lens in *top-down* geometry** — •Felix Fromm[1], Martin Hundhausen[2], Michl Kaiser[3], Julia Krone[1], and Thomas Seyller[1] — [1]TU Chemnitz, Institut für Physik — [2]FAU Erlangen-Nürnberg, Lehrstuhl für Laserphysik — [3]FAU Erlangen-Nürnberg, Lehrstuhl für Werkstoffwissenschaften

We present a study of epitaxial graphene by recording Raman spectra from the backside through the silicon carbide (SiC) substrate. In that *top-down* geometry we profit from the fact, that the graphene layer emits approximately 96 % of the Raman intensity into the SiC [1]. However, we only observe an intensity enhancement of approximately a factor of 4 compared to the conventional *top-up* geometry. This is because the solid angle of detection is decreased by refraction at the SiC/air interface and is limited by the total internal reflection. To further improve the detection efficiency, we use a high refractive index solid immersion lens (SIL) made of cubic zirconia combined with a suitable immersion liquid. By that, the angle of total internal reflection, as well as the solid angle of detection are increased. We eventually observe an increase of the detected Raman intensity towards the *top-up* geometry to a factor of 25. As an additional advantage, the background signal of the two-phonon Raman modes of the SiC is suppressed to a large extent.

[1] F. Fromm et al., New J. Phys. 15, 113006 (2013)

O 65.6 Wed 17:00 P1

**Growth of graphene on 6H-SiC(0001) under ammonia/argon**

**atmosphere** — •Christian Raidel, Felix Fromm, Samir Mammadov, Martina Wanke, and Thomas Seyller — TU Chemnitz, Insitut für Physik, Germany

In this work we investigated the nitrogen incorporation into epitaxial grown monolayer graphene by using ammonia as process gas within argon flow during thermal decomposition of SiC. The growth parameters as temperature and ammonia concentration were studied by various surface sensitive methods as XPS, LEED, RAMAN, AFM, and STM. ARPES shows that the ammonia grown graphene shows more p-type doped graphene than undoped graphene on SiC(0001). Due to the dissociation of ammonia during the growth process etch pits are produced. Vacancy associated nitrogen incorporation was observed by XPS and STM.

O 65.7 Wed 17:00 P1

**Characterization and transfer of 2D dichalcogenides produced by anodic bonding** — •Philipp Nagler, Gerd Plechinger, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

Atomically thin $MoS_2$ and $WS_2$ structures have attracted growing attention as promising 2D semiconductors. As monolayers, both materials exhibit a direct bandgap and therefore are suitable candidates for future opto-electronical devices. We produced singlelayer $MoS_2$ and $WS_2$ by means of anodic bonding. In this process, the material is bonded by electrostatic forces on a borosilicate glass substrate. Compared to mechanical exfoliation, this technique usually yields larger flakes. Anodic bonded $MoS_2$ flakes were characterized by Raman and photoluminescence (PL) spectroscopy. Performing low-temperature PL measurements, we observed similar behaviour as in $SiO_2$-supported $MoS_2$. Furthermore, PL measurements for anodic bonded $WS_2$ are presented. By applying the wedging transfer technique, we transferred anodic bonded monolayer $WS_2$ from the glass to a $SiO_2$ substrate. Additionally, using this method, heterostructures consisting of various 2D materials could be produced and characterized.

O 65.8 Wed 17:00 P1

**Graphene nanostructures produced from transfered layers** — •Christopher Belke, Dmitri Smirnov, Johannes C. Rode, Hennrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover, Germany

Graphene consists of carbon atoms, which are arranged in a two-dimensional honeycomb lattice. It has unique electronic properties, which can be examined in high quality samples [1]. These are often prepared by mechanical exfoliation on a silicon wafer with silicon dioxide on top. This substrate has a strong influence on the transport properties due to charge traps and surface roughness [2]. To reduce these effects or to produce novel complexe layersystems, graphene sheets can be stacked by a transfer methode e. g. onto other substrates or one upon the other to fabricate twisted flakes. The latter has been done and was under examination with magnetotransport measurements.

Graphene is exfoliated on a thin PMMA layer, which can be detached from the silicon wafer. This layer is then placed on another graphene mono- or bilayer flakes. The samples were characterized at low temperatures and in dependence of a magnetic field. Magnetic field independent oscillations could be observed in a multilayer system.

[1] K. S. Novoselov et al. Science **306**, 666 (2004)

[2] P. Barthold et al. NJP **13**, 0433020 (2011)

O 65.9 Wed 17:00 P1

**Twisted graphene bilayers, folded via atomic force microscope** — •Johannes C. Rode, Dmitri Smirnov, Christopher Belke, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

Naturally occurring double-layer graphene consists of two hexagonal lattices in Bernal stacking. We investigate the folding of single-layer graphene via atomic force microscope (AFM) and the electronic properties of thusly created bilayers. The crystal lattices of these are twisted against each other which affects the interlayer coupling, giving rise to interesting electronic properties like a screening effect and reduced Fermi velocities at higher twist angles. Furthermore, the influence of a moiré-superlattice or twist induced van-Hove-singularities can be expected at lower twist angles. Our samples are obtained by micromechanical cleavage of natural graphite and placed on a silicon substrate with a top layer of silicon dioxide. The atomic force microscope then serves as a tool to mechanically manipulate the sample by programmed tip movements. We show AFM-induced folding of graphene on a $\mu$m-scale which can afterwards be contacted via e-beam lithography. Magnetotransport measurements over the folded areas show interesting signatures like multiple origins of landau fans in the charge carrier concentration.

O 65.10 Wed 17:00 P1

**The Effect of the Chemical Potential of Graphene on THz Detection** — •Markus Göthlich[1], Fathi Gouider[1], André Müller[2], Yuri B. Vasilyev[3], and Georg Nachtwei[1] — [1]Institut für Angewandte Physik, Technische Universität Braunschweig, Mendelssohnstraße 2, D-38106 Braunschweig — [2]Physikalisch Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig — [3]A.F.Ioffe Physical Technical Institute, RU-194021 St.Petersburg, Russia

One particular fact about graphene is its remarkable Landau quantization $E_n = \mathrm{sgn}(n)\sqrt{\Delta^2 + 2\hbar e v_F^2 |n| B}$ with $n$ being the Landau level (LL) index. This would allow a transition at 2.4 THz (corresponding to an energy of about 10 meV) to happen at a magnetic field as low as 0.2 T. But theoretical investigations show the opening of a bandgap and a high chemical potential in epitaxial graphene on Si-face SiC due to graphene–substrate interactions. On the other hand our calculations—based on Gusynin et al. Phys. Rev. Lett. 98, 157402 (2007)—show that at high chemical potential the photoresponse can only be observed at higher magnetic fields of some Tesla. Gating is difficult due to the insolating behaviour of SiC substrate on the one hand and THz intransparency of top gates on the other hand. Therefore our aim is to design a new sample geometry that allows the manipulation of the chemical potential of the graphene while not blocking the THz radiation before reaching the detector.

O 65.11 Wed 17:00 P1

**Gate-controlled STM study of magnetic impurities on a graphene surface** — •Paul Punke[1], Christian Dette[1], Roberto Urcuyo[1], Christopher Kley[1], Sören Krotzky[1], Rico Gutzler[1], Marko Burghard[1], Soon Jung Jung[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Graphene has been regarded as an ideal material for post silicon electronic application due to its unique electronic properties. To realize a field effect transistor for logic applications out of graphene, there has been a lot of effort to understand the gating effect on the charge-carrier-density-dependent properties of graphene, such as electronic scattering, spin based phenomena and collective excitations. We have designed a gatable low temperature scanning tunneling microscope (STM) by adding contacts to the sample holder. To prepare the gate-tunable graphene devices, we use graphene grown by chemical vapor deposition (CVD), transferred with or without a supporting layer of polymethylmethacrylate (PMMA) or polystyrene (PS), on an insulating layer of SiO2 or hexagonal boron nitride (h-BN) on SiO2. We also grow the graphene on h-BN directly on Ni substrate by CVD method. The quality of these samples will be compared by means of optical microscopy, atomic force microscopy (AFM), Raman spectroscopy and STM. Finally, we will present the gate-controlled electronic structure of graphene.

O 65.12 Wed 17:00 P1

**Ion Implantation of Graphene - Toward IC Compatible Technologies** — •H. Hofsäss[1], U. Bangert[2,3], W. Pierce[2], D. M. Kepaptsoglou[3], Q Ramasse[3], R Zan[1], M. H. Gass[3,4], J.A. van den Berg[5], C. Boothroyd[6], and J Amani[1] — [1]II. Physikalisches Institut, Georg-August-Universität Göttingen, Göettingen, Germany — [2]School of Materials, The University of Manchester, Manchester, United Kingdom — [3]SuperSTEM Laboratory, Daresbury, United Kingdom — [4]AMEC, Walton House, 404 The Quadrant, Birchwood, United Kingdom — [5]School of Computing, Science and Engineering, University of Salford, Salford, United Kingdom — [6]Ernst Ruska-Centre for Microscopy and Spectroscopy, Juelich Research Centre, Juelich, Germany

Doping of graphene via ultra low energy ion implantation could open possibilities for fabrication of nanometer-scale patterned graphene-based devices as well as for graphene functionalization compatible with large-scale integrated semiconductor technology. Using advanced electron microscopy/spectroscopy methods, we show for the first time directly that graphene can be doped with B and N via ion implantation of mass selected ions at energies of 20 - 30 eV and that the retention is in good agreement with predictions from calculation-based literature values. Atomic resolution high-angle dark field imaging (HAADF) combined with single-atom electron energy loss (EEL) spectroscopy reveals that for sufficiently low implantation energies ions are predominantly substitutionally incorporated into the graphene lattice with a very small fraction residing in defect-related sites.

## O 66: Invited Talk (Manos Mavrikakis)

Time: Thursday 9:30–10:15 Location: HSZ 01

**Invited Talk** O 66.1 Thu 9:30 HSZ 01

**Fundamental mechanistic studies in formic acid decomposition on transition metal surfaces** — •Manos Mavrikakis — University of Wisconsin - Madison

Formic acid (HCOOH) is a simple molecule that is an abundant product of biomass processing and can serve as an internal source of hydrogen for oxygen removal and upgrading of biomass to chemicals and fuels. In addition, HCOOH can be used as a fuel for low temperature direct fuel cells. We present a systematic study of the HCOOH decomposition reaction mechanism starting from first-principles and including reactivity experiments and microkinetic modeling. In particular, periodic self-consistent Density Functional Theory (DFT) calculations are performed to determine the stability of reactive intermediates and activation energy barriers of elementary steps. Pre-exponential factors are determined from vibrational frequency calculations. Mean-field microkinetic models are developed and calculated reaction rates and reaction orders are then compared with experimentally measured ones. These comparisons provide useful insights on the nature of the active site, most-abundant surface intermediates as a function of reaction conditions and feed composition. Trends across metals on the fundamental atomic-scale level up to selectivity trends will be discussed. Finally, we identify from first-principles alloy surfaces, which may possess better catalytic properties for selective dehydrogenation of HCOOH than monometallic surfaces, thereby guiding synthesis towards promising novel catalytic materials.

## O 67: Graphene-like Materials: Silicene, MoS2 and Relatives (HL jointly with DY, MA, O, TT)

Time: Thursday 10:00–12:30 Location: POT 081

O 67.1 Thu 10:00 POT 081

**Many-body effects in 2D hexagonal semimetals and semiconductors** — •Tineke Stroucken, Johanna Grönqvist, and Stephan W. Koch — Department of Physics and Material Sciences Center, Philipps University Marburg, Renthof 5, D-35032 Marburg, Germany

Recently, a variety of graphene-analogues materials like h-BN, silicene or transition-metal dichalcogenides have been fabricated. Similar to graphene, these novel material systems display exciting new physical properties, distinct from their bulk counterparts.

Owing to the symmetry of the hexagonal lattice, band edge carriers are described by massive Dirac Fermions. Typically, the Fermi-velocity is in the range of $c/300$ or below. This yields effective fine structure constants $\alpha = e^2/\epsilon\hbar v_F \gtrsim 2/\epsilon$, implying prominent Coulomb interaction and relativistic effects. Particularly, $\alpha \gtrsim 1$ indicates an excitonic instability of the noninteracting ground state.

In this presentation, we discuss conditions for strong Coulomb coupling in 2D hexagonal crystals and identify experimentally observable signatures signaling an excitonic ground state. To this end, the gap equations are solved self consistently with the polarization function, which depends on the interacting band structure.

[1] T. Stroucken *et al.*, Phys. Rev. B 84, 205445 (2011)
[2] J. H. Grönqvist *et al.*, EPJ B 85, 12 (2012)
[3] T. Stroucken *et al.*, Phys. Rev. B. 87, 245428(2013)
[4] T. Stroucken *et al.*, Appl. Phys. Lett. 103, 163103 (2013)

O 67.2 Thu 10:15 POT 081

**Single and Multi-Layer Silicene: Growth, Properties and Perspectives** — •Patrick Vogt[1], Thomas Bruhn[1], Andrea Resta[2], Paola De Padova[3], and Guy Le Lay[2] — [1]Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Aix-Marseille University, CNRS- PIIM UMR 7345, F-13397 Marseille Cedex 20, France — [3]Instituto di Struttura della Materia, Consiglio Nazionale delle Ricerche -ISM, via Fosso del Cavaliere, 00133 Roma, Italy

Silicene, a new silicon allotrope with a graphene-like honeycomb structure, has recently attracted considerable interest, because its topology confers to it the same remarkable electronic properties as those of graphene, with the potential advantage of being easily integrated in current Si-based nano/micro-electronics offering novel technological applications.

We will discuss the epitaxial formation of single layer silicene on Ag substrates and its structural and electronic properties [1-2]. Based on these results we will look at the growth of silicene multi-layers which can be explained by stacking of single silicene sheets [3-4]. Different experimental techniques are used to investigate atomic structure and electronic properties of this layered system and to discuss its similarities to graphite.

1) Vogt, P. et al., Phys. Rev. Lett. 108, 155501 (2012).
2) Avila, J. et al., J. Phys.: Condens. Matter 25, 262001 (2013).
3) De Padova, P.; Vogt, et al. Appl. Phys. Lett. 102, 163106 (2013).
4) Resta, A. et al., Sci. Rep. 3, 2399 (2013).

O 67.3 Thu 10:30 POT 081

**Optical and vibrational properties of MoS2** — •Ludger Wirtz[1], Alejandro Molina-Sanchez[1], and Kerstin Hummer[2] — [1]Physics and Materials Science Research Unit, University of Luxembourg — [2]Faculty of Physics, University of Vienna, Austria

Monolayer MoS2 is currently receiving a lot of attention as a potential alternative to graphene. Its band gap of about 2eV (depending on the dielectric environment) makes it a suitable candidate for thin-film electronics. The optical and vibrational properties of mono-layer, few-layer, and bulk are seemingly straightforward to calculate. Nevertheless some surprises occur: the phonon dispersion displays an anomalous Davydov splitting and the optical absorption spectra display a rich structure of excitonic peaks in the band-gap and in the continuum of interband transitions. We give a short review of the state-of-the art and discuss recent advances in the understanding of the influence of the substrate on the vibrations and electronic excitations.

O 67.4 Thu 10:45 POT 081

**Carrier- and valley dynamics of singlelayer $MoS_2$** — •Gerd Plechinger[1], John Mann[2], Christian Schüller[1], Ludwig Bartels[2], and Tobias Korn[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Chemistry, Physics, and Materials Science and Engineering, University of California, CA 92521 Riverside, USA

Consisting of an only 0.7 nm thin S-Mo-S sheet and offering a direct bandgap at the K-points in the Brillouin zone, singlelayer $MoS_2$ represents a promising semiconductor material for flexible and transparent optoelectronic applications. By means of chemical vapor deposition (CVD), large-area films (several $mm^2$) of singlelayer $MoS_2$ can be produced. These were characterised by photoluminescence and Raman spectroscopy. In order to investigate the carrier dynamics, we performed pump-probe measurements in the spectral range of the optical transitions in singlelayer $MoS_2$. Helicity-resolved PL measurements have demonstrated an efficient valley polarisation of the $K^+$ or $K^-$ valley at near-resonant excitation. We probe these valley dynamics with Kerr spectroscopy and find a biexponential decay of the valley polarisation with decay times of a few tens of ps and a few hundreds of ps at low temperatures.

**Coffee break (15 min.)**

O 67.5 Thu 11:15 POT 081

**Photocurrent studies on semiconducting MoS2** — Marina Hoheneder, •Eric Parzinger, Alexander Holleitner, and Ursula Wurstbauer — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching

The current interest in transition metal dichalcogenides is stimulated by their peculiar electrical and optoelectrical properties and their potential for novel device applications. We investigate the semiconductor MoS2, which shows a crossover from an indirect to a direct bandgap semiconductor by thinning it down to a monolayer. We prepare MoS2 samples through micromechanical exfoliation and characterize the thin flakes with Raman spectroscopy. We further study photocurrent generation of single and few layer MoS2 in dependence of wavelength and power of the exciting light. We gratefully acknowledge financial support by BaCaTec.

O 67.6 Thu 11:30 POT 081

**Resonant Inelastic Light Scattering on $MoS_2$** — •Bastian Miller, Eric Parzinger, Alexander Holleitner, and Ursula Wurstbauer — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching (Germany)

Two-dimensional layered 'van-der Waals' materials are of increasing interest for fundamental research due to their peculiar band-structure.

We utilize inelastic light scattering - a contactless and extremely versatile tool - to study phonon excitation spectra of mono- and fewlayer $MoS_2$. The phonon modes are unique fingerprints of the material properties and are sensitive to defects, strain, doping and the number of $MoS_2$ -layers.

We observe signatures of multistep scattering processes involving phonon-phonon, electron-phonon as well as electronic excitations under resonant conditions, where the incoming or outgoing light meets the energy of a fundamental optical transition of the system.

O 67.7 Thu 11:45 POT 081

**The effect of substrate and environment on the elementary excitations of $MoS_2$** — •Eric Parzinger[1], Marina Hoheneder[1], Bastian Miller[1], Anna Cattani-Scholz[1], Alexander Holleitner[1], Joel W. Ager[2], and Ursula Wurstbauer[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching (Germany) — [2]Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley, California 94702 (United States)

The novel two-dimensional layered 'van-der Waals' material Molybdenum disulfide ($MoS_2$) is investigated using inelastic and resonant light scattering - a contactless and extremely versatile tool - to study phonon and electronic excitations. In particular, we focus on the influence of different supporting materials ($SiO_2$, sapphire and SAMs of organic molecules) as well as various environmental conditions (ambient, vacuum and water) on the low energy excitations of $MoS_2$. We find that both, different substrate and environment give rise to a significant modification of the most prominent Raman modes, whereas a monolayer is most effected by the environmental conditions. We gratefully acknowledge financial support by BaCaTec.

O 67.8 Thu 12:00 POT 081

**Spin-orbit coupling, quantum dots, and qubits in transition metal dichalcogenides** — •Andor Kormanyos[1], Viktor Zolyomi[2], Neil Drummond[2], and Guido Burkard[1] — [1]Universität Konstanz — [2]Lancaster University

We derive an effective Hamiltonian describing the dynamics of electrons in the conduction band of transition metal dichalcogenides (TMDC) in the presence of perpendicular electric and magnetic fields. We discuss both the intrinsic and Bychkov-Rashba spin-orbit coupling (SOC) induced by an external electric field. We identify a new term in the Hamiltonian of the Bychkov-Rashba SOC which does not exist in III-V semiconductors. We point out important differences in the spin-split conduction band between different TMDC compounds. A significant consequence of the strong intrinsic SOC is an effective out-of-plane $g$-factor for the electrons which differs from the free-electron $g$-factor $g \simeq 2$. Using first-principles calculations, we give estimates of the various parameters appearing in the theory. Finally, we consider quantum dots (QDs) formed in TMDC materials and derive an effective Hamiltonian allowing us to calculate the magnetic field dependence of the bound states in the QDs. We find that all states are both valley and spin split, which suggests that these QDs could be used as valley-spin filters. We explore the possibility of using spin and valley states in TMDCs as quantum bits, and conclude that, due to the relatively strong intrinsic SOC in the conduction band, the most realistic option appears to be a combined spin-valley (Kramers) qubit at low B fields.

O 67.9 Thu 12:15 POT 081

**Analytical approach to excitonic properties of MoS2** — •Gunnar Berghäuser and Ermin Malic — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We present an analytical investigation of the optical absorption spectrum of monolayer molybdenum disulfide (MoS2). Based on the density matrix formalism [1], our approach gives insights into the microscopic origin of excitonic transitions, their relative oscillator strength, and binding energy [2]. We show analytical expressions for the carrier-light coupling element, which contains the optical selection rules and well describes the valley- selective polarization in MoS2 . In agreement with experimental results, we find the formation of strongly bound electron-hole pairs due to the efficient Coulomb interaction. The absorption spectrum of MoS2 on a silicon substrate features two pronounced peaks at 1.91 eV and 2.05 eV corresponding to the A and B exciton, which are characterized by binding energies of 420 meV and 440 meV, respectively. Our calculations reveal their relative oscillator strength and predict the appearance of further low-intensity excitonic transitions at higher energies. The presented approach is applicable to other transition metal dichalcogenides and can be extended to investigations of trion and biexcitonic effects.

[1] E. Malic and A. Knorr, Graphene and Carbon Nanotubes: Ultrafast Optics and Relaxation Dynamics, 1st ed. (Wiley-VCH, Berlin, 2013).

[2] Gunnar Berghäuser and Ermin Malic, arXiv:1311.1045 (2013)

# O 68: Spintronics II (HL jointly with MA, O, TT)

Time: Thursday 10:00–12:15 Location: POT 151

O 68.1 Thu 10:00 POT 151

**Magnetotransport in nanostructured InAs-based Heterostructures** — •Olivio Chiatti[1], Sven S. Buchholz[1], Wolfgang Hansen[2], Mehdi Pakmehr[3], Bruce D. McCombe[3], and Saskia F. Fischer[1] — [1]Neue Materialien, Institut für Physik, Humboldt-Universität zu Berlin, D-10099 Berlin — [2]FG Wachstum, Institut für Angewandte Physik, Universität Hamburg, D-20148 Hamburg — [3]Dept. of Physics, University at Buffalo, the State University of New York, Buffalo, NY 14260-1500 USA

The control of spin-polarized currents entirely by electrical fields is of great interest in the field of spintronics. The spin-orbit coupling in narrow-gap semiconductors has been identified as a possible tool to this end, because it couples the momentum of an electron to its spin. Nanostructures can be used to filter specific momentum modes and offer the possibility to create and detect spin-polarized currents. [1] Quantum point contacts (QPCs) in nominally symmetric InAs quantum well structures have been reported to generate spin-polarized currents, when asymmetric gate voltages are applied. [2]

We have fabricated Hall-bars and QPCs with in-plane gates in InAs quantum well structures, and performed transport measurements at low temperatures and in high magnetic fields. We investigate the effects of symmetric and asymmetric gate voltages. Here, we present the results of our measurements and discuss their implications for investigations of the spin-orbit coupling in InAs.

[1] Silsbee, *J. Phys.: Condens. Matter* **16**, R179 (2004)

[2] Debray *et al.*, *Nature Nanotech.* **4**, 759 (2009)

O 68.2 Thu 10:15 POT 151

**Acoustic charge and spin transport in GaAs (111)B quantum wells** — •Alberto Hernández-Mínguez, Klaus Biermann, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The special properties of electron spin dynamics in GaAs (111) quantum wells (QWs) have been subject of study during the last years. Recently, it has been experimentally shown that, to first order in the electron wavevector, the in-plane component of the spin-orbit interaction can be suppressed simultaneously for all electrons in the QW just by applying an electric field of a certain amplitude perpendicularly to the QW plane. As a consequence, by tuning the amplitude of the electric field, the spin polarization lifetime of an electron ensemble is varied from a few hundred picoseconds to tens of nanoseconds.

In addition, surface acoustic waves (SAWs) have proved to be an useful tool for the controlled transport and manipulation of electron spins in GaAs QWs: the piezoelectric field accompanying the SAW allows the spatial confinement of electrons and their transport, with the well defined SAW velocity, over distances of several tens of micrometers. In this contribution, we explore the generation of SAWs in GaAs (111) QWs, as well as their combination with vertical electric fields for the acoustic transport of long living electron spins. In this way, we observe acoustic charge transport along 40$\mu$m distance, and spin transport around 15 $\mu$m.

O 68.3 Thu 10:30 POT 151

**Indirect Excitons Spin manipulation in GaAs/Al$_x$Ga$_{1-x}$As double quantum wells** — •Adriano Violante[1], Snežana Lazić[2], Klaus Biermann[1], Rudolph Hey[1], Paulo Santos[1], Kobi Kohen[3], and Ronen Rapaport[3] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Departamento de Física de Materiales, Universidad Autónoma de Madrid, Madrid, Spain — [3]Racah Institute of Physics, Hebrew University of Jerusalem, Jerusalem, Israel

A spatially indirect exciton (IX) is a bound state of an electron and a hole localized in different quantum wells (QWs) of a double quantum well structure (DQW). In an IX, the spatial separation of electrons and holes reduces the exchange interaction, thus significantly enhancing the spin lifetime with respect to the direct QW excitons. [1] In this contribution, we show that spin-polarized IXs created using a circularly polarized laser beam diffuse up to distances 15 $\mu$m away from the generation point, revealing spatial oscillations of the polarization degree $\rho_z$. The latter are attributed to the precession of the spin vector in the spin-orbit effective magnetic field $B_{SO}$ as they move away from the excitation spot, which can be modulated both with electric and magnetic fields. The IXs spin transport using acoustic fields is also discussed.

[1] J. R. Leonard, Y. Y. Kuznetsova, S. Yang, L. V. Butov, T. Ostatnick, A. Kavokin, and A. C. Gossard. Nano Lett. 9, 4204-4208 (2009)

O 68.4 Thu 10:45 POT 151

**Time- and space-resolved measurements of spin diffusion in high-mobility GaAs-based 2D electron systems** — •Markus Schwemmer[1], Roland Voelkl[1], Tobias Korn[1], Sergey Tarasenko[2], Dieter Schuh[1], Werner Wegscheider[3], and Christian Schüller[1] — [1]Institute of Experimental and Applied Physics, Faculty of Physics,University of Regensburg, Germany — [2]A. F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, St. Petersburg, Russia — [3]ETH Zurich, Switzerland

Two-dimensional electron systems embedded in (110)-grown, symmetrically doped GaAs/AlGaAs QWs are highly interesting for spintronics. They combine high carrier mobility with long spin dephasing times. Previously, we have studied these systems in different experiments, which either gave temporal or spatial resolution. By using a two-beam Hanle-MOKE method we could observe diffusion lengths of more than 125 $\mu$m at low temperatures. As a next step, the experimental setup was modified in order to achieve temporal and spatial resolution with the help of a single pulsed TiSa laser. The main issue is the spectral separation of the pump and the probe beams, which are collinearly focused onto the sample. Due to the broad spectrum of the femtosecond laser pulse, this can be realized using bandpass filters. Besides the mapping of the temporal propagation of the spins via diffusion, this experimental setup should also allow to visualize the evolution of a drifting spin packet. Financial support by the DFG via SFB 689 and SPP 1285 is gratefully acknowledged.

O 68.5 Thu 11:00 POT 151

**Direct measurement of the spin splitting in GaAs quantum wells** — •Christoph Schönhuber[1], Matthias Walser[2], Christian Reichl[3], Werner Wegscheider[3], Gian Salis[2], Tobias Korn[1], and Christian Schüller[1] — [1]Universität Regensburg, 93040 Regensburg, Germany — [2]IBM Research-Zurich, 8803 Rüschlikon, Switzerland — [3]ETH Zurich, 8093 Zurich, Switzerland

We investigate the spin splitting in the conduction band of GaAs quantum wells employing Raman scattering experiments. The investigated system consists of a 12-nm-wide (001)-oriented GaAs/AlGaAs QW, which is asymmetrically Si modulation doped to reach a balanced Rashba and Dresselhaus SOI contribution.

The performed measurements on intrasubband transitions reveal a double peak structure for the [11] direction, while in [1-1] direction there is only a single peak. This anisotropic behavior in the spin splitting is probed for a wide range of transfered wavevectors and in good agreement with the prediction for a system with comparable magnitudes of Rashba and Dresselhaus SOI.

O 68.6 Thu 11:15 POT 151

**Hole g-factor anisotropy in coupled GaAs/AlAs quantum wells** — •Christian Gradl, Michael Kempf, Dieter Schuh, Dominique Bougeard, Christian Schüller, and Tobias Korn — Universität Regensburg, D-93040 Regensburg, Germany

We performed time-resolved Kerr rotation measurements on undoped [110]- and [113]-grown double quantum well (QW) structures to resolve the spin dynamics of hole ensembles at low temperatures. For these growth directions, a strong anisotropy of the hole g-factor with respect to the in-plane magnetic field direction is theoretically predicted.

Our gated system consists of two QWs with different well widths, which we use for the spatial separation of the optically excited electron-hole pairs. Thus, we are able to create hole ensembles with spin lifetimes of several hundreds of picoseconds in the broader QW without any doping. This also allowed an observation of a strong hole g-factor anisotropy by varying the magnetic field direction in the QW plane. Moreover, our extracted values are in a very good agreement with theoretical predictions.

O 68.7 Thu 11:30 POT 151

**Polarization oscillations in spin-polarized vertical-cavity**

**surface-emitting lasers controlled by multiple excitation pulses** — •Henning Höpfner, Markus Lindemann, Nils C. Gerhardt, and Martin R. Hofmann — Photonics and Terahertz Technology, Ruhr-University Bochum, D-44780 Bochum, Germany

Spin-polarized lasers offer many potential advantages over their conventional counterparts, including threshold reduction, polarization control and ultrafast dynamics for increased modulation bandwidth [1].

Upon excitation with circularly polarized light that creates spin-polarized carrier in a vertical-cavity surface-emitting laser (VCSEL), the VCSEL shows oscillations of the circular polarization degree. These polarization oscillations can be much faster than the relaxation oscillations of the carrier-photon system. From calculations based on a rate-equation model we show that these oscillations can be switched on and off in a controlled manner using multiple circularly polarized optical excitation pulses. The results are verified experimentally, showing spin-induced polarization oscillation in conventional, electrically biased VCSELs subject to optical spin injection. We show polarization oscillation bursts with possible modulation frequencies far beyond the device's electrical modulation bandwidth.

[1] Gerhardt et al., Applied Physics Letters 99 (15), 151107 (2011)

O 68.8 Thu 11:45 POT 151

**Spin polarization of electron states in GaAs quantum wells** — •Pavel Streda — Institute of Physics ASCR, Praha, Czech Republic

The standard method to establish the spin orientation of electron states, for zinc-blende semiconductors like GaAs, is based on the effective medium approach represented by the Luttinger Hamiltonian. For a two-dimensional electron gas, confined within a potential well, the real eigenfunctions of bound states across the well has been approximated by an envelope function. It leads to the conclusion that along main crystallographic axis, $[1, 0, 0]$ and $[0, 1, 0]$, the spin orientation is parallel or antiparallel with velocity directions. This contradicts to the tendency of the spin to be perpendicular to the velocity direction, observed in bulk structures.

The question arises if an envelope function approach, which suppresses the effect of local environment, is not too crude approach for real quantum wells, which are usually wider than ten lattice constants. To answer this question the empirical pseudopotential method has been used to establish energy dispersions and spin expectation values for two-dimensional electron gas confined within quantum wells of the different width. In all cases the tendency of the spin to be perpendicular to the velocity direction has been observed. For wide enough wells the obtained spin structure approaches that given by the bulk GaAs crystal with $k_z = 0$.

O 68.9 Thu 12:00 POT 151

**Spin injection efficiency dependence on MgO tunnel barrier thickness** — •Lennart-Knud Liefeith, Tomotsugu Ishikura, Zhixin Cui, and Kanji Yoh — Research Center for Integrated Quantum Electronics, Japan

We study non-local spin valves in inverted InAlAs/InGaAs high-electron mobility transistors on InP(001). On the ferromagnet (FM) side, permalloy electrodes are employed. On the semiconductor (SC) side the electron system resides in a two-dimensional InAs channel. It has been argued that direct FM/SC contacts provide negligible spin polarization in the SC if the transport is diffusive, known as the conductivity mismatch problem[1]. In the ballistic transport regime efficient spin injection is predicted[2]. For devices basing on ballistic transport, a low contact resistance between FM and SC is essential. An strategy to tackle the conductivity mismatch problem is the insertion of a tunnel barrier at the FM/SC interface. We thus study ballistic structures with MgO tunnel barriers of varied thickness. Here we will compare spin injection efficiencies in non-local spin valve structures with either no or a 2 nm-thick MgO tunnel barrier at the FM/SC interface.

[1] G. Schmidt, „Fundamental obstacle for electrical spin injection from a ferromagnetic metal into a diffusive semiconductor“, Physical Review B 62, R4790 (2000)

[2] M. Zwierzycki, „Spin-injection through an Fe/InAs interface“, Physica Status Solidi A: Applications and Materials Science 1, 25-28 (2003)

## O 69: Focussed Session: Towards a Quantitative Understanding of Complex Adsorption Structures: Surface Science goes Organic II

Time: Thursday 10:30–13:15 Location: HSZ 01

**Topical Talk** O 69.1 Thu 10:30 HSZ 01

**Injection/extraction barriers in donor-acceptor blends on metals through core-level spectroscopy** — •Enrique Ortega[1,2], Afaf El-Sayed[1], Patrizia Borghetti[2], Eli Goiri[2], Celia Rogero[2], Luca Floreano[3], Yutaka Wakayama[4], Jose Luis Cabellos-Quiroz[2], Duncan Mowbray[2], Angel Rubio[2], and Dimas Oteyza[1,2] — [1]Departamento de Física Aplicada I, UPV/EHU, San Sebastian — [2]Centro de Física de Materiales and DIPC, San Sebastian — [3]Cons. Naz. Ric.-IOM, L. N. TASC, Trieste — [4]National Institute Material Science, Tsukuba

The active interface in charge injection devices can be generally defined by a monolayer-thick blend of donor/acceptor molecules in contact with a metal surface, where electron and hole injection/extraction barriers are determined by the offset of HOMO/LUMO molecular levels with respect to $E_F$. HOMO/LUMO alignment is not easy to elucidate in complex multi-component systems from valence band photoemission. Alternatively, we explored core-level photoemission, as a way to transparently assess molecular level alignment in donor-acceptor/metal interfaces. We performed systematic experiments combining acceptor-like fluorinated phthalocyanine (F16CuPc) and perfluoropentacene (PFP) with pentacene (PEN) and copper phthalocyanine (CuPc), respectively, on Au(111), Ag(111) and Cu(111). We observe, as a function of the donor/acceptor ratio, a characteristic binding energy shift in all core-levels, irrespectively of the donor/acceptor/metal combination. The meaning and the exceptions to such general behavior will be discussed. [See A. El-Sayed et al. ACS Nano **7**, 6914 (2013)]

O 69.2 Thu 11:00 HSZ 01

**Charge Localization at Inorganic/Organic Interfaces** — •Oliver T. Hofmann, Patrick Rinke, and Matthias Scheffler — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Understanding the mechanism behind level alignment at heterointerfaces is of fundamental importance for a variety of fields, including organicelectronics. Using density functional theory, we investigate the atomistic details of the level alignment of organic acceptors adsorbed on different surfaces. For adsorbates in direct contact with an Ag(111) surface, we observe the formation of hybrid states. This induces density of states at the Fermi energy and all molecules in the layer become partially and uniformly charged. Preventing the hybridization by inserting an NaCl layer between the adsorbate and the metal leads to a drastic change in the charge transfer behaviour. While semi-local density functionals still predict a fractional electron transfer, more sophisticated hybrid functionals break the translational symmetry and result in the integer charging of only a fraction of the molecules. The associated molecular states are found several tenth of an eV below the Fermi energy. This charge localization is accompanied by a distortion of the molecular geometry and can be interpreted as polaron. It affects several observables including core-level shifts or the electrostatic potential in the vicinity of the surface. Furthermore, a qualitatively different dependence of the adsorption-induced work-function change on the coverage is found.

O 69.3 Thu 11:15 HSZ 01

**Simulating X-ray absorption spectra of large organic adsorbates with DFT: possible pitfalls on the example of free-base porphine on Ag(111) and Cu(111)** — •Katharina Diller, Reinhard J. Maurer, and Karsten Reuter — Technische Universität München, Germany

Near-edge X-ray Absorption Fine-Structure (NEXAFS) spectroscopy is widely used in Surface Science for the characterisation of adsorbate-substrate systems. Especially for large organic molecules, however, the spectral features consist of a set of overlapping peaks and cannot be disentangled easily. For many systems an independent first-principles simulation of the respective spectra is therefore indispensable for the analysis of the experimental data. Particularly for stronger chemisorbed adsorbates the (often applied) approximation to restrict the calculations to the isolated gas-phase molecule is bound to fail. On the other hand, explicit consideration of in particular extended metal surfaces faces multiple challenges that mostly arise from the need to keep the calculations computationally tractable. Using the adsorption of free-base porphine on Ag(111) and Cu(111) as example we conduct density functional theory (DFT) simulations using both all-electron (FHI-aims) and pseudopotential (CASTEP) based implementations to investigate the efficiency and reliability of prevalent approaches to achieve the actual core-excitation, to ensure the localization of the core-hole, and to properly describe all final states of interest.

**Topical Talk** O 69.4 Thu 11:30 HSZ 01

**Core and valence spectroscopy of physisorbed molecules: Role of substrate** — •Claudia Draxl — Humboldt-Universität zu Berlin, Berlin

The interplay between weak intermolecular bonding and molecule-substrate interaction governs orientation, alignment, conformation, and packing of molecules. These geometrical aspects, in turn, determine the electronic and optical properties of the molecular layer(s). The substrate can, however, play an even more important role. It may affect the electronic structure in terms of charge transfer, polarization, and vibrational effects. To this extent, theoretical results obtained by density-functional theory and many-body perturbation theory will be analyzed and confronted with various microscopic and spectroscopic experimental probes. I will show how, for example, the molecular HOMO and LUMO levels are shifted by image-charge effects induced by a metal surface, and how small amounts of transferred charge can alter the molecular orbitals. Finally, the impact of electron-phonon coupling on x-ray absorption spectra of low-dimensional systems will be discussed.

O 69.5 Thu 12:00 HSZ 01

**Substrate induced intermolecular dispersion and observed hybridisation: Pentacene on Cu(110)** — •Thomas Ules[1], Eva Reinisch[1], Markus Ostler[2], Georg Koller[1], Daniel Lüftner[1], Peter Puschnig[1], and Michael Ramsey[1] — [1]Institute of Physics, Karl-Franzens University Graz, 8010 Graz, Austria — [2]University of Erlangen-Nürnberg, Erlangen, Germany

The 5A monolayer on Cu(110) has been studied by Angle Resolved UPS (ARUPS). The tomographic analysis of the ARUPS data cube into band (E vs. k) and momentum (kx vs. ky) maps reveal changes in both the substrate and molecule electronic structure upon the formation of the monolayer. In the region down to 1eV below the Fermi edge the momentum maps clearly show a 5A LUMO intensity distribution with a remarkably large dispersion of ˜ 0.7eV in the direction of the long molecular axes. This contrasts to the calculated dispersion of a free standing 5A monolayer of only 20 meV and a truly significant enhancement of intermolecular dispersion is claimed. The strong periodic potential of the 5A overlayer leads to an apparent opening of a band gap in the Cu sp band which will be argued to be the result of the change of Cu sp states to molecular LUMO character.

O 69.6 Thu 12:15 HSZ 01

**Time-resolved simulation of angular resolved photoemission** — •Matthias Dauth and Stephan Kümmel — University of Bayreuth, Germany

We present an approach for calculating angular resolved photoemission spectra (ARPES) by explicit simulation of the photoemission process in real-time. This allows us to go beyond the frequently employed molecular-orbital and eigenvalue-based interpretation of photoemission. In the latter, electrons are assumed to be emitted from single particle orbitals and final states are implictly assumed to be plane waves. Our approach lifts these approximations. We use the framework of time dependent density functional theory to propagate the electronic system under the influence of an external ionizing laser field. Electron interaction and dynamical effects such as internal relaxation are thus explictly taken into account. We simulate the energy and angular resolved photoelectron detection by evaluating the kinetic energy spectrum of the outgoing time-dependent electron density. The dynamic ionization process is analyzed in detail and compared to results that are obtained from the molecular orbital picture in combination with the plane wave approximation.

O 69.7 Thu 12:30 HSZ 01

**Adsorption geometry and electronic structure of iron phthalocyanine on Ag surfaces revealed by photoelectron momentum mapping** — •Vitaliy Feyer[1,2], Martin Graus[3,4], Pascal Nigge[3,4], Michael Wiessner[3,4], Robert G. Acres[2], Carsten Wiemann[1], Claus M. Schneider[1,5], Achim Schöll[3,4], and Friedrich Reinert[3,4] — [1]Research Center Jülich, 52425 Jülich, Germany — [2]Sincrotrone Trieste, 34012 Basovizza, Trieste, Italy — [3]Universität Würzburg, 97074 Würzburg, Germany — [4]Karlsruher Institut für Technologie KIT, 76021 Karlsruhe, Germany — [5]Universität Duisburg-Essen, D-47048 Duisburg, Germany

We report a comprehensive study of the adsorption behavior of iron phthalocyanine on the low-index crystal faces of silver. Experiments were carried out at the NanoESCA beamline of the Elettra synchrotron. The experimental setup includes a non-magnetic, electrostatic photoelectron emission microscope and a double-pass hemispherical analyzer that directly images a parallel momentum component of photoelectron at a fixed binding energy. A combination of photoelectron momentum mapping (PMM) and low-energy electron diffraction (LEED) provides access to the superstructure unit cell and the arrangement of the molecules within the unit cell. Additionally, momentum patterns give information about the electronic structure at the interface and the symmetry of molecular orbitals. Comparative analysis of the PMM of the lowest unoccupied molecular orbitals (LUMO) of FePc on the substrates with different symmetry indicates that both degenerate LUMOs receive charge transfer from the substrate.

O 69.8 Thu 12:45 HSZ 01

**Phase Determination of Electronic Wavefunctions utilizing the Circular Dichroism in the Angular Distribution of Photoelectrons** — •Martin Graus[1,2], Michael Wiessner[1,2], Pascal Nigge[1,2], Achim Schöll[1,2], and Friedrich Reinert[1,2] — [1]Universität Würzburg, 97074 Würzburg, Germany — [2]Karlsruher Institut für Technologie KIT, 76021 Karlsruhe, Germany

The experimental measurement of molecular orbitals by angle resolved photoelectron spectroscopy (ARPES) respectively photoemission electron microscopy (PEEM) is on the edge of providing three dimensional images of the respective electronic density distribution. This provides unprecedented insight into the structural, electronic and chemical properties of molecular materials, which are of practical relevance for future molecular electronics. A challenge in gathering the full orbital information lies in the determination of the quantum mechanical phase since it is usually lost by the conventional process of measuring solely the square of the wave function's absolute value. However, the phase is highly desired as the key parameter for the backwards Fourier Transform, which is necessary to create real space images out of the measured k-space data. We demonstrate an experimental approach to solve the phase problem taking advantage of interference patterns in the circular dichroism angular distribution (CDAD), whereby the handedness is introduced by the experimental geometry. This key experiment evidently shows that the determination of the full quantum mechanical wave function is possible by simultaneous measurement of intensity and phase.

O 69.9 Thu 13:00 HSZ 01

**3D Tomographic Imaging of Molecular Orbitals in Real Space** — •Pascal Nigge[1,2], Martin Graus[1,2], Vitaliy Feyer[3,4], Michael Wiessner[1,2], Achim Schöll[1,2], and Friedrich Reinert[1,2] — [1]Universität Würzburg, 97074 Würzburg, Germany — [2]Karlsruher Institut für Technologie KIT, 76021 Karlsruhe, Germany — [3]Research Center Jülich, 52425 Jülich, Germany — [4]Sincrotrone Trieste, 34012 Basovizza, Trieste, Italy

The imaging of molecular orbitals by angle resolved photoelectron spectroscopy (ARPES) or photoemission electron microscopy (PEEM) has shown to be a very powerful tool for the investigation of molecular materials. By mapping the angle dependent intensity patterns of photoelectrons this technique provides tomographic images of the density distribution of the orbitals in k-space. The full potential of the tomographic mapping of molecular orbitals becomes obvious by providing three-dimensional images of orbitals in real space. While this has already been proposed theoretically, the practical realization requires access to variable photon energies at a synchrotron. We present first experimental data that demonstrates how 3D-imaging of molecular orbitals is feasible with a PEEM, which allows reconstruction of the molecular orbital in momentum space from the hemispherical k-space tomograms. Utilizing the additional phase information derived from experiments with circular light polarization, the full molecular orbital can be uncovered in 3D in real space by a Fourier transformation, thus providing unprecedented insight into the electronic structure of molecules.

# O 70: Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale VI

Time: Thursday 10:30–13:15 Location: TRE Ma

**Topical Talk** O 70.1 Thu 10:30 TRE Ma

**Localization at the edge of 2D topological insulator by Kondo impurities** — •Boris Altshuler[1], Igor Aleiner[1], and Vladimir Yudson[2] — [1]Physics Department, Columbia University, New York, NY 10027, USA — [2]Institute for Spectroscopy, Russian Academy of Sciences,Troitsk, Moscow 142190, Russia

Recent interest to the topological insulators [1] is inspired by the fact that their boundaries host gapless electronic excitations, which are extended and make the system conductive even in the presence of a potential disorder. 1D edge of a 2D topological insulator is predicted to have perfect conductance (2e2/h): right and left moving electrons carry opposite spins and potential disorder cannot flip spins and thus causes neither back-scattering nor the usual 1D localization.

What if there are localized spins coupled to the edge electrons? It turns out that the conductivity is still perfect provided that this coupling conserves the z-projection of the total spin of the impurities and electrons. Magnetic anisotropy violates this conservation and causes the backscattering even at T=0, i.e. an arbitrary small density of the spins with arbitrary weak anisotropy of the coupling leads to Anderson localization of the edge states in long enough samples [3]. The conclusion follows from the mapping of the electron-spin coupling to the well-studied problem [2] of disordered Luttinger liquid.

1. M.Z. Hasan and C.L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
2. T.Giamarchi and H.J.Schulz, Phys. Rev. B 37, 325 (1988).
3. B.L.Altshuler, I.L.Aleiner, V.I. Yudson Phys. Rev. Lett 111, 086401 (2013)

O 70.2 Thu 11:00 TRE Ma

**Multiple Exciton Generation in Si and Ge Nanoparticles with high pressure core structures** — •Stefan Wippermann[1], Marton Vörös[2], Dario Rocca[3], Adam Gali[4], Gergely Zimanyi[2], and Giulia Galli[2] — [1]Max-Planck-Institute for Iron Research, Düsseldorf — [2]University of California, Davis — [3]Universite de Lorraine, Nancy — [4]Budapest University of Technology and Economics

Multiple exciton generation (MEG) in semiconductor nanoparticles (NPs) is a promising path towards surpassing the Shockley-Queisser limit in solar energy conversion efficiency. Recent studies demonstrate MEG to be more efficient in NPs than in the bulk, including Si. However, the increased efficiency is observed only on a relative energy scale in units of the gap: quantum confinement (QC) effects believed to be responsible for efficient MEG in NPs, also increase their optical gap, swiftly shifting the MEG threshold beyond the solar spectrum.

We present density functional and many body perturbation theory calculations of the electronic, optical, and impact ionization properties of Si and Ge nanoparticles (NPs) with core structures based on high-pressure bulk Si and Ge phases. Si and Ge particles with a BC8 or ST12 core structure exhibit significantly lower optical gaps and multiple exciton generation (MEG) thresholds, and an order of magnitude higher MEG rate than diamondlike ones of the same size (1).

(1) S. Wippermann et al., Phys. Rev. Lett. 110, 046804 (2013)

O 70.3 Thu 11:15 TRE Ma

**Advanced time-evolution method for optical absorption spectra calculations** — •Tobias Sander and Georg Kresse — Computational Materials Physics, University of Vienna, Sensengasse 8/12, 1090 Vienna, Austria

The Green's function formalism from many-body perturbation theory gives access to electronic structure calculation within the quasiparticle picture, as well as provides for calculating optical absorption spectra. Within the traditional ansatz [1], a Bethe-Salpeter like equation for the polarizability is solved. This requires to diagonalize an in general non-hermitian and complex matrix (BSE matrix). Usually, the off-diagonal elements of the BSE matrix are neglected and this is referred to as Tamm-Dancoff approximation. The computational effort can be reduced by using the time-evolution ansatz [2] which avoids the matrix diagonalization. We present a method based on the time-evolution algorithm, that finally avoids storing and diagonalizing the BSE matrix. This leads to a reduction of the scaling w.r.t the system size N from $N^5$ to $N^3$. Finally, we present first results for typical systems.

[1] S. Albrecht, L. Reining, R. Del Sole, G. Onida, PRL 80, 4510 (1998)
[2] W. G. Schmidt, S. Glutsch, P. H. Hahn, F. Bechstedt, PRB 67, 085307 (2003)

O 70.4 Thu 11:30 TRE Ma

**New starting point for the calculation of optical properties** — •Igor Reshetnyak[1,2] and Lucia Reining[1,2] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, F-91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF)

The Bethe-Salpeter Equation based on Hedin's GW approximation to the self-energy is a powerful approach for describing electron-hole interactions in optical properties and photo-absorption spectra. However, in its current formulation it is both computationally heavy and displays cancellation effects not accounted for analytically. We discuss the sources of these cancellations and the possibility of putting them forward explicitly. We furthermore assess alternative formulations and sets of approximations to the BSE. For each of them we examine its behavior on model systems as well as their computational applicability. Finally we suggest possible directions for further investigations.

O 70.5 Thu 11:45 TRE Ma

**Electron-Energy Loss and Inelastic X-ray Scattering of CuO from First Principles** — •Claudia Rödl, Francesco Sottile, Matteo Gatti, and Lucia Reining — Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau cedex, France and European Theoretical Spectroscopy Facility (ETSF)

Even though the strongly correlated transition-metal oxide CuO has many fields of application (potential absorber material in photovoltaic devices, pigment in glass and ceramics, building block of cuprate superconductors,...), surprisingly little is known about its electronic excitations from a theoretical point of view. The band gap and all electronic excitations in its vicinity are governed by the intricate interplay between itinerant O $2p$ and localized Cu $3d$ electrons. Complex many-body effects, that are still not well understood nowadays, determine the screening of the electron-electron interaction.

Electron-energy loss and inelastic x-ray scattering experiments yield direct access to the wave-vector- and frequency-dependent loss function $-\operatorname{Im}\varepsilon^{-1}_{\mathbf{GG}'}(\mathbf{q},\omega)$, and, hence, to the screened Coulomb interaction $W$. We use time-dependent density-functional theory (TDDFT) to calculate the loss spectrum of CuO and discuss the occurring *d-d* and plasmon excitations. This allows us, by comparing theory and experiment, to assess the quality of the screened Coulomb interaction which is a key quantity for many-body approaches, for instance, *GW* and Bethe-Salpeter calculations.

O 70.6 Thu 12:00 TRE Ma

**Optical Spectra from Molecules to Solids: Insight from Many-Body Perturbation Theory** — •Caterina Cocchi and Claudia Draxl — Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

The spurious long-range behavior of time-dependent (TD) density functional theory (DFT) is a well known source of error in describing bound excitons in solids. Remarkably, TD-DFT is often able to capture the optical features of isolated systems, even with the most simple exchange-correlation kernels, like the TD local density approximation. With the example of molecular crystals, we aim at solving the puzzle when and why TD-DFT can be relied on. We answer this question by confronting TD-DFT with many-body perturbation theory (GW and Bethe-Salpeter equation), which is the most accurate methodology to describe optical excitations in solids. Our results are obtained with the all-electron code "exciting" (http://exciting-code.org), where all the quantities entering the two formalisms are treated on the same footing [1]. In-depth analysis allows us to identify the shortcomings of TD-DFT in predicting the excitonic spectra of extended systems and to understand when this methodology is capable of providing correct results.

[1] S. Sagmeister and C. Draxl, Phys. Chem. Chem. Phys. 11, 4451 (2009)

O 70.7 Thu 12:15 TRE Ma

**Relativistic Solar Cells** — •Paolo Umari[1], Edoardo Mosconi[2], and Filippo De Angelis[2] — [1]Dipartimento di Fisica e Astronomia, Università di Padova, via Marzolo 8, I-35131 Padova, Italy — [2]Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), CNR-ISTM, Via Elce di Sotto 8, I-06123, Perugia, Italy

Hybrid $AMX_3$ perovskites (A=Cs, $CH_3NH_3$; M=Sn, Pb; X=halide) have revolutionized the scenario of emerging photovoltaic technologies. Indeed, a rapid evolution led, very recently, up to 15% efficient solar cells. $CH_3NH_3PbI_3$ has so far dominated the field, while the similar $CH_3NH_3SnI_3$ has not been explored for photovoltaic applications, despite the reduced band-gap. Replacement of Pb by the more environment-friendly Sn would facilitate the large uptake of perovskite-based photovoltaics. Despite the extremely fast progress, the materials electronic properties which are key to the photovoltaic performance are relatively little understood. Here we develop an effective GW method incorporating spin-orbit coupling which allows us to accurately model the electronic, optical and transport properties of $CH_3NH_3SnI_3$ and $CH_3NH_3PbI_3$, opening the way to new materials design. The different $CH_3NH_3SnI_3$ and $CH_3NH_3PbI_3$ properties are discussed in light of their exploitation for solar cells, and found to be entirely due to relativistic effects.

O 70.8 Thu 12:30 TRE Ma

**Solar nanocomposites with complementary charge extraction pathways for electrons and holes: Si embedded in ZnS** — •Stefan Wippermann[1], Marton Vörös[2], Adam Gali[3], Francois Gygi[2], Gergely Zimanyi[2], and Giulia Galli[2] — [1]Max-Planck-Institute for Iron Research, Düsseldorf — [2]University of California, Davis — [3]Budapest University of Technology and Economics

We propose that embedding silicon nanoparticles (NP) into amorphous, non-stoichiometric ZnS leads to promising nanocomposites for solar energy conversion. Using ab initio molecular dynamics simulations we show that upon high temperature amorphization of the host chalcogenide, sulfur atoms are drawn to the NP surface. We found that the sulfur content may be engineered to form a type II heterojunction, with complementary charge transport channels for electrons and holes, and that sulfur capping is beneficial to lower the nanoparticle gap, with respect to that of NPs embedded in oxide matrices. Our analysis was conducted using density functional theory with local and hybrid functionals and many body perturbation theory at the GW level.

O 70.9 Thu 12:45 TRE Ma

**Ultraviolet photo-emission spectroscopies from Koopmans-compliant functionals** — •Ngoc Linh Nguyen[1], Giovanni Borghi[1], Andrea Ferretti[2], Ismaila Dabo[3], and Nicola Marzari[1] — [1]Theory and Simulations of Materials, École Polytechnique Fédérale de Lausanne, Station 12, 1015 Lausanne, Switzerland. — [2]Centro S3, CNR-Istituto Nanoscienze, I-41125 Modena, Italy — [3]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, USA.

We study the photo-electron properties of organic photovoltaic molecules using Koopmans-compliant functionals [1] as well as the Perdew-Zunger self-interaction correction (PZ-SIC) [2] to density-functional theory. A simple method for simulating ultraviolet photoemission spectra (UPS) of molecules has been implemented. It is based on a plane-wave approximation for the final states to account for the spectra intensities. Our calculations show that Koopmans-compliant functionals provide ionization potentials and electron affinities closely comparable with those obtained by many-body perturbation theory (GW). In addition, we find that UPS spectra computed imposing the Koopmans' condition on the PZ-SIC functional are in remarkable agreement with experimental results.

Refs: [1] I. Dabo, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, and M. Cococcioni, Phys. Rev. B 82, 115121 (2010); [2] J. P. Perdew and A. Zunger, Phys. Rev. B 23, 5048 (1981).

O 70.10 Thu 13:00 TRE Ma

**Self-consistent dynamical embedding in real space** — •Wael Chibani[1], Xinguo Ren[1,2], Patrick Rinke[1], and Matthias Scheffler[1] — [1]*Fritz Haber Institute of the Max Planck Society, Berlin, Germany* — [2]*Key Laboratory of Quantum Information, USTC, Hefei, China*

Density-functional theory with its local-density (LDA) and generalized gradient approximations (GGA) is known to fail for localized states. To extend *ab initio* approaches to this domain, we have devised an embedding scheme that facilitates the treatment of the physically important part of a system with electronic structure methods, that are computationally too expensive for periodic systems, whereas the rest of the periodic system is treated with computationally less demanding approaches, i.e. LDA/GGA, in a self-consistent manner. Our scheme is based on the concept of dynamical mean-field theory (DMFT) [1]. However, in contrast to the original DMFT formulation for correlated model Hamiltonians, we consider here the unit cell as embedded cluster in an *ab initio* way, that includes all electronic degrees of freedom. The performance of our scheme is demonstrated by treating the embedded region with hybrid functionals for simple bulk systems, e.g. Si or NiO. The total energy and the density of states converge rapidly with respect to the computational parameters and approach their bulk limit with increasing cluster size. By treating the embedded region with *GW* we were able to improve the band gap using only a small cluster. The effect of self-consistency in *GW* for the embedded region will also be addressed. [1] A. Georges *et al.*, Rev. Mod. Phys. **68**,14 (2006)

## O 71: Plasmonics and Nanooptics III

Time: Thursday 10:30–13:00 Location: GER 38

O 71.1 Thu 10:30 GER 38

**Photochromic switching of Fano resonances in metallic photonic crystals** — •Felix Bleckmann[1], Sandra Cordes[2], Eduard Maibach[2], Clayton Shallcross[2], Klaus Meerholz[2], and Stefan Linden[1] — [1]Physikalisches Institut, Universität Bonn, Nußallee 12, 53115 Bonn, Germany — [2]Institut fürr Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, 50939 Köln, Germany

We study switchable metallic photonic crystals composed of a gold grating embedded in a photochromic waveguide. For that purpose we coated the gold grating on top of an ITO-covered glass substrate with the photochromic material XDTE. The interaction of localized plasmonic resonances and delocalized waveguide modes forms waveguide-plasmon polaritons (WPPs) and thus gives rise to a typical Fano line shape in the extinction spectra. The layer thicknesses as well as the shape and period of the gold grating were optimized for the design wavelength of the maximal switching efficiency of the XDTE layer ($\lambda = 610$ nm). By illumination of the sample with UV light, XDTE becomes absorptive in the red part of the spectrum and the damping of the waveguide mode strongly increases. As a result, the Fano dip is strongly suppressed. The low absorpion state is recovered by illumination with orange light. Compared to a simple XDTE film of the same thickness, our approach doubles the switching efficiency at the design wavelength $\lambda = 610$ nm.

O 71.2 Thu 10:45 GER 38

**Tuning propagating surface phonon polaritons at mid-infrared frequencies using a phase-change material** — •Tao Wang, Peining Li, Ann-Katrin Michel, Dmitry N. Chigrin, Matthias Wuttig, and Thomas Taubner — 1st Institute of Physics (IA), RWTH Aachen University, 52056, Aachen, Germany

Plasmonic antennas are crucial components for nano-optics and have been extensively used to enhance sensing, spectroscopy, light emission, photodetection and others [1, 2]. Nowadays, there is a trend to search for new plasmonic materials with low intrinsic loss at new plasmon frequencies. Alternative to metals, polar crystals have a negative real part of permittivity in the Reststrahlen band and support surface phonon polaritons (SPhP) with weak damping. Recently, we experimentally demonstrated single circular microcavities with well-defined, size-tunable SPhP resonances possessing high Q factors around 60 which are much higher than those in surface plasmon polariton resonators with similar structures [3]. In this work, we present that the dispersion of propagating surface phonon polaritons and the resonances of circular SPhP microcavities can be tuned by the phase change of a thin-layer germanium antimony telluride (GST). The tunability of the propagating SPhP dispersion and resonance pave the way for realizing single active antennas with high Q-factors at mid-infrared frequencies.

[1] L. Novotny et al., Nat. Photonics 5, 83-90 (2011). [2] P. Biagioni,et al., Rep. Prog. Phys. 75, 024402 (2012). [3] T. Wang et al., Nano Lett. 13, 5051-5055 (2013).

O 71.3 Thu 11:00 GER 38

**Probing coherent surface plasmon polaritons propagation in gold films using ultrabroadband spectral interferometry** — •Dongchao Hou, Heiko Kollmann, Martin Silies, and Christoph Lienau — AG Ultraschnelle Nano-Optik, Institut für Physik, Fakultät V, Universität Oldenburg, 26111 Oldenburg, Deutschland

Surface Plasmon Polaritons (SPP), generated by ultrashort laser pulses at thin dielectric-metal interfaces can transport energy in metallic structures over mesoscopic distances. They can then be used to couple far-field radiation into nanoscopic dimensions reaching extreme light intensities, e.g. at the end of metallic nanotips [1,2].

These SPPs propagate as coherent wavepackets and with propagation properties that are defined by the geometry of the material and the composition of the metal film, e.g. grain boundaries and surface quality. So far, coherent SPP propagation in metallic nanostructures has been studied to a limit extent.

Here, we introduce a new ultrabroadband far-field spectral interferometry method to characterize coherent SPP propagation in metallic nanostructures. Group velocity and dispersion of SPPs are determined with high precision in a wide frequency range in the visible and near-infrared region. Our results shed new light on the interplay between nanostructure geometry and coherent SPP propagation.

[1] S. Schmidt et al., ACS Nano 6, 6040-6048 (2012)

[2] C.C. Neacsu et al., Nano Letters 10, 592-596 (2010)

O 71.4 Thu 11:15 GER 38

**Plasmo-Emission: Nonlinear Emission of Electrons from the Plasmonic Field** — •Philip Kahl, Andreas Makris, Simon Sindermann, Michael Horn-von Hoegen, and Frank-J. Meyer zu Heringdorf — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

Nonlinear Photoemission Electron Microscopy (PEEM) using ultrashort ($< 20$ fs) laser pulses in a normal incidence geometry has been demonstrated to be capable of observing Surface Plasmon Polaritons (SPPs) in space and time. The advantage of the normal incidence geometry over the commonly used grazing incidence geometry is the fringe spacing of the observed Photoemission pattern, which resembles the SPP wavelength. Furthermore, due to the cylindrical symmetry of this incidence geometry, all propagation directions of SPPs on the surface are imaged equally. This opens the possibility to perform Plasmon-Nanooptics measurements, in which SPPs can be observed propagating in different directions and also being reflected, all with sub-wavelength resolution. In the overlap region of two counter-propagating SPPs the formation of a standing wave can be observed. Curved grating couplers can be used to focus two SPPs propagating in opposite directions into a joint focal point. The resulting standing wave pattern has a characteristic time, space and energy signature of SPP-emitted electrons (Nonlinear Plasmo-Emission) and arises without the need of additional light to trigger Photoemission (classical nonlinear Photoemission).

O 71.5 Thu 11:30 GER 38

**Interplay between strong coupling and radiative damping of excitons and surface Plasmon polaritons in hybrid nanostructures** — Wei Wang[1], Parinda Vasa[1,2], Robert Pomraenke[1], Ralf Vogelgesang[1], Antonietta de Sio[1], •Ephraim Sommer[1], Margherita Maiuri[3], Cristian Manzoni[3], Giulio Cerullo[3], and Christoph Lienau[1] — [1]Institut für Physik, Universität Oldenburg, 26129 Oldenburg — [2]Indian Institute of Technology Bombay, 400076 Mumbai — [3]Dipartmento di Fisica, Politecnico di Milano, Milano

Strongly coupled exciton - surface plasmon polariton systems (X-SPP) are of great interest, as they carry a high potential for realizing all-optical plasmonic circuits and devices [1]. For such applications it is imperative to tailor the radiative damping of the coupled system. So far, however, little is known about radiative damping of strongly coupled systems. We therefore study the optical response of a strongly coupled J-aggregate/SPP hybrid [1] by means of coherent angle-resolved spectral interferometry and ultrafast pump-probe spectroscopy. We find large differences between the radiative lifetimes of the hybrid upper (UP) and lower (LP) polariton mode. This indicates that two different energy transfer channels between X and SPP coexist: (i) coherent resonant dipole-dipole interaction [1] and (ii) an incoherent exchange due to spontaneous emission of a photon by one emitter and its subsequent reabsorption by another. The interplay between both pathways results in a pronounced modification of the radiative damping due to the formation of sub- and super-radiant polariton states.

1. Vasa, P. et al, Nature Photon. 7, 128-132, 2013

O 71.6 Thu 11:45 GER 38

**k-space resolved nano-imaging with an adiabatic nanofocusing SNOM** — •Simon F. Becker, Martin Esmann, Jens H. Brauer, Petra Gross, Ralf Vogelgesang, and Christoph Lienau — Carl von Ossietzky Universität, 26111 Oldenburg, Germany

Adiabatic nanofocusing of surface plasmon polaritons (SPP) propagating on metallic tapers promises to largely reduce unwanted background contributions in apertureless scanning near-field optical microscopy (SNOM) [1,2]. SPP wavepackets launched on a grating-coupler come to a complete halt at the taper apex for an ideal cone-shaped waveguide. Hence, a single point-dipole like light source is formed which bears great potential for nano-imaging and spectroscopy applications.

Recently, we have developed and implemented a k-space imaging technique to characterize this nano-scale light-source and to separate contributions from different taper eigenmodes [3]. Only the lowest, rotationally symmetric eigenmode is expected to contribute to near-fields at the taper apex. Here, using Stokes polarimetry k-space imaging, we isolate the emission from this lowest eigenmode and demonstrate its radial polarization. This allows us to implement a new adaptive optics scheme (based on [4]) to optimize the emission of this fundamental mode. For the first time, we apply k-space resolved polarimetry to nano-imaging of metallic nanostructures and investigate the near-field coupling between probe and sample.

[1] M.I. Stockman, PRL 93, 137404 (2004); [2] S. Schmidt et al., ACS Nano 6, 6040 (2012); [3] M. Esmann et al., BJ Nano 4, 603 (2013); [4] S. Schmidt et al., Opt. Express 21, 26564 (2013).

O 71.7 Thu 12:00 GER 38

**Low-temperature scattering scanning near-field optical microscopy** — •Jonathan Döring, Susanne C. Kehr, and Lukas M. Eng — IAPP, George-Bähr-Straße 1, 01069 Dresden

We present a fully operating low-temperature scattering scanning near-field optical microscope (LT-s-SNOM) with access to a tunable free-electron laser (FEL) source. The light scattered off an AFM tip strongly depends on the tip-sample near-field interaction, and thus enables mapping of optical properties with a resolution ways below the diffraction limit. The FEL provides spectrally narrow laser radiation in the regime from 4 to 250 $\mu m$ at a high power density. By the novel and unique combination of LT-s-SNOM and FEL, optical properties of materials can be measured at specific wavelengths as well as at temperatures down to $4K$. Our device is therefore perfectly suited for investigating phase transitions of sample materials featuring phonon resonances in the mid-to-far-infrared regime.

We present measurements of the tetragonal-to-orthorhombic phase transition of barium titanate (BTO), a prototype perovskite ferroelectric material. At room temperature BTO features a characteristic domain pattern, which changes dramatically below the transition temperature of $253K$ as the alteration of the crystal structure is accompanied by a realignment of the spontaneous polarisation axes. We imaged the anisotropy contrast between such ferroelectric domains by LT-s-SNOM [1] above and below the phase transition temperature and confirmed our results by piezo-response force microscopy (PFM).

[1] Kehr et al., Phys. Rev. Lett. 100, 256403 (2008)

O 71.8 Thu 12:15 GER 38

**Topological optical-phase transitions in superlensing imaging** — •Peining Li[1], Thomas Taubner[1], Jon Schuller[2], Mark Brongersma[2], Chris Fietz[3], Yaroslav Urzhumov[3], Dmitriy Korobkin[3], Gennady Shvets[3], and Rainer Hillenbrand[4] — [1]I. Institute of Physics (IA), RWTH Aachen University, Aachen 52056, Germany — [2]Geballe Lab for Advanced Materials, Stanford University, Stanford, California 94306, USA — [3]Department of Physics and Center for Nano and Molecular Science and Technology, The University of Texas at Austin, Austin, Texas 78712, USA — [4]CIC nanoGUNE Consolider, 20018 Donostia-San Sebastián, Spain

Metamaterials show great capabilities to artificially engineer the light-matter interactions. It has been recently shown that tuning the optical dispersion of metamaterials from ellipsoidal dispersion to hyperbolic dispersion enables a substantial intensity-enhancement of high-spatial-frequency (or high-k) optical fields. In this work, we focus on the phase behavior of high-k fields within the dispersion transition of metamaterials. By using interferometric scanning near-field optical microscopy, we are able to record phase information of the superlens, which is usually lost in the intensity-recording measurements. We experimentally reveal a phase transition of optical near fields in an infrared metamaterial superlens when its dispersion altering between two different kinds of hyperbolic dispersions. Our results illuminate the important role of phase imaging in superlensing, which are also useful for understanding phase behaviors in other metamaterial-based imaging devices such as perfect-lens, hyperlens and meta-lens.

O 71.9 Thu 12:30 GER 38

**Near-field nanospectroscopy on perovskite-based superlenses** — •Susanne C. Kehr and L.M. Eng — Institut für Angewandte Physik/Photophysik, Technische Universität Dresden, 01061 Dresden

A planar slab with negative permittivity acts as a superlens: it transforms the evanescent fields from the object located on one side of the slab, to form a sub-diffraction-limited image on the opposite side. We study superlenses based on perovskite oxides that show superlensing in the mid-IR. These materials have little material absorption at the wavelengths of interest and, moreover, can be grown epitaxially in high quality, which reduces any losses due to scattering at the interfaces.

We examine multilayer lenses by scattering-type near-field optical microscopy (s-SNOM) in combination with a free-electron laser. This unique setup allows us to address precisely the superlensing resonance, to record the local images created by the lenses, and to measure their spectral response. We found that different perovskites can be combined to form superlenses at different wavelengths that match perfectly theoretical predictions [1]. All of these superlenses form images beyond the diffraction limit. Moreover, we found that the spectral behavior of the lenses reflects a special probe-sample coupling that is mediated by the superlens [2], which might be of interest for functionalized coupling of nanosized objects. Furthermore, the special properties of perovskites such as colossal magnetoresistance, ferroelectricity, and superconductivity may allow for further applications and variations of superlensing.

[1] S.C. Kehr et al., Opt. Mater. Express 1, 1051 (2011).

[2] S.C. Kehr et al., Nat. Commun. 2, 249 (2011).

O 71.10 Thu 12:45 GER 38

**Modified Solid Immersion Lens Design for Efficient Light Extraction** — •Andreas W. Schell, Tanja Neumer, and Oliver Benson — Humboldt-Universität zu Berlin, Institut für Physik, AG Nanooptik, D-12489 Berlin, Germany

For solid-state single photon emitters, like quantum dots or defect centers like the nitrogen vacancy (NV) center in diamond, it usually is very difficult to efficiently extract the photons. Due to the high refractive index of the host material, many photons are totally internal reflected at the material's planar interface – photons which are basically lost. An elegant way to circumvent this problem is to use of so called solid immersion lenses (SILs). In analogy to the immersion oil in oil immersion microscopy these lenses are made to suppress total internal reflection. Standard SILs are based on a spherical geometry, with the hemispherical SIL being most common.

Here, we will show a design based on ellipsoids and verify its usefulness via three-dimensional finite difference time domain (FDTD) simulations. These structures can be easily produced using the process of two-photon direct laser writing, a process which also allows for direct integration of single photon emitters [1]. Our modified SILs are able to not only collect light, but also do also make use of controlled total internal reflection to direct the light into a very small solid angle while maintaining a high overlap with a Gaussian beam, solving two drawbacks of standard SIL designs at once.

[1] A. W. Schell et al., Scientific Reports 3, 1577 (2013).

## O 72: Competition for the Gerhard Ertl Young Investigator Award

Time: Thursday 10:30–13:00 Location: PHY C 213

O 72.1 Thu 10:30 PHY C 213

**Fundamental aspects of germanium surface passivation by gas phase oxidation and liquid phase sulfidation** — •Claudia Fleischmann[1], Koen Schouteden[2], Michel Houssa[3], Sonja Sioncke[4], Matthias Müller[5], Chris Van Haesendonck[2], Kristiaan Temst[1], and Andre Vantomme[1] — [1]Instituut voor Kern- en Stralingsfysica, KU Leuven, Celestijnenlaan 200D, BE-3001 Leuven, Belgium — [2]Laboratorium voor Vaste-Stoffysica en Magnetisme, KU Leuven, Celestijnenlaan 200D, BE-3001 Leuven, Belgium — [3]Laboratory of Semiconductor Physics, KU Leuven, Celestijnenlaan 200D, BE-3001 — [4]imec, Kapeldreef 75, BE-3001, Leuven, Belgium — [5]Physikalisch-Technische Bundesanstalt, Abbestrasse 2-12, D-10587 Berlin, Germany

To fully explore the potential germanium may offer for device application the effective and reliable passivation of defect states is essential (A.Dimoulas et al. 2007). In this contribution we will present two promising passivation schemes for Ge(100) surfaces: The in situ oxidation and ex situ sulfidation. By applying complementary analysis techniques we were able to investigate -at the atomic level- the adsorption mechanisms and surface properties of these O/Ge(100) and S/Ge(100) systems. We will show that both treatments result in discontinuous (sub-monolayer) self-limiting adsorbate layers. The adsorption geometry is comparable between both passivation schemes, and similarities are observed in view of passivation of intrinsic unoccupied defect states in the Ge band gap. The overall quality of the passivation layer appears to be limited by intrinsic and extrinsic constraints.

O 72.2 Thu 11:00 PHY C 213

**Unraveling Elementary Electron Scattering Processes Using Ultrafast Photoemission** — •Patrick Kirchmann — Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park CA, USA

Femtosecond time- and angle resolved photoemission spectroscopy is becoming a powerful tool for resolving elementary electron scattering processes directly in the time domain. Measurement of the transient single-particle function grants simultaneous access to single- and many-body information with energy and momentum resolution only few methods can deliver. In this contribution, we highlight these exciting capabilities by discussing (i) quasi-particle lifetimes due to electron-electron scattering in quasi-two-dimensional Pb quantum wells and their relation to Fermi liquid theory [1], (ii) optical excitation pathways and phonon-mediated surface-to-bulk scattering in the topological insulator compound $Bi_2Se_3$ [2], and (iii) the collective response of the amplitude mode in the charge density wave compound $TbTe_3$ [3]. These results provide qualitatively new insights into the dynamics of optically excited electrons and the collective response of emergent phases in quantum materials.

[1] Nature Physics 6, 782 (2010)

[2] PRL 108, 117403 (2012); PRL 111, 136802 (2013)

[3] Science 321, 1649 (2008)

O 72.3 Thu 11:30 PHY C 213

**Digging up the band structure of buried layers** — •Jill Miwa[1], Philip Hofmann[1], Oliver Warschkow[2], Damien Carter[3], Nigel Marks[3], Michelle Simmons[4], and Justin Wells[5] — [1]Aarhus University, Denmark — [2]University of Sydney, Australia — [3]Curtin University, Australia — [4]UNSW, Australia — [5]NTNU, Norway

Atomically precise dopant placement opens up an exciting new arena for exploring complex valley physics in novel materials and quantum electronic devices. Atomic scale devices derived from phosphorus $\delta$-layers in silicon have been recently demonstrated, including a single-atom transistor. A $\delta$-layer is formed several nanometers beneath the surface of silicon because of a one-atom-thick plane of phosphorus dopants which are placed there. The local but strong doping leads to confined 2D electron states, separated by an energy referred to as valley splitting. The magnitude of the valley splitting has implications for critical device properties. Hitherto only indirect information on the electronic structure of the 2D states and valley splitting was available and a reliance on calculations has been necessary. We directly measure the band structure of a buried $\delta$-layer using ARPES. Although the $\delta$-layer is deeply buried, relative to the photoelectron mean free path, photoemission is still possible at very low kinetic energies, or when a resonant enhancement is invoked. By engineering a favourable surface Umklapp process, we can resolve the $\delta$-layer states and measure a valley splitting of 132meV, which falls centrally within reported calculated values. Electronic properties, such as valley splitting, are central in understanding $\delta$-layers and their use in atomic-scale devices.

O 72.4 Thu 12:00 PHY C 213

**PdZn and CuZn model catalysts for methanol steam reforming - Structure selectivity correlations obtained by in-situ surface spectroscopy and catalytic testing** — •Christoph Rameshan[1], Werner Stadlmayer[2], Christian Weilach[1], Harald Lorenz[2], Michael Hävecker[3], Raoul Blume[3], Tulio Rocha[3], Detre Teschner[3], Axel Knop-Gericke[3], Robert Schlögl[3], Norbert Memmel[2], Dmitry Zemlyanov[4], Günther Rupprechter[1], and Bernhard Klötzer[2] — [1]Institute of Materials Chemistry, Vienna University of Technology, Lehargasse 9, 1060 Wien — [2]Institute of Physical Chemistry, University of Innsbruck, Innrain 52a, 6020 Innsbruck — [3]Department of Inorganic Chemistry, Fritz-Haber-Institute of the Max-Planck_society, Faradayweg 4-6, 14195 Berlin — [4]Brick Nanotechnology Centre, Purdue University, 1205 West State Street, West Lafayette, In 47907-2057, USA

Methanol Steam Reforming is a promissing reaction for the reneable Energy Scenario. The reaction must be carried out with a high selectivity, avoiding the undesired by-product CO, which poissons the fuell-cell electro catalyst. Apart from advanced copper based catalysts, reduced states of Pd/ZnO or Pd/Ga2O3 have been identified as promising candidates. This work was focused on PdZn and CuZn model catalysts and their activity and selectivity. Exact correlation between their catalyst structure and the catalytic performance were shown through synchrotron based in-situ ambient pressure XPS measurements. It could be shown that only a sufficient thick PdZn intermetallic phase with a corrugated surface (Zn out, Pd in) is an excellent catalyst.

O 72.5 Thu 12:30 PHY C 213

**Cost-Effective Catalysis on Early Transition Metal Carbides Surfaces** — •Francesc Viñes — Universitat de Barcelona, Barcelona, Spain

Most of the reactions carried out in the industry are catalyzed on the surface of materials, which oftentimes are late transition metals, given its ideal properties as catalytic active phases. However, coinage and Pt-group metals can be quite expensive mainly due to their scarcity, which leaded to the utilization of metal nanoparticles supported on oxide supports, thus partially alleviating the economic burden.

Early transition metal carbides have been introduced in the last decase as a low-cost alternative to late transition metals. Beyond the comparable electric and thermic conductivities, they present physical robustness, and, eventually, a catalytic activity comparable, or even superior, to late transition metals. Here we show, by ab initio density functional calculations combining experimental results, how different surfaces of such carbides are adequate catalytic active phases for a variety of reactions, including the water-gas-shift reaction and the dissociation of small molecules, such as oxygen, hydrogen, and even carbon dioxide. Moreover, theses carbides result to be excellent supports for late transition metal clusters, playing also the role of promoters; the carbide surface is able to polarize the late transition metal electron density, leading to an enhanced catalytic activity, as shown to be critical in the decomposition of sulfur-containing species such as sulphur dioxide and tiophene. Future fields of applications are envisaged.

## O 73: Scanning Probe Methods II

Time: Thursday 10:30–13:15 Location: WIL A317

O 73.1 Thu 10:30 WIL A317

**Friction contrast in Dynamic Friction Force Microscopy** — •Felix Mertens, Thomas Göddenhenrich, and André Schirmeisen — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, D-35392 Gießen

Dynamic Friction Force Microscopy is a measuring technique for the investigation of friction properties on the nanometer scale. The off-resonance modulation of the sample excites bending oscillations of the cantilever if the tip is in contact with the sample surface. Contrast at surface steps and grain boundaries on HOPG demonstrate, that the third-harmonic lock-in detection is a selective method for the investigation of different tip-sample interactions. Furthermore, the signal on antimony nanoparticles shows the dependence on modulation amplitude and frequency for different materials as well as the influence caused by the particle topography.

O 73.2 Thu 10:45 WIL A317

**Artifacts in combined STM/AFM due to non-ideal ground in an STM pre-amplifier** — •Nirmalesh Kumar Sampath Kumar, Alfred John Weymouth, and Franz Josef Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

In AFM, it is normal to apply a bias voltage between the tip and the sample, most often to compensate for the contact potential difference. In order to perform simultaneous STM, the tunneling current must be measured. This usually involves a pre-amplifier that holds its current input terminal at a virtual ground that is ideally equal to real ground. Limitations of amplifier bandwidth, gain and slew rate lead to time-dependent deviations of virtual ground from zero, causing a time-dependent variation of the electrostatic force between tip and sample. These time-dependent deviations can lead to artifacts in apparent dissipation and even to an apparent "self" excitation of the cantilever. Here, we monitor virtual ground and discuss the effect of virtual ground deviations to apparent dissipation.

O 73.3 Thu 11:00 WIL A317

**Dynamic local work function measurement and the role of topography** — •Ferdinand Huber[1], Sonia Matencio[2], Alfred J. Weymouth[1], and Franz J. Giessibl[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute of Material Science of Barcelona (ICMAB-CSIC), Campus UAB, 08193 Bellaterra, Spain

Performing simultaneous STM/AFM allows the electronic structure of the surface to be investigated. Two common methods are Kelvin Probe Force Microscopy (KPFM) and current-distance ($I$-$z$) spectroscopy. With KPFM, the tunneling current channel is difficult to interpret because the applied bias is not constant. $I$-$z$ spectroscopy is usually performed at low temperature in order to minimize drift and creep. We propose an alternate technique called *dynamic $\kappa$ measurement* based on Refs. [1] and [2], in which we measure the decay constant of the tunneling current taking advantage of the oscillating conducting tip. We explain this technique and compare it to measurements at low temperature. Furthermore we discuss the influence of topography on the local work function.

[1] G. Binnig, H. Rohrer, Surf. Sci. **126**, 236 (1983)

[2] M. Herz, Ch. Schiller, F. Giessibl and J. Mannhart, Appl. Phys. Lett. **86**, 153101 (2005)

O 73.4 Thu 11:15 WIL A317

**The STM as Microwave resonator: Josephson currents interacting with the environment** — •Berthold Jäck[1], Matthias Eltschka[1], Maximilian Assig[1], Markus Etzkorn[1], Christian R. Ast[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, D-70569 Stuttgart — [2]École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne

We investigated the Josephson Effect in Vanadium tunnel junctions by using an STM operating at a temperature of 15 mK [1]. As the STM junction geometry is of very small capacitance our measured current-voltage characteristics exhibit clear indications for Coulomb blockade dominated tunneling in the overdamped regime. Next to the supercurrent we observe harmonic sub-gap features at energies of about 100 *eV. By varying the STM tip length and the tip-sample geometry we are able to tune both resonance energy as well as its intensity. We explain these findings with photon-assisted tunneling of

Cooper pairs driven by an electro-magnetic mode localized on the STM tip. The mode is excited by GHz radiation which is emitted from the Josephson junction driven in the AC regime. Our physical picture is substantiated with finite-element-method simulations on the electrodynamic properties of our 3D tip-sample geometry. We will discuss these findings in the framework of Josephson junctions coupled to an electro-magnetic environment [2] and also give an outlook in view of possible applications as GHz-source on the atomic scale.

[1] M. Assig et al., Rev. Sci. Instrum. 84, 033903 (2013)

[2] G.-L. Ingold et al., Phys. Rev. B 50, 1 (1994)

O 73.5 Thu 11:30 WIL A317

**The Zeeman Effect in dimensionally confined, superconducting STM tips** — •C. R. Ast[1], M. Eltschka[1], B. Jäck[1], M. Assig[1], M. Etzkorn[1], O. V. Kondrashov[2], M. A. Skvortsov[2,3], and K. Kern[1] — [1]MPI for Solid State Research, Stuttgart — [2]Moscow Institute of Physics and Technology, Moscow, Russia — [3]Landau Institute for Theoretical Physics, Chernogolovka, Russia

It has been shown in the 1970s that in thin films superconductivity persists in much higher magnetic fields than in the bulk. The resulting Zeeman splitting of the spin-polarized electrons has been used to measure the absolute spin-polarization of electrons in planar tunnel junctions. Transferring this concept to the superconducting tip in a scanning tunneling microscope, it is not *a priori* clear that the dimensional confinement at the tip apex is suitable to produce a similar effect. We show both experimentally and theoretically that this effect can be observed in scanning tunneling spectroscopy. The parameters for successful tip preparation as well as possible applications will be discussed.

O 73.6 Thu 11:45 WIL A317

**Multi-Tip STM / Nanoprober for electrical characterization at the nanoscale** — •Bert Voigtländer, Vasily Cherepanov, Peter Coenen, Stefan Korte, Marcus Blab, and Hubertus Junker — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

We present design and performance of an ultra compact four tip STM which integrates four independent STM units within a diameter of 50 mm resulting in a mechanical stability which enables atomic resolution imaging with each tip. The heart of this STM is a new type of piezoelectric coarse approach called KoalaDrive. The coarse positioning of the tips is done under the control of an SEM. This multi-tip instrument offers the capability to perform current and voltage measurements at the nanoscale. Due to its small size this instrument is ideally suited for integration into a cryostat. The control electronics allows each tip to be used as current probe or voltage probe. The software allows virtually any possible "concerted" spectroscopic measurements involving the four tips and the sample. We demonstrate the potential of the instrument to perform charge transport measurements at the nanoscale by various examples: Resistance/dopant profiling at freestanding GaAs nanowires, distance dependent four point measurements at Si surfaces, and gate dependent charge transport measurements on graphene.

O 73.7 Thu 12:00 WIL A317

**Atomically resolved STM imaging with a single-crystal diamond tip** — Vladimir I. Grushko[1], •Olaf Lübben[2], Alexander N. Chaika[2,3], Nikolay V. Novikov[1], Evgeniy I. Mitskevich[1], A. P. Chepugov[1], Oleg G. Lysenko[1], Barry E. Murphy[2], Sergey A. Krasnikov[2], and Igor V. Shvets[2] — [1]V. Bakul Institute for Superhard Materials, Kiev, 04074, Ukraine — [2]Centre for Research on Adaptive Nanostructures and Nanodevices, School of Physics, Trinity College, Dublin 2, Ireland — [3]Institute of Solid State Physics RAS, Chernogolovka, Moscow district 142432, Russia

The spatial resolution of a scanning tunneling microscope (STM) can be enhanced using light element-terminated probes with spatially localized electron orbitals at the apex atom. Conductive diamond probes can provide carbon atomic orbitals suitable for STM imaging with sub-Ångström lateral resolution and high apex stability crucial for the small tunneling gaps necessary for high-resolution experiments. Here we demonstrate that high spatial resolution can be achieved in STM experiments with single crystal diamond tips. The results of STM experiments with a heavily boron-doped, diamond probe on a graphite surface; density functional theory calculations of the tip and surface electronic structure; and first principles tunneling current calculations demonstrate that the highest spatial resolution can be achieved with diamond tips at tip-sample distances of 3-5 Å when the $p$ orbitals of the tip provide their maximum contribution to the tunneling current. At the same time, atomic resolution is feasible even at extremely small gaps with very high noise in the tunneling current.

O 73.8 Thu 12:15 WIL A317

**STM imaging of HOPG: Tip geometry effects** — •Gábor Mándi[1], Gilberto Teobaldi[2], and Krisztián Palotás[1] — [1]Budapest University of Technology and Economics, Department of Theoretical Physics, Budafoki út 8., H-1111 Budapest, Hungary — [2]Stephenson Institute for Renewable Energy, and Surface Science Research Centre, Department of Chemistry, University of Liverpool, L69 3BX Liverpool, UK

Highly oriented pyrolytic graphite (HOPG) is an important substrate in technological applications, particularly in scanning tunneling microscopy (STM) calibration. Therefore, the proper interpretation of the experimentally observed STM image contrasts is very important [1]. Using a three-dimensional (3D) Wentzel-Kramers-Brillouin (WKB) tunneling model [2,3] combined with first principles electronic structure calculations, we demonstrate that the tip orientation has a considerable effect on the simulated STM images. We show that the local rotation of the apex of the STM tip can cause a triangular-hexagonal contrast change. By comparing STM topographic data between experiment [1] and large scale simulations, we can determine particular tip orientations that are most likely present in the STM experiment.

[1] G. Teobaldi et al., Phys. Rev. B 85, 085433 (2012).

[2] K. Palotás et al., Phys. Rev. B 86, 235415 (2012).

[3] G. Mándi et al., J. Phys.: Condens. Matter 25, 445009 (2013).

O 73.9 Thu 12:30 WIL A317

**A new low temperature near-field optical scanning microscope** — •Julia Janik[1], Claudio Dal Savio[2], and Achim Hartschuh[1] — [1]Department Chemie and CeNS, LMU München, 81377 München, Germany — [2]attocube systems AG, 80539 München, Germany

The characterisation of nanostructures with high spatial resolution and detection sensitivity can be achieved by tip-enhanced near-field optical microscopy (TENOM) [1]. Up to now nearly all TENOM measurements were performed at room temperature. Low temperature measurements on the other hand would reveal even more detailed information about material properties, for example due to reduced spectral broadening. We describe a new scheme for implementing TENOM at low temperatures. For initial experiments and testing well known quasi 1D semiconducting model systems such as single-walled carbon nanotubes (SWCNT) and cadmium selenide (CdSe) nanowires were used [2]. Here we describe our efforts and first results on our way towards low temperature near-field optical microscopy.

We acknowledge financial support by NIM and the ERC (NewNanoSpec).

[1] N. Mauser and A. Hartschuh, Chem. Soc. Rev., DOI: 10.1039/C3CS60258C (2014)

[2] M. Böhmler et al., Angew. Chem. Int. Ed. 50, 11536 (2011)

O 73.10 Thu 12:45 WIL A317

**Secondary Electron Analysis with Topografiner Techonlogy** — •Lorenzo G. De Pietro, Danilo A. Zanin, Hugo Cabrera, Mehmet Erbudak, Andreas Fognini, Thomas U. Michlmayr, Yves M. Acremann, Danilo Pescia, and Urs Ramsperger — ETH Zurich, Switzerland

In Near Field-Emission Scanning Electron Microscopy (NFESEM), based on the topografiner techonlogy, cold field emitted electrons from a sharp polycrystalline W-tip are the source of a primary electron beam. The applied voltage for field emission (between the tip and the sample) accelerates these electrons up to some tens of eV. After having interacted with the sample, secondary and backscattered electrons are detected, while an STM controller is used to scan the tip at a constant distance (10 to 20 nm) from the sample surface. This technique has been used to take topography images of various metals and semiconductors achieving subnanometer lateral resolution. In case of a W(110) surface partially covered by Fe a chemical contrast was observed. After having implemented energy analysis to this technique, we present a series of images generated by collecting only electrons with selected energies, i.e. true secondary electrons. This represents an important step in view of adding a spin polarization analysis and use the NFESEM as an instrument to investigate magnetic surfaces at a nanometer scale.

O 73.11 Thu 13:00 WIL A317

**High-Resolution Imaging and nano-FTIR Spectroscopy using Synchrotron Radiation at the Metrology Light Source** — •Peter Hermann[1], Arne Hoehl[1], Piotr Patoka[2], Bernd Kästner[1], Georg Ulrich[2], Eckart Rühl[2], Burkhard Beckhoff[1], and Gerhard Ulm[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany — [2]Physikalische und Theoretische Chemie, Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

Infrared radiation provided by an electron storage ring can be regarded as an ideal source for spectroscopic applications since it is up to 1000 times brighter and covers a much broader spectral range than the radiation emitted from a conventional thermal light source. The achievable spatial resolution is, however, limited by diffraction, thus preventing a resolution below the diffraction limit. This limitation can be circumvented by using near-field approaches which are based on the use of a sharp metallic probe tip acting as a nano-scale light source when irradiated by a focused synchrotron radiation (SR) beam. In the following, we report on the use of broadband SR provided by the Metrology Light Source (MLS) for near-field imaging and acquisition of nano-FTIR spectra in a wide spectral range. By using SR for imaging of Si-based samples a spatial resolution below 50 nm can be achieved. The near-field signal detection in nano-FTIR measurements is confirmed by the acquisition of spectra from a SiC sample showing the characteristic strong phonon resonance near 927 cm-1. Additionally, further results obtained from various solid matter samples are presented.

## O 74: Surface and Interface Magnetism II (O jointly with MA)

Time: Thursday 10:30–13:00 Location: WIL C107

O 74.1 Thu 10:30 WIL C107

**Spin excitations in nanostructures on a Cu(111) surface: Access to the electron self-energy from first-principles** — •Benedikt Schweflinghaus, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Magnetic excitation spectra of nanostructures are nowadays accessible by low-temperature inelastic scanning tunneling spectroscopy, see *e.g.* [1]. We developed a first-principles description of such spectra by combining time-dependent density functional theory and many-body perturbation theory, implemented in a code based on the Korringa-Kohn-Rostoker Green function method [2,3]. The coupling of the electrons to the spin-excitation within the adsorbate is given in terms of the electron self-energy. We analyze this key quantity for a number of clusters with different geometries placed on a Cu(111) substrate. We spin-characterize their excitation spectra and discuss how they change with the number of involved atoms, their kind, and their arrangement on the surface.

This work is supported by the HGF-YIG Programme VH-NG-717 (Functional Nanoscale Structure and Probe Simulation Laboratory, Funsilab).

[1] A. A. Khajetoorians *et al.*, Phys. Rev. Lett. **106**, 037205 (2011).
[2] S. Lounis *et al.*, Phys. Rev. Lett. **105**, 187205 (2010).
[3] S. Lounis *et al.*, Phys. Rev. B **83**, 035109 (2011).

O 74.2 Thu 10:45 WIL C107

**Calculation of magnetoelectric coupling at Fe/BaTiO$_3$ and Fe/SrTiO$_3$ interfaces** — •Hannes Behrend, Brahim Belhadji, and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, 24098 Kiel, Germany

The magnetoelectric coupling effect in composites built out of piezoelectric and ferromagnetic materials has attracted great interest, e.g for sensor applications. The objective of our work is to calculate the magnetoelectric coupling that occurs locally, on an atomic scale, at the Fe/BaTiO$_3$ and Fe/SrTiO$_3$ interfaces by means of spin-density functional calculations. The program VASP by Kresse, Hafner *et al.* from the University Wien is applied. The magnetization density and magnetic moment induced by an external electric field are calculated for electric field strengths chosen sufficiently small so that the system stays in the linear response regime. Currently most of the results refer to frozen-in atomic positions,with additional first results for atomic geometries relaxed under the influence of the electric field. A detailed comparison of the Fe/BaTiO$_3$ and Fe/SrTiO$_3$ interfaces will be given. This will be complemented by a calculation of the magnetoelectric coupling coefficient for Fe/Cu layers, for which we have observed an unexpectedly sensitive dependence of the result on the thickness of the Fe slab. The spacial variation of the induced magnetization density as opposed to the induced electronic charge density will be addressed.

O 74.3 Thu 11:00 WIL C107

**Control of ferromagnetism in epitaxial La$_{0.7}$Sr$_{0.3}$MnO$_3$ films via BaTiO$_3$ substrate phase transitions investigated by XMCD and XLD** — •Arndt Quer[1], Erik Kröger[1], Kerstin Hanff[1], Lars Oloff[1], Rohit Soni[2], Adrian Petraru[2], Matthias Kalläne[1], Herrmann Kohlstedt[2], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institute of Experimental and Applied Physics, University of Kiel, Germany — [2]Department of Nanoelectronics, University of Kiel, Germany

It is known that La$_{0.7}$Sr$_{0.3}$MnO$_3$ thin films grown on BaTiO$_3$ can undergo strain-controlled giant, sharp, and persistent magnetization changes as a result of substrate structural phase transitions. In order to investigate the interplay between lattice strain, magnetism, and electronic structure in this system, we have performed X-ray magnetic circular dichroism (XMCD) and X-ray linear dichroism (XLD) measurements on 20-nm thin, epitaxial La$_{0.7}$Sr$_{0.3}$MnO$_3$ films grown by pulsed laser deposition on single-crystalline BaTiO$_3$. Here, we report the obtained results. Experiments were performed at the BACH beamline of the Elettra syncrotron storage ring (Trieste, Italy). This work was supported by the DFG (German Research Foundation) through SFB 855 (Collaborative Research Centre 855) "Magnetoelectric Composites - Future Biomagnetic Interfaces".

O 74.4 Thu 11:15 WIL C107

**Spin Excitations in STM Evaluated in Perturbation Theory** — •Markus Ternes — Max-Planck Institut für Festkörperphysik, Heisenbergstr. 1, 70569 Stuttgart, Germany

Inelastic spin flip spectroscopy has been very successful to characterize and manipulate the properties of single spins as well as coupled spin structures on surfaces. I will show that a perturbative approach of the interactions between the localized spin system, the probing tip, and the supporting substrate can results in fits to experimental data with unprecedented accuracy. The employed model is based on a transport Hamiltonian which accounts for spin-flip and Coulomb scattering of the tunneling electrons with the magnetic impurity system. Higher order and correlations effects are considered by including spin-spin scattering between the impurity and substrate electrons and by solving the corresponding rate-equations up to 3rd order. Despite its simplicity, the model enables a deeper understanding of the relevant couplings in such systems and provides an easy access to the dynamical properties and correlations in atomic scale spin systems.

O 74.5 Thu 11:30 WIL C107

**Interplay between Kondo effect and molecular quenching in magnetic molecules at metal substrates from first principles** — •David Jacob[1], Maria Soriano[2], and Juan José Palacios[2] — [1]MPI für Mikrostrukturphysik, Halle, Germany — [2]Universidad Autónoma de Madrid, Madrid, Spain

When a magnetic molecule is deposited on a metallic substrate or attached to metal leads, the Kondo effect can take place, thereby screening its magnetic moment. On the other hand strong coupling of the transition metal center to the organic ligands also leads to quenching of the spin. Using our DFT based ab initio approach for nanoscale devices explicitly taking into account the dynamic correlations originating from strong electronic interactions [1,2], we calculate the electronic structure and STM spectra of high spin complexes on metal surfaces. Our calculations reveal the complex interplay of the Kondo effect and molecular quenching processes in these systems [3]. Furthermore we find that Kondo screening via the organic ligands leads to novel features in the spectral function near the Fermi level different from the usual Kondo peaks. [1] D. Jacob *et al.*, PRL **103**, 016803 (2009); [2] M. Karolak *et al.*, PRL **107**, 146604 (2011); [3] D. Jacob *et al.*, PRB

**88**, 134417 (2013).

O 74.6 Thu 11:45 WIL C107

**Protection of excited spin states by a superconducting energy gap** — •Benjamin W. Heinrich[1], Lukas Braun[1], José I. Pascual[1,2], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]CIC nanoGUNE, San Sebastián, and Ikerbasque, Basque Foundation for Science, Bilbao, Spain.

The ability to tune the magnetism of individual atoms or molecules and to control their interaction with the environment is a key requirement for their use in potential spintronic applications. We employ scanning tunneling microscopy and spectroscopy at 1.2 K to characterize the spin state of individual metal-organic complexes, namely Fe(III)-Octaethylporphyrin-Chloride, adsorbed on a superconducting Pb(111) surface. The organic ligand provides an anisotropic environment for the spin of the Fe ion ($S = 5/2$), which leads to a zero field splitting of the spin eigenstates. The superconducting gap in the density of states of the substrate now stabilizes excited spin states of the Fe as it hinders the exchange of energy and angular momentum between the substrate's quasi-particles and the molecular spin. This allows for lifetimes of $\approx$ 10 ns of the excited spin state [1]. Furthermore we examine the influence of our probe, the STM tip, on the zero field splitting of the Fe ion. Even at a distance of several Angstrom between tip and molecule a sizable change of the magnetic anisotropy is detected.

[1] B. W. Heinrich *et al.* Nature Physics, doi:10.1038/nphys2794.

O 74.7 Thu 12:00 WIL C107

**Scanning tunneling microscopy and spectroscopy of transition metal phthalocyanines on noble metal surfaces** — •Jens Kügel, Jacob Senkpiel, Pin-Jui Hsu, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Transition metal phthalocyanine (TM-Pc) molecules adsorbed on metal substrate have recently attracted considerable interest, as they offer a versatile platform to study magnetic interaction of the central metal ion with the substrate. Especially the Kondo effect, a collective interaction phenomena with the substrate, arising from unscreened magnetic moments of the metal ion, has been intensively studied [1,2]. In this contribution we present low-temperature ($T = 5\,\mathrm{K}$) scanning tunneling microscopy and spectroscopy data of CuPc and MnPc adsorbed on different noble metal substrates [Ag(001), Cu(001)]. The different molecular spectra will be compared and analyzed in terms of their electronic and magnetic properties. In particular we will focus on the Kondo effect and discuss how superimposed states can lead to misinterpretation of the Kondo temperature.

[1] E. Minamitani *et al.*, Phys. Rev. Lett. **109**, 086602 (2012).
[2] A. Stróżecka *et al.*, Phys. Rev. Lett. **109**, 147202 (2012).

O 74.8 Thu 12:15 WIL C107

**Engineering Giant Magnetic Anisotropy and Kondo Resonances in Cobalt Adatoms on the h-BN Nanomesh** — •Peter Jacobson[1], Tobias Herden[1], Markus Ternes[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

The magnetic properties of Cobalt adatoms on the h-BN/Rh(111) nanomesh have been investigated by scanning tunneling microscopy at low temperatures (1.5 K) and high magnetic fields (10 T). Isolated Co adatoms show a pronounced Kondo resonance consistent with a spin-1 system with an estimated Kondo temperature well below 1 K possessing negligible magnetic anisotropy. Addition of hydrogen to the Co adatoms results in a remarkable shift in the magnetic properties, the Kondo resonance disappears and inelastic spin flip excitations are observed. The Co-H species remains in a spin-1 state and the spin flip excitations indicate that this species has a substantial magnetic anisotropy of 5 meV. The large magnetic anisotropy is attributed to an unquenched orbital moment. Given the dramatic changes upon hydrogen adsorption, we consider the 'molecular' Co-H system an ideal test system for engineering the magnetic anisotropy in molecular magnets.

O 74.9 Thu 12:30 WIL C107

**tuning spin-related transport properties of FePc on Au(111) by single-molecule chemistry** — •Jian Shang — BNLMS, college of chemistry and molecular engineering, Peking University, 100871, Beijing, China

Tuning spin-related transport properties at the single molecule level is crucial not only for a fundamental understanding of charge and spin interactions but also represents a prerequisite for development of molecular electronics and spintronics. Here we deposited FePc on Au(111) and then, tuned its spin-related transport properties step by step by single-molecule chemistry. After removing 2H, 4H, 6H and 8H from the molecule, Kondo effect, spin transition, Kondo effect and spin transition were observed in differential conductance spectra, sequentially.

O 74.10 Thu 12:45 WIL C107

**Spin state of spin-crossover complexes: from single molecules to ultra-thin films** — •Manuel Gruber[1,2], Vincent Davesne[1,2], Martin Bowen[1], Samy Boukari[1], Eric Beaurepaire[1], Wulf Wulfhekel[2], and Toshio Miyamachi[2,3] — [1]IPCMS (UMR 7504 Université de Strasbourg-CNRS), Strasbourg, France — [2]Physikalisches Institut, Karlsruher Institut für Technologie, Germany — [3]Institute for Solid State Physics, University of Tokyo, Chiba, Japan

The spin-state bi-stability of spin-crossover molecules [1] can, in principle, be used as building blocks of memory devices. However, it is not obvious if such complexes deposited on surfaces can sustain their controllable bi-stability. In this work, using a scanning tunneling microscope in ultra-high vacuum at 4K, we investigated Fe(1,10-phenanthroline)2(NCS)2 molecules on Cu(100) and Cu(111) surfaces for coverage going from single molecules to ultra-thin films. For submonolayer coverage both spin species coexist at low temperatures [2] while this coexistence seems to be lost for the second-layer molecules. We give insights about the origin of this unexpected spin-state coexistence based on the adsorption geometry. Furthermore, we observe voltage-dependent topographies of the second-layer molecules that we tentatively ascribe to a voltage-dependent steady-state combination of HS and LS in a proportion that reflects the bias- and current-dependent switching rates to/from the HS state [3].

[1] P. Gütlich et al., Chem. Soc. Rev. 29, 419 (2000). [2] T. Miyamachi et al., Nat. Commun. 3, 938 (2012). [3] M. Gruber et al., in preparation.

# O 75: Plenary Talk (Lukas Novotny)

Time: Thursday 14:00–14:45 Location: HSZ 02

**Plenary Talk** O 75.1 Thu 14:00 HSZ 02

**Optical Antennas for Enhanced Light-Matter Interactions** — •Lukas Novotny — ETH Zürich, Photonics Laboratory, 8093 Zürich

Optical antennas consisting of plasmonic materials provide extreme light localization and small mode volumes, thereby boosting the sensitivity and signal-to-noise ratio in applications ranging from single photon sources to photodetection. Optical antennas can also be employed to efficiently control and manipulate light on the nanometer scale and to achieve directional emission. I will review the physical properties of optical antennas, present recent results, and discuss applications.

# O 76: Invited Talk (Carsten Busse)

Time: Thursday 15:00–15:45 Location: TRE Ma

**Invited Talk** O 76.1 Thu 15:00 TRE Ma

**Quasi free-standing graphene** — •Carsten Busse — II. Physikalisches Institut, Universität zu Köln, Germany

Following its successful isolation from graphite in 2004, graphene has risen to one of the most researched topics in solid state physics with e.g. whole sessions at this conference devoted to this material only. A widespread method to produce graphene is epitaxial growth on metal surfaces. Here, Ir(111) sticks out as it allows the growth of extended layers with a high degree of structural perfection where the interaction between the carbon sheet and its substrate is comparably weak. However, the close proximity of the metal surface modifies the behavior of charge carriers (opening of minigaps), quenches the characteristic phonon modes, decreases the lifetime of plasmons, and precludes mechanical exfoliation of graphene.

Intercalation of an additional species as alkali metals or oxygen reduces the graphene-substrate interaction and renders graphene quasi free-standing. I will highlight the structure of the resulting graphene intercalation compounds measured using scanning tunneling microscopy (STM) with superior lateral resolution and x-ray standing waves (XSW) with high vertical resolution. The electronic structure as determined by Fourier transform scanning tunneling spectroscopy and angular resolved photoemission spectroscopy (ARPES) shows unperturbed graphene bands, often strongly shifted in energy due to significant charge transfer (doping) from the intercalant to the carbon layer. I will show that graphene nanoflakes can act as quantum dots and confine image potential states as well as Dirac states.

# O 77: Focussed Session: Towards a Quantitative Understanding of Complex Adsorption Structures: Surface Science goes Organic III

Time: Thursday 16:00–19:00 Location: TRE Phy

**Topical Talk** O 77.1 Thu 16:00 TRE Phy

**Infrared-Spectroscopy applied to ultrathin organic films.** — •Peter Jakob — Physics Department, Philipps-University Marburg, 35032 Marburg, Germany

IR-spectroscopy is commonly referred to as a fingerprint technique to identify molecular species. However, this method can do better! The high spectral resolution and polarization dependence of vibrational modes allows to distinguish between different local environments (→ lateral interactions), bonding configurations (→ adsorption site and orientation), and phases (monolayer, bilayer, bulk) of large organic molecules with high selectivity. Thereby IR spectroscopy is non-invasive/destructive, obeys strict selection rules, and provides adequate sensitivity to detect even slight differential changes within grown films. Selected examples of various effects and curiosities associated with ultra-thin molecular layers will be presented, demonstrating the excellent quality and potential of infrared spectroscopy in studying such systems. Notably, for molecular species exhibiting a partially filled (former) LUMO, IR spectra are influenced by interfacial dynamical charge transfer (IDCT) between molecule and metal substrate /1/. By means of line-shape analysis of the associated Fano-like absorption profiles the electron dynamics (electron transfer time) between contact primer layer and metal substrate can be estimated.
/1/ F.S. Tautz, Progress in Surface Science 82 (2007) 479-520.

O 77.2 Thu 16:30 TRE Phy

**Diffusion and site selection of PTCDA on KCl(100) studied by fluorescence spectroscopy and STM** — Alexander Paulheim, Christian Marquardt, Qinmin Guo, and •Moritz Sokolowski — Institut für Physikalische und Theoretische Chemie der Universität Bonn Wegelerstraße 12, 53115 Bonn, Germany

We report an investigation on the optical properties of the model molecule PTCDA at very low coverages (below 1% of a monolayer) on thin epitaxial KCl(100) films. From STM data we derive a statistical adsorption of isolated molecules at low temperature. Upon thermal activation, diffusion to steps edge sites occurs, comparable to that on other alkali halide surfaces [1]. This scenario was investigated also by fluorescence spectroscopy (FL) and FL excitation spectroscopy, exploiting its high sensitivity. Different adsorption sites lead to different optical transition energies due to differences in the molecule substrate interactions [2]. In addition, from the external vibronic modes we conclude that the PTCDA molecule is distorted from its planar geometry by the interaction with the KCl surface. [1] H. Karacuban et al., Nanotech., 2011, 22, 295305; [2] Paulheim et al., Phys. Chem. Chem. Phys., 2013, 15, 4906.

O 77.3 Thu 16:45 TRE Phy

**Site specific mobility boost of caged bisphenol A trimers on Ag(111)** — •Özge Sağlam, Julian A. Lloyd, Anthoula C. Papageorgiou, Sybille Fischer, Seung Cheol Oh, Katharina Diller, David A. Duncan, Francesco Allegretti, Florian Klappenberger, Joachim Reichert, and Johannes V. Barth — Physik Department E20, Technische Universität München, Garching, Germany

Artificial molecular rotors, which have been a focus of attention in the last decade of nanoscience, are fascinating subjects not only in terms of fundamental understanding of molecular motion but also due to their promising potential in the context of molecular scale machinery. The construction of regularly oriented two-dimensional arrays of molecular rotors, rather than isolated single rotors, is a key requirement to demonstrate and miniaturize functional systems for signal processing or sensing. Such a molecular system of regular arrays of molecular rotors has been achieved by utilizing a single layer of bisphenol A (BPA) molecules on the weakly corrugated Ag(111) surface. We employ a combined experimental approach using STM, XPS and NEXAFS providing complementary insights regarding self-assembled networks built with BPA molecules on the Ag(111) surface under UHV conditions. Our data reveal temperature-dependent polymorphism, where mobile molecules undergo rotational movements when trapped in the cavities of a nanoporous network. We propose molecular models stabilized by intermolecular hydrogen bonding, and explain the rotational motion of the caged species by their specific adsorption sites.

O 77.4 Thu 17:00 TRE Phy

**Structure and ordering of thin organic layers on silicon surfaces** — •Thomas Schmidt, Christian Schulz, Torsten Wilkens, and Jens Falta — Universität Bremen, Germany

The adsorption and growth of organic layers on silicon surfaces offers the opportunity to combine the application potential of organic materials with silicon technology, e.g., for hybrid solar cells, transistors, or biosensors [1–3].

We investigated thin films of 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) and copper phthalocyanine (Cu-PC) on Si(111) surfaces that had been passivated with monolayer deposits of either Ag or Bi. Scanning tunneling microscopy and high-resolution low-energy electron diffraction show a drastic improvement of the structural order and morphology as compared to deposition on clean Si(111).

PTCDA forms smooth layers with a herringbone structure on Ag-terminated as well as Bi-terminated Si(111). For the latter case, x-ray photoelectron spectroscopy indicates a charge transfer from the carbonyl oxygen of the anhydride groups to the substrate. Additional structural phases are observed in the initial growth stages, which can be suppressed by deposition at elevated temperatures.

With respect to the structural order of Cu-PC films, Ag turns out to be superior to Bi as passivating agent and leads to well-ordered domains with rhombic (nearly square) unit cells.

[1] D.R.T. Zahn et al., Solar Energy **80**, 707 (2006).
[2] L. De Stefano et al., Sensors **7**, 214(2007).
[3] Zhongming Wei et al., Appl. Phys. Lett. **95**, 033304 (2009).

O 77.5 Thu 17:15 TRE Phy

**Growth of 2D molecular crystals: The role of the substrate topology** — •Daniel Schwarz[1], Caroline Henneke[1], Raoul van Gastel[2], Harold Zandvliet[2], Bene Poelsema[2], and Christian Kumpf[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich and Jülich Aachen Research Alliance (JARA) – Fundamentals of Future Information Technology, 52428 Jülich, Germany — [2]Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, NL-7500 AE Enschede, The Netherlands

We present a LEEM study on the initial growth dynamics and the influence of the substrate topology on 2D molecular crystals. We have selected BDA and PTCDA, which both are elongated flat organic molecules with oxygen atoms at their ends. Deposited on Cu(001) both molecules form well-ordered 2D crystals. However, despite the similarities, the interaction of the molecules with Cu-steps is quite different, resulting in distinct differences in the domain growth dynamics. Steps are permeable for the smaller BDA molecule, which leads to a growth instability of the Mullins-Sekerka type: Domains grow very fast along the steps and much slower perpendicular to the steps. PTCDA, on the other hand, interacts strongly with steps, which makes them impermeable for molecules and hence does not exhibit the Mullins-Sekerka instability.

O 77.6 Thu 17:30 TRE Phy

**Combined 2PPE and photoluminescence study of electron and exciton dynamics at the PTCDA/Ag(111) interface** — •Andreas Namgalies, Manuel Marks, Sangam Chatterjee, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg

The presence of a metal contact can drastically alter the electron and exciton dynamics of organic semiconductors. For a study of the fundamental processes that govern this dynamics as well as the dynamics of carrier transfer at the metal/organic interface, we combine the advantages of time resolved 2-photon-photoemission (2PPE) and time-resolved photoluminescence in one experiment and investigate well-ordered and characterized thin films of PTCDA/Ag(111). Our luminescence setup enables monolayer sensitivity and a time resolution of approximately 700 fs using a streak camera.

It will be shown that a long-lived component of hot electrons in the 2PPE spectrum, whose lifetime and intensity strongly increases as a function of layer thickness, arises at the metal interface as a result of exciton decay of PTCDA. Systematic studies as a function of film thickness reveal, that Foerster-like dipole-dipole coupling is important for the decay in the regime of several monolayers, whereas exciton hopping between PTCDA layers and quenching and the interfaces dominates the decay for thicker films.

O 77.7 Thu 17:45 TRE Phy

**Molecular Geometry Determination by Atomic Force Microscopy** — •Nikolaj Moll, Leo Gross, Bruno Schuler, Fabian Mohn, Alessandro Curioni, and Gerhard Meyer — IBM Research – Zurich, Säumerstrasse 4, CH-8803 Rüschlikon, Switzerland

Using functionalized tips, the atomic resolution of a single organic molecule can be achieved by atomic force microscopy (AFM) operating in the regime of short-ranged repulsive Pauli forces while the van-der-Waals and electrostatic interactions only add a diffuse attractive background [1]. To theoretically describe the atomic contrast a simple model is introduced in which the Pauli repulsion is assumed to follow a power law as a function of the probed charge density. Even, different bond orders of individual carbon-carbon bonds in organic molecules can be distinguished by AFM [2]. The adsorption geometry of single molecules with intramolecular resolution were measured. The lateral adsorption position was determined with atomic resolution, adsorption height differences, and tilts of the molecular plane with very high precision [3].

[1] L. Gross, F. Mohn, N. Moll, P. Liljeroth, and G. Meyer, Science 325, 1110 (2009).

[2] L. Gross, F. Mohn, N. Moll, B. Schuler, A. Criado, E. Guitián, D. Peña, A. Gourdon, and G. Meyer, Science 337, 1326 (2012).

[3] B. Schuler, W. Liu, A. Tkatchenko, N. Moll, G. Meyer, A. Mistry, D. Fox, and L. Gross, Phys. Rev. Lett. 111, 106103 (2013).

O 77.8 Thu 18:00 TRE Phy

**Quantifying molecule-surface interactions using AFM-based single-molecule manipulation** — •Christian Wagner[1,2], Norman Fournier[1], Victor G. Ruiz[3], Chen Li[4], Michael Rohlfing[5], Alexandre Tkatchenko[3], F. Stefan Tautz[1], and Ruslan Temirov[1] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Universiteit Leiden, Leiden, The Netherlands — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [4]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [5]Universität Münster, Münster, Germany

Scanning probe microscopy plays an important role in the investigation of molecular adsorption. Promising is the possibility to probe the molecule-surface interaction while tuning its strength through AFM tip-induced single-molecule manipulation. Here, we outline a strategy to achieve quantitative understanding of such manipulation experiments [1,2]. The example of qPlus sensor based 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) molecule lifting experiments is used to demonstrate how different aspects of the molecule-surface interaction, namely the short-range adsorption potential [2], the asymptotic van der Waals potential, and local chemical bonds which are the source of the surface corrugation can be quantified by the help of force-field simulations.

[1] N. Fournier et al., *Phys. Rev. B* **84**, 035435 (2011)
[2] C. Wagner et al., *Phys. Rev. Lett.* **109**, 076102 (2012)

O 77.9 Thu 18:15 TRE Phy

**Accessing 4f-states in single-molecule spintronics** — •Frank Matthes[1,4], Sarah Fahrendorf[1,4], Nicolae Atodiresei[2,4], Claire Besson[3,4], Vasile Caciuc[2,4], Stefan Blügel[2,4], Paul Kögerler[3,4], Daniel E. Bürgler[1,4], and Claus M. Schneider[1,4] — [1]Peter Grünberg Institute, Electronic Properties, Forschungszentrum Jülich, Germany — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Quantum Theory of Materials, Forschungszentrum Jülich, Germany — [3]Institute of Inorganic Chemistry, RWTH Aachen University, Germany — [4]Jülich-Aachen Research Alliance, Fundamentals for Future Information Technology, Forschungszentrum Jülich, Germany

Magnetic molecules are potential functional units for molecular and supramolecular spintronic devices. However, charge transfer and hybridization may modify the electronic structure and thereby influence or even quench the molecular magnetic moment. Yet, detection and manipulation of the molecular spin state by means of charge transport, that is, spintronic functionality, mandates a certain level of hybridization of the magnetic orbitals with electrode states. Here we show how a judicious choice of the molecular spin centres determines these critical molecule-electrode contact characteristics. In contrast to late lanthanide analogues, the 4f-orbitals of single bis(phthalocyaninato)-neodymium(III) molecules adsorbed on Cu(100) can be directly accessed by scanning tunneling microscopy[1]. Hence, they contribute to charge transport, whereas their magnetic moment is sustained as evident from comparing spectroscopic data with ab initio calculations.

[1] S. Fahrendorf *et al.*, Nature Commun. 4, 2425 (2013)

O 77.10 Thu 18:30 TRE Phy

**Structure-dependent reactions of tetraphenylporphyrin with Cu(111)** — •Ole Lytken, Michael Röckert, Matthias Franke, Quratulain Tariq, Michael Stark, Stefanie Ditze, Hubertus

Marbach, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen, Egerlandstraße 3, Germany

As tetraphenylporphyrin (2HTPP) is deposited on Cu(111) and heated, several distinct reactions happen: First the porphyrin molecule picks up a copper atom from the surface and metalates forming copper(II)tetraphenylporphyrin (CuTPP), which subsequently dehydrogenates, first loosing 8 hydrogen atoms and later the remaining 20. The first dehydrogenation reaction is proposed to link the phenyl rings with the pyrrole rings, and the last dehydrogenation reaction is proposed to be the loss of the remaining hydrogen atoms producing an ill-defined, interlinked, nitrogen-doped carbon network on the surface. The rate of the metalation and the first dehydrogenation both depends strongly on coverage, with an abrupt change as the coverage is increased and the structure of the adsorbed 2HTPP layer changes. Using XPS, STM and TPD (of both deuterated and undeuterated molecules) the reaction rates and the different intermediates on the surface have been investigated in the temperature range from 200-1000 K as a function of the structure of the initial 2HTPP layer.

O 77.11 Thu 18:45 TRE Phy

**DFT calculations addressing a possible imaging mechanismin the Scanning Tunneling Hydrogen Microscope** — •Uwe Friedel and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

The Scanning Tunneling Hydrogen Microscope (STHM) [1] can resolve intramolecular structures of adsorbed organic molecules and even produce intermolecular contrast along lines of expected hydrogen bondings. The method does not only work with hydrogen, which gave the method its name, but also with other molecules such as CO and nobel gas atoms. Still, the reasons for the improved contrast in the STHM are not fully understood yet.

This talk will present dispersion corrected DFT calculations (DFT-D3 [2]) addressing the interaction of a CO molecule positioned between a tip and a pentacene molecule. The distance of the CO molecule from the tip has been monitored as a function of its lateral position above the naphthalene molecule. We will discuss whether an explanation based on Tersoff-Hamann theory [3] can be established in order to understand the improved contrast in the STHM.

[1] C. Weiss *et al.*, J. Am. Chem. Soc. **132**, 11864 (2010)
[2] S. Grimme *et al.*, J. Chem. Phys. **132**, 154104 (2010)
[3] J. Tersoff and D.R. Hamann, Phys. Rev. Lett. **50**, 1998 (1983)

## O 78: Graphene: Spintronics, Transistors, and Sensors (HL jointly with DY, MA, O, TT)

Time: Thursday 15:00–18:00 Location: POT 081

O 78.1 Thu 15:00 POT 081

**Graphene's RF Potential: How harmful is the Zero Bandgap?** — Kyle D. Holland[1], Navid Paydavosi[1], Neophytos Neophytou[2], •Diego Kienle[3], and Mani Vaidyanathan[1] — [1]Department of Electical and Computer Engineering, University of Alberta — [2]Institute for Microelectronics, Technical University of Vienna — [3]Institute of Theoretical Physics I, University of Bayreuth

With the aid of self-consistent quantum-mechanical simulations and simple expressions for the radio-frequency (RF) metrics, we examine the impact of a lack of a bandgap on limiting the RF potential of graphene transistors. Considering various RF figures of merit, we show that the lack of a bandgap leads to all RF metrics being optimal when the bias point is chosen such that the drain Fermi level aligns with the Dirac point at the midpoint of the channel. We further quantify the precise extent to which the lack of a bandgap limits the transistor's cutoff frequencies, an issue that has been flagged as requiring crucial attention to make graphene transistors competitive. For an 18-nm channel length, we show that the extrinsic unity-current-gain frequency could be improved by 300 GHz and the unity-power-gain frequency could be doubled if a bandgap could be introduced to reduce the output conductance to zero. [1] K. D. Holland, N. Paydavosi, N. Neophytou, D. Kienle, and M. Vaidyanathan, IEEE Trans. Nanotechnol. 12, 566 (2013).

O 78.2 Thu 15:15 POT 081

**Atomic layer deposited aluminum oxide on epitaxial graphene without surface activation** — •Peter Wehrfritz[1], Florian Speck[2], Felix Fromm[1], Stefan Malzer[3], and Thomas Seyller[1] — [1]TU Chemnitz, Institut für Physik, Chemnitz, Deutschland — [2]FAU Erlangen-Nürnberg, Department Physik, Erlangen, Deutschland — [3]FAU Erlangen-Nürnberg, Angewandte Physik, Erlangen, Deutschland

Graphene with its high charge carrier mobility is a promising material for analog RF field effect transistors. The preparation of the required insulating layer is still challenging. Atomic layer deposition (ALD) has been extensively studied in the context of alternative dielectrics for silicon-based field effect transistors owing to its capabilities to produce high-quality, homogeneous oxide layers. However, nucleation of ALD growth is strongly suppressed on inert graphene surfaces.

In this contribution we present an approach to obtain conformal aluminum oxide ($Al_2O_3$) on epitaxial monolayer graphene on silicon carbide (SiC). We demonstrate that closed layers of $Al_2O_3$ can be deposited on the so called buffer layer. This buffer layer covered by ALD-$Al_2O_3$ can then be decoupled from the SiC substrate by means of hydrogen intercalation yielding quasi-freestanding monolayer graphene with an insulating dielectric on top. We investigated the quality of the graphene layer and ALD-$Al_2O_3$ using X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, AFM, and Hall effect measurements.

O 78.3 Thu 15:30 POT 081

**Spin-dependent negative differential resistance in composite graphene superlattices** — •Christopher Gaul[1,2], Javier Munárriz[2], Andrey V Malyshev[2], Pedro A Orellana[3], Cord A Müller[4], and Francisco Domínguez-Adame[2] — [1]Max-Planck-Institut für Physik Komplexer Systeme, Dresden — [2]Universidad Complutense de Madrid, Spain — [3]Universidad Técnica Federico Santa María, Casilla 110 V, Valparaíso, Chile — [4]Fachbereich Physik, Universität Konstanz

We propose and study a compound system of a graphene nanoribbon and a set of ferromagnetic insulator strips deposited on top of it. The periodic array of ferromagnetic strips induces a proximity exchange splitting of the electronic states in graphene, resulting in the appearance of a superlattice with a spin-dependent energy spectrum. We find clear signatures of spin-dependent negative differential resistance. The electric current through the device can be highly polarized and both the current and its polarization manifest non-monotonic dependence on the bias voltage. The device operates therefore as an Esaki spin diode, which opens possibilities to design new spintronic circuits.

Phys. Rev. B 88, 155423 (2013)

O 78.4 Thu 15:45 POT 081

**Exchange coupling between localized defect states in graphene nanoflakes** — •Matthias Droth and Guido Burkard — University of Konstanz, Germany

Graphene nanoflakes are interesting because electrons are naturally confined in these quasi zero-dimensional structures, thus eluding the need for a bandgap. Defects inside the graphene lattice lead to localized states and the spins of two such localized states may be used for spintronics. We perform a tight-binding description on the entire system and, by virtue of a Schrieffer-Wolff-transformation on the bonding and antibonding states, we extract the coupling strength between the localized states. The coupling strength allows us to estimate the exchange coupling, which governs the dynamics of singlet-triplet spintronics.

O 78.5 Thu 16:00 POT 081

**Novel fabrication method of lateral spin valve devices based on graphene on hexagonal boron nitride** — Marc Drögeler[1], Frank Volmer[1], •Maik Wolter[1], Bernat Terrés[1], Kenji Watanabe[3], Takashi Taniguchi[3], Gernot Güntherodt[1], Christoph Stampfer[1,2], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany, EU — [2]Peter Grünberg Institute (PGI-8/9), Forschungszentrum Jülich, 52425 Jülich, Germany, EU — [3]National Institute for

Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

Despite tremendous efforts in improving graphene-based spin transport devices the measured spin lifetimes are still orders of magnitude less than theoretically predicted. Contact-induced spin dephasing has recently been identified as the bottleneck for spin transport through Co/MgO spin injection and detection electrodes. It can, however, significantly be suppressed for devices with large contact resistance area products [1]. Simultaneously, a strong reduction of the charge carrier mobility is usually observed. We present a new method to fabricate graphene-based non-local spin valves on hexagonal boron nitride yielding spin lifetimes above 3 ns, spin diffusion length above 10 $\mu$m and large charge carrier mobilities above 30.000 cm$^2$/Vs.

[1] F. Volmer *et al.*, Phys. Rev. B **88**, 161405(R) (2013).

This work has been supported by DFG through FOR 912 and by EU through Graphene Flagship.

O 78.6 Thu 16:15 POT 081

**Suppression of contact-induced spin dephasing in graphene/Co/MgO$_x$ spin-valve devices by successive oxygen treatments** — Frank Volmer, •Christopher Franzen, Marc Drögeler, Eva Maynicke, Nils von den Driesch, Maren Laura Boschen, Gernot Güntherodt, and Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

By successive oxygen treatments of graphene non-local spin-valve devices we achieve a gradual increase of the contact resistance area products $R_cA$ of the Co/MgO$_x$ spin injection and detection electrodes and a transition from linear to non-linear characteristics in the corresponding $dV/dI$-curves. With this manipulation of the contacts both spin lifetime and amplitude of the spin signal can significantly be increased by a factor of seven in the same device. This demonstrates that contact-induced spin dephasing is the bottleneck for spin transport in graphene devices with small $R_cA$ values [1]. With increasing $R_cA$ we furthermore observe the appearance of a second charge neutrality point (CNP) in gate dependent resistance measurements. Simultaneously we observe a decrease of the gate voltage separation between the two CNPs. The strong enhancement of the spin transport properties as well as the charge transport will be explained by the same gradual suppression of a Co/graphene interaction by improving the oxide barrier.

Work was supported by DFG/FOR 912 and EU/Graphene Flagship.

[1] F. Volmer *et al.* Phys. Rev. B **88**, 161405 (2013).

## Coffee break (15 min.)

O 78.7 Thu 16:45 POT 081

**Development of an amperometric H2O2 sensor based on graphene** — •Masoumeh Sisakhti[1], Alexander Zöpfl[2], Jonathan Eroms[1], Thomas Hirsch[2], and Christoph Strunk[1] — [1]Institut für Experimentelle und Angewandte Physik,Universität Regensburg — [2]Institut für analytische Chemie,Universität Regensburg

The precise detection of Hydrogen peroxide (H2O2) has been a widely researched topic and the focus of a vast amount of attention, owing to its vital role in biological systems, as well as its utility in food, pharmaceutical and biochemical industries.

The objective of this work is to investigate a novel nonenzymatic, amperometric sensor for reliable determination of H2O2 based on graphene.

We produced graphene sensors based on three types of graphene: exfoliated graphene, CVD grown graphene and reduced graphene oxide and carried out cyclic voltammetry and amperometric experiments using a CH Instrument electrochemical analyzer. We demonstrate that all three graphene materials show excellent sensitivity to the catalytic reduction of H2O2 and are able to detect H2O2 concentrations down to 0.1 mM. rGO as well as graphene prepared by CVD are promising candidates for sensor applications since they are able to detect hydrogen peroxide with high sensitivity at moderate electrode potentials. Both materials are superior in the signal-to-noise ratio compared to exfoliated graphene. A further conjugation of enzymes to the defects within the carbon nano material as well as the assembly of 2D-layered composite materials will be perspective to biosensor applications.

O 78.8 Thu 17:00 POT 081

**Controlled chemical modification of graphene for applications in biosensing** — •Marco R. Bobinger, Max Seifert, Anna Cattani-Scholz, and Jose A. Garrido — Walter Schottky Institut, Technische Universität München, Germany

Given its exceptional chemical and mechanical stability as well as its unique electronic properties, graphene is an extremely promising platform for biosensors. In order to use graphene in the biological environment and to improve sensing specificity and device performance, chemical functionalization schemes are needed to allow stable grafting of organic and bioorganic molecules onto graphene. In particular for applications in bioelectronics, the influence of the chemical functionalization of graphene on the generation of defects, strain, and doping has to be balanced with the desired modulation of the electronic properties of the produced graphene-organic hybrid material. In this work the effect of the controlled chemical modification of large area CVD-grown graphene via ozone treatment is investigated. This process creates sp3-like defects, related to covalently bound surface groups, e.g. OH-. Such ozone-treated surfaces are characterized by Raman- and X-ray photoelectron spectroscopy in order to investigate the degree of surface modification and the chemical composition of the surface terminations. The generated anchor groups are further used as binding sites for the modification of graphene with organic molecules.

O 78.9 Thu 17:15 POT 081

**Functionalization of Graphene for Bioelectronic Applications** — •Alina Lyuleeva[1], Lucas Hess[1], Frank Deubel[2], and Jose Antonio Garrido[1] — [1]Walter Schottky Institut, TU München, 85748 Garching — [2]Wacker Chemie AG, 81379 München, Germany

With its fascinating structural, chemical and electronic properties, graphene outperforms many materials and is expected to pare the way for a vast range of applications such as transparent electrodes, energy storage devices, high-frequency electronics, or biosensors. The performance of the devices for these various applications can be enhanced with the help of surface functionalization, allowing a versatile modification of the properties of this material. Here, we report on the covalent and thus robust functionalization of CVD graphene with enzymes for the development of novel devices for bioelectronic applications. Graphene solution-gated field-effect transistors (SGFETs) are functionalized using a controlled grafting of polymethacrylate (PMA) brushes. We will show how this material platform can be used for further functionalization with the enzyme acetylcholinesterase (AChE). The enzymes' activity can be monitored with the modified-graphene transistor allowing both the measurement of the concentration of the neurotransmitter acetylcholine as well as the inhibition of the enzyme by neurotoxins such as nerve agents or pesticides. Our study demonstrates the potential of graphene-based functionalized transistors for biosensing and bioelectronic application.

O 78.10 Thu 17:30 POT 081

**Coupling of electrogenic cells to graphene devices** — Michael Sejer Wismer, Felix Rolf, Damia Viana, •Martin Lottner, Lucas Hess, and Jose A. Garrido — Walter Schottky Institut - Technische Universität München, Am Coulombwall 4, 85748 Garching

In this contribution, we will demonstrate the electrical coupling between electrogenic cells and graphene-based solution-gated field effect transistors (SGFETs). To this end, HEK293 and HL1 cells were cultured on 8x8 arrays of graphene SGFETs with feature sizes of 10 mu x 20 mu. Graphene was grown by chemical vapour deposition (CVD) on copper foil and transferred to sapphire substrates, on which field effect transistors were fabricated using standard semiconductor technology. The devices show a typical maximum transconductance of >100 muS at 0.1 V drain-source voltage. This value is stable over months of storage. HEK293 cells were used to analyse the electrical coupling between cells and transistors. A model considering the distribution of ions within the cell transistor cleft and ion sensitivity of the graphene SGFETs fits the measured signals very well. Additionally, nano-transistors were defined by e-beam lithography, which allowed feature sizes down to 50 nm. With these nanoscale devices a signal-to-noise ratio of 2.5 could be obtained within single recordings of HL1 activity. Analysis of the measured ionic currents allowed to draw conclusions about local inhomogeneities of ion channel concentration within the membrane. Further, experiments for the stimulation of PC12 cells using arrays of graphene SGFET and graphene-based microelectrode arrays (MEAs) are under preparation.

O 78.11 Thu 17:45 POT 081

**Graphene solution-gated field effect transistors on flexible substrates** — •Andrea Bonaccini Calia, Benno M. Blaschke, Lucas H. Hess, Max Seifert, and Jose A. Garrido — Walter Schottky Institut, Technische Universität München, Germany

Graphene based solution-gated field effect transistors (SGFETs) hold great promise for biosensors and bioelectronic applications. Due to its unique combination of electronic, mechanical, and chemical properties, such as high charge carrier mobility, flexibility and good biocompatibility, graphene has been shown to be an excellent material for sensing in electrolyte environments. Sensors based on graphene SGFETs have already been realized on rigid substrates for various analytes, as well as for the detection of cell signals. However, this technology hold some severe problems for biomedical and in vivo applications. One of the major problems is the rigidity of the substrate itself, which does not allow a proper mechanical matching to the biological tissue, resulting in the formation of scar tissue. Therefore, flexible devices are currently considered as a major step towards the development of more biocompatible implants. In this work, an array of graphene SGFETs is fabricated on a flexible polymer substrate. We present a detailed electrical characterization of the flexible graphene SGFETs in electrolyte and compare their performance to graphene SGFETs on rigid substrates. In addition, we analyze the effect of changes in the electrolyte's pH and ionic strength on the transistor performance and present a model to explain the obtained results. Furthermore, the low-frequency noise performance of graphene devices on flexible substrates is discussed.

# O 79: Plasmonics and Nanooptics IV

Time: Thursday 16:00–18:30 Location: TRE Ma

O 79.1 Thu 16:00 TRE Ma

**A Plasmon Autocorrelator** — •Christoph Lemke[1], Till Leissner[1], Jörn Radke[1], Jacek Fiutowski[2], Jakob Kjelstrup-Hansen[2], Horst-Günter Rubahn[2], and Michael Bauer[1] — [1]University of Kiel, IEAP, Leibnizstraße 19, 24118 Kiel, Germany — [2]University of Southern Denmark, Mads Clausen Institute, NanoSYD, Alsion 2, DK-6400 Sønderborg, Denmark

Surface plasmon polaritons (SPP) are considered as a main component in future broadband and ultrafast nanophotonic devices. This perspective asks for methods that enable one to determine in-situ the temporal and spectral properties of ultrashort SPP pulses.

In this contribution we demonstrate the realization of a plasmonic autocorrelator [1] for the characterization of SPP pulse parameters. A wedge shaped structure is used to continuously increase the time delay between two interfering SPPs. The autocorrelation signal is monitored by non-linear two-photon photoemission electron microscopy. The presented approach is applicable to other SPP sensitive detection schemes that provide only moderate spatial resolution and may therefore be of general interest in the field of ultrafast plasmonics.

[1] Lemke, C. et al. Measurement of surface plasmon autocorrelation functions. Opt. Express 21, 4700-4705 (2013).

O 79.2 Thu 16:15 TRE Ma

**Helical Plasmonic Nanostructures for Strong Chiral Near-Fields** — •Martin Schäferling[1], Xinghui Yin[1], Nader Engheta[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Centers SCoPE and SimTech, University of Stuttgart, Germany — [2]Department of Electrical and Systems Engineering, University of Pennsylvania, Philadelphia, USA

Chiral electromagnetic fields are used to probe the handedness of natural chiral objects. The strength of the chiroptical interaction can be quantified by the so-called optical chirality [1]. Plasmonic nanostructures can tailor the optical chirality of their near-fields [2]. Even achiral structures can generate chiral near-fields. However, their properties strongly depend on the phase between incident and scattered fields [3].

We numerically demonstrate that the eigenmodes of helical nanostructures generate near-fields with strong optical chirality. Our design with multiple helices optimizes simultaneously the strength of the optical chirality and the coupling to the external field. This structure exhibits non-trivial dependencies on the pitch of the helices due to coupling effects. We show that the optimum design strategy depends strongly on the size of the whole structure. These nanostructures with chiral eigenmodes are model devices for enantiomer sensors with improved sensitivity. Our design theoretically enhances the interaction with chiral molecules by almost two orders of magnitude.

[1] Y. Tang and A. E. Cohen, Science **332**, 333 (2011).
[2] M. Schäferling et al., Phys. Rev. X **2**, 031010 (2012).
[3] M. Schäferling et al., Opt. Express **20**, 26326 (2012).

O 79.3 Thu 16:30 TRE Ma

**Chiral Plasmonic Fano Resonance** — •Xinghui Yin, Martin Schäferling, and Harald Giessen — 4. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

Chiral plasmonic structures are able to enhance the sensitivity in chiroptical spectroscopy methods. They provide superchiral fields that interact strongly with chiral molecular environments on the nanoscale. [1] At the same time, their inherent chiral spectral features are modified by such an interaction and thus serve as probes that can be readily accessed in far-field measurements. [2] From conventional refractive index based plasmonic sensors, it is known that their sensitivity is maximal for geometries that exhibit a Fano-dip. [3] Prominent examples are plasmonic oligomers with the pentamer as a special C4-symmetric case. Here, we show that stacking two Pentamers on top of each other with a relative rotation angle of 22.5° about the center particle, translates the sharp Fano feature into the circular dichroism spectrum of the thus created three-dimensional chiral plasmonic oligomer. Assessing the electromagnetic properties of the structure reveals that it additionally provides strong superchiral fields, rendering it the ideal candidate for highly-sensitive enhanced chiroptical spectroscopy.

[1] Y. Tang and A. E. Cohen, Science 332, 333 (2011).
[2] E. Hendry et al., Nature Nanotechnology 5 (11), 783 (2010).
[3] B. Gallinet et al., ACS Nano 7, 6978 (2013).

O 79.4 Thu 16:45 TRE Ma

**Simulations of plasmonic nano-structures using the hydrodynamic DGTD method** — •Matthias Moeferdt[1], Christian Wolff[2], Christian Matyssek[1], Rogelio Rodriguez-Oliveros[1], and Kurt Busch[1,2] — [1]Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik und Photonik, Newtonstr. 15, 12489 Berlin, Germany — [2]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany

We present scattering simulations for plasmonic nano-structures, using the Discontinuous Galerkin Time Domain method (DGTD).

A classical nonlocal and nonlinear hydrodynamic material description is employed where the electron gas inside the metal is described by the hydrodynamic Euler equations and the pressure is implemented according to the Thomas-Fermi theory.

This constitutes a versatile computational framework that enables us to reliably obtain second harmonic spectra, to investigate the role of bulk plasmons, and to compute the field enhancement of nano-gap structures.

A comparison with corresponding simulations using a Drude material description allows us to discern nonlocal and nonlinear effects in the field enhancement.

O 79.5 Thu 17:00 TRE Ma

**Angular resolved electron energy-loss spectroscopy on plasmonic nanostructures** — •Felix von Cube[1,2,3], Jens Niegemann[4], Stephan Irsen[2], David C. Bell[3], and Stefan Linden[1] — [1]Physikalisches Institut, Universität Bonn, 53115 Bonn, Germany — [2]Electron Microscopy and Analytics (EMA), Center of Advanced European Studies and Research (caesar), 53175 Bonn, Germany — [3]School of Engineering and Applied Sciences, Harvard University, Cambridge MA 02138, USA — [4]Laboratory for Electromagnetic Fields (IFH), ETH Zurich, 8092 Zurich, Switzerland

We investigate the plasmonic near-field of a lithographically defined metallic nanostructure with angular resolved electron energy-loss spectroscopy in a scanning transmission electron microscope. By tilting the sample, different electric field components of the plasmonic modes can be probed with the electron beam. The electron energy-loss spectra recorded under oblique incidence can feature plasmonic resonances that are not observable under normal incidence. Our experimental findings are reproduced by full numerical calculations based on the discontinuous Galerkin time-domain method.

O 79.6 Thu 17:15 TRE Ma

**Plasmon Dynamics in Noble Metal Nanorods with Femtosecond Pulse-Shaping** — •Alberto Comin, Richard Ciesielski, Kevin Donkers, Giovanni Piredda, and Achim Hartschuh — Ludwig-Maximilians-Universitaet Muenchen

Plasmonic nanostructures exhibit localized surface plasmon resonances (LSPR) which greatly enhance optical absorption, scattering, and the near-field component of the electric field. LSPR are coherent, broadband and intrinsically ultrafast collective electronic excitations, with a lifetime of 5-15 fs. Here we present a time resolved study on the femtosecond plasmon dynamics of single metallic nano-particles using confocal microscopy. Broadband 10 fs laser pulses were controlled in amplitude and phase using a 4f shaper configuration. For pulse characterization in the focus of a high numerical aperture objective we developed an extension of the method of multiphoton intrapulse interference phase scans (MIIPS), which we called Gated-MIIPS. This technique allowed us to obtain an accurate characterization of the phase profile of the broadband pulses, which was valuable in achieving reliable characterization of plasmonic nanostructures in the femtosecond time range. In this contribution we will briefly discuss the newly developed Gated-MIIPS technique and the first results on the plasmon dynamics of metallic nanostructures.

O 79.7 Thu 17:30 TRE Ma

**Plasmonically enhanced thin film Faraday effect with up to 4 degrees rotation** — •Dominik Floess[1], Jessie Chin[1], Akihito Kawatani[1], Daniel Dregely[1], Hanns-Ulrich Habermeier[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCOPE, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

Light propagation is usually Lorentz-reciprocal. However, a static magnetic field along the propagation direction can break the Lorentz-reciprocity in the presence of magneto-optical (MO) materials. The Faraday effect in such materials rotates the polarization plane of light, and when light travels backward the polarization is further rotated. The enhancement of the Faraday rotation in MO thin films is of particular interest due to the demand of optical isolation devices in integrated optics. We hybridized MO materials with plasmonic structures and achieved 4 degrees of Faraday rotation for 200 nm thick structures. This large Faraday rotation is accompanied with a reasonably low relative insertion loss of 5.2 dB.

O 79.8 Thu 17:45 TRE Ma

**Plasmoelectrons: Electron emission by decay of confined bulk plasmons in epitaxial ultrathin Mg films** — •Ulrich Hagemann and Hermann Nienhaus — Faculty of Physics and Center for Nanointegration (CeNIDE), University of Duisburg-Essen, D-47048 Duisburg, Germany

A novel electron emission process is observed for epitaxially grown Mg layers on Si(111)-7x7 surfaces. The metal film thickness ranges between 5 and 50 monolayers and the surface (SS) as well as quantum well states (QWS) are well resolved by ultraviolet photoelectron spectroscopy (UPS). Intensive replica peaks of the SS and QWS structures are detected in the UPS spectra on the secondary electron background at a constant kinetic energy independent of the energy of the incident photons (HeI, NeI, ArI, ArII). The emission structures are up to two orders of magnitude more intense than the photoelectron peaks. Since they appear for an excitation energy of 10.3 eV, i.e., the Mg bulk plasmon energy, the emission is explained by the decay of optically excited bulk plasmon modes confined in the ultrathin metal film. Such modes couple effectively to the QWS and SS of the Mg film. This plasmoelectron emission is only present for well-ordered and ultrathin Mg films. At 300 ML Mg films, the effect vanishes. A threshold photon energy for the plasmoelectron excitation is found between 12 and 13eV. First experiments with Mg and Al thin films demonstrate that a similar but weaker effect is found for surface plasmons as well.

O 79.9 Thu 18:00 TRE Ma

**Coupled photon-exciton modes in CHPI-based devices** — •David Leipold[1], Wendy Niu[2], Lindsey Ibbotson[2], Vijaya Prakash[3], Jeremy Baumberg[2], and Erich Runge[1] — [1]Institut für Physik, Technische Universität Ilmenau, Germany — [2]Cavendish Laboratory, University of Cambridge, UK — [3]Nanophotonics Research Group, Indian Institute of Technology Delhi, India

Almost all designs proposed for future active all-optical data processing devices with subwavelength dimensions involve the coupling of electromagnetic excitations in or on metal (mostly plasmons) with nonlinear optics in dielectric materials (mostly due to excitons).

Candidates for the nonlinear materials are low-dimensional semiconductor heterostructures and organic dyes. While the former are hard to build close enough to the metal, the latter are generally chemically unstable at room temperature and high optical intensities.

Recently, CHPI ($(C_6H_9C_2H_4NH_3)_2PbI_4$), a lead iodide based inorganic-organic hybrid material gained a lot of interest because it promises to combine the best of both worlds: like many organic dyes, CHPI can be spin-coated from a solution directly onto the metal interface. After drying, it forms self-assembled 2D semiconductor sheets. Thus, the CHPI combines the stability of an inorganic semiconductor nano-structure and the simple processing of an organic dye layer.

In this talk, we will present experiments and calculations with CHPI-covered metal gratings. Several optical modes can be identified which are predominantly localized in the slits of the grating. These show strong coupling with CHPI exciton resonances.

O 79.10 Thu 18:15 TRE Ma

**Multi-photon photoelectron microscopy of porphyrin thin films in contact with plasmonic silver structures** — •Klaus Stallberg and Winfried Daum — Intstitute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstraße 4, 38678 Clausthal-Zellerfeld

Porphyrins represent a prominent class of molecules with extended $\pi$-electron system extensively studied for light harvesting and solar energy conversion. Recent studies showed strong coupling of molecular excitations in J-aggregates of porphyrins with surface plasmons of metallic films and plasmonic nanostructures. We study the interaction of magnesium-tetraphenylporphyrin (Mg:TPP) excited states ($S_2$ level, Soret band) with localized surface plasmons (LSPs) in silver nanostructures by energy-resolved photoemission electron microscopy (PEEM) and by photoelectron excitation with short laser pulses for time-resolved single particle spectroscopy. As a first step in this direction we fabricated silver nanoparticles with a broad distribution of sizes and LSP resonances by evaporation of silver through a mask of polysterene spheres onto a natively oxidized silicon substrate. By variation of the photon excitation wavelength we identify LSP resonances that match the Mg:TPP Soret band. We also report on wavelength-dependent PEEM experiments with Mg:TPP films deposited on substrates with more homogeneous Ag nanoparticles prepared from solutions. First results from time-resolved 2- and 3-photon photoemission pump-probe experiments on Mg:TPP films are presented.

# O 80: Surface Dynamics I

Time: Thursday 16:00–19:00 Location: GER 38

O 80.1 Thu 16:00 GER 38

**High Remanent Spin Injection into GaAs(110): Strong Electron Energy Dependence with Steep Fall-Off** — •Svenja Mühlenberend, Markus Gruyters, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany

The spin polarization of electrons injected into GaAs from a magnetic tip of a scanning tunneling microscope is determined from the polarization of the induced electroluminescence. At low temperatures, unexpectedly high polarization values are observed. Moreover, the polarization exhibits a drastic electron energy dependence. Electron transport occurs at remanence, i.e. no external magnetic field is necessary to obtain a high spin injection efficiency.

O 80.2 Thu 16:15 GER 38

**Spin-resolved electron transmission through chiral molecules and proteins on metal surfaces** — •Matthias Kettner[1], Benjamin Göhler[1], Debabrata Mishra[2], Tal Z. Markus[2], Georg F. Hanne[1], Ron Naaman[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Chemical Physics, Weizmann Institute, Rehovot, Israel

Electron spin polarization has been measured for photoelectrons emitted from aluminum and gold substrates and transmitted through adsorbed layers of the chiral membrane protein bacteriorhodopsin and the amino acid alanine. The samples are irradiated by 213nm laser radiation exciting photoelectrons within the metal substrate. These photoelectrons are then transmitted through the chiral layer and analyzed by a Mott polarimeter. The case of bacteriorhodopsin which is physisorbed on an aluminum substrate, electron spin polarization values of up to +15% are obtained independent of the polarization of the incident light. Taking earlier studies of bacteriorhodopsin on a gold substrate into account, spin-orbit-coupling of the substrate seems to have a minor influence [1]. Moreover the electron spin polarization shows a dependence on the coverage of the substrate. These studies are extended to the chiral amino acid polyalanine which is self-assembled on a gold surface. The results indicate that also in this case the interaction of chiral layers with the electrons depends on the spin orientation. This effect may enable the design of efficient spin filters for spintronic applications.

[1] D. Mishra, et al., PNAS 110, 14872 (2013)

O 80.3 Thu 16:30 GER 38

**A photoinduced change of $k_\mathrm{F}$ in Bi2212 revealed by femtosecond time- and angle-resolved photoemission spectroscopy** — •S. Freutel[1], J.D. Rameau[2], L. Rettig[1], I. Avigo[1], S. Thirupathaiah[1], M. Ligges[1], G.D. Gu[2], H. Eisaki[3], P.D. Johnson[2], and U. Bovensiepen[1] — [1]Faculty of Physics, University of Duisburg-Essen, Duisburg, Germany — [2]Brookhaven National Laboratory, New York, USA — [3]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

Optical excitation and subsequent ultrafast electronic relaxation leads to quasiparticle redistribution, which potentially changes the chemical potential, or the Fermi momentum $k_\mathrm{F}$, in systems with non-constant density of states. Here, we report on time- and angle resolved photoemission spectroscopy on optimally doped Bi2212 in the pseudogap phase. We observed a change in $k_\mathrm{F}$ that appears as a photoinduced change of the effective doping level caused by an electron-hole asymmetry. Along the nodal line this effect scales linearly with the optical excitation density of 35 to 300 $\mu$J/cm$^2$ and peaks at a delay of 100 fs. Since the change in $k_\mathrm{F}$ relaxes within 1 ps, we consider the excitation of secondary electrons and subsequent electron phonon coupling as the underlying processes. Additional results on chemically underdoped Bi2212 show that the shift in $k_\mathrm{F}$ increases for larger momenta which suggests a quantitative comparison and discussion of static chemical and transient photoinduced doping.

We acknowledge support by the DFG through SFB616 and the Mercur Research Center Ruhr through PR-2011-0003.

O 80.4 Thu 16:45 GER 38

**Ultrafast electron dynamics in Pb nanowire arrays on Si(557)** — Abdul Samad Syed[1], Vesna Mikšić Trontl[1], •Manuel Ligges[1], Mathias Sandhofer[1], Ishita Agarwal[1], Isabella Avigo[1], Daniel Lükermann[2], Christoph Tegenkamp[2], Herbert Pfnür[2], and Uwe Bovensiepen[1] — [1]Fakultät für Physik, Univ. Duisburg-Essen — [2]Institut für Festkörperphysik, Leibnitz Univ. Hannover

Quasi-1D materials are expected to exhibit exotic properties that are considerably different from those of their corresponding bulk material counterparts. As a consequence of the strong real-space anisotropy of these systems, significant differences in, e.g., electron scattering rates along and perpendicular to the wire structure can be expected. We investigate this particular aspect using time- and angle-resolved two photon photoemission from the Pb/Si(557) nanowire system. We present results regarding the unoccupied electronic structure and ultrafast relaxation of optically excited carriers probed as a function of two mutually independent in-plane momentum directions along and perpendicular to the nanowire orientation. We gratefully acknowledge funding by the DFG through FOR1700.

O 80.5 Thu 17:00 GER 38

**Time-resolved photoemission spectroscopy on $1T$–TaSe$_2$: Mott physics at the surface?** — •Christian Sohrt, Ankatrin Stange, Lutz Kipp, Michael Bauer, and Kai Rossnagel — Institute for Experimental and Applied Physics, University of Kiel, Germany

According to angle-resolved photoelectron spectroscopy and scanning tunneling microscopy studies, the surface of $1T$–TaSe$_2$ displays Mott insulating behavior in connection with a commensurate $\sqrt{13} \times \sqrt{13}$ charge-density wave, in a similar way as observed in $1T$–TaS$_2$ [1,2]. But the question is whether the observed spectral gap at the Fermi level is really a Mott gap.

A possible smoking-gun experiment to answer this question is time- and angle-resolved photoelectron spectroscopy (trARPES), which in principle enables us to distinguish between Peierls and Mott gaps by direct determination of the gap quenching times [3].

Here, we present the results of a comparative momentum-dependent trARPES study on $1T$–TaSe$_2$ and $1T$–TaS$_2$. In contrast to the prevailing view, no indications for Mott dynamics are found at the surface of $1T$–TaSe$_2$.

[1] L. Perfetti *et al.*, Phys. Rev. Lett., **90**, 166401 (2003)
[2] S. Colonna *et al.*, Phys. Rev. Lett., **94**, 036405 (2005)
[3] S. Hellmann *et al.*, Nat. Commun., **3**, 1069 (2012)

O 80.6 Thu 17:15 GER 38

**Time- and angle-resolved 2PPE of unoccupied electronic states of topological insulators Sb$_2$Te$_3$ and Sb$_2$Te$_2$S** — •Johannes Reimann, Jens Güdde, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg

Topological insulators with their unique protected surface state offer promising potentials for a wide field of applications. In order to make use of the conducting properties of the surface state it is important to know the properties of both the occupied and the unoccupied electronic states close to the Fermi-energy.

In this work the unoccupied electronic states of the topological insulators Sb$_2$Te$_3$ and Sb$_2$Te$_2$S have been investigated by time- and angle-resolved two-photon photoemission (2PPE) along $\overline{\Gamma}$-$\overline{\mathrm{K}}$- and $\overline{\Gamma}$-$\overline{\mathrm{M}}$-direction. Both materials show a linear dispersive electronic state near Fermi-energy, resembling the typical Dirac-Cone structure. Additional bulk and surface states at higher energies can be identified. The experimental spectroscopic results will be compared with theoretical calculations of the surface and bulk band structure. First results on the electron-dynamics using time- and angle-resolved 2PPE are presented. While both materials show similar dynamics at room temperature, the dynamics at low temperatures differs.

O 80.7 Thu 17:30 GER 38

**Bulk- and surface electron dynamics in a p-type topological insulator SnSb$_2$Te$_4$** — •Sebastian Otto, Daniel Niesner, Volker Hermann, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Time-resolved two-photon photoemission is used to study the electronic structure and dynamics at the surface of SnSb$_2$Te$_4$, a p-type topological insulator. The topological surface state is centered at $0.32 \pm 0.03$ eV above the Fermi level with a group velocity of 3.4 eVÅ.

Electrons from the conduction band minimum are scattered on a time scale of 43 ± 4 fs to the Dirac cone. From there they decay to the partly depleted valence band with a time constant of 78 ± 5 fs. The short time scales are attributed to the large overlap with the bulk bands. Higher doped samples show even shorter time constants indicating that the unoccupied bulk valence band provides the final states for decay. The infrared-pumped scattering processes above the Dirac cone in the conduction band are described by a rate equation model. States are populated by the pump pulse and electrons decaying from higher-lying states and decay into lower-lying states. The good agreement between filling and depleting decay rates of neighboring energy levels shows that the decay occurs mostly within the conduction band.

O 80.8 Thu 17:45 GER 38

**2PPE measurement on $Sb_2Te_2S$ with an angle-resolving time-of-flight spectrometer** — •Thomas Kunze[1,2], Sophia Ketterl[1], Thorsten U. Kampen[2], Evgeny Chulkov[3], and Martin Weinelt[1] — [1]FU Berlin, Germany — [2]SPECS GmbH, Germany — [3]UPV/EHU San Sebastián, Spain

We present two-photon photoemission measurements on the p-doped topological insulator $Sb_2Te_2S$. The Dirac cone of this system lies above the Fermi energy and is therefore only accessible using two-photon photoemission.

We detect the photoemitted electrons with an angle-resolving time-of-flight spectrometer. This instrument allows us to measure the kinetic energy $E$ as a function of $k_{x\|}$ and $k_{y\|}$ without rotating the sample. Our laser system with two OPAs gives us the opportunity to tune the photon energy of the infrared and ultraviolet pulse independently. This allows us to create a resonant population and efficient probing of the Dirac cone.

$Sb_2Te_2S$ shows a Dirac cone with direction-dependent linear dispersion close above the Fermi level and hexagonal warping at higher energies. Polarization-dependent measurements manifest the spin texture of the Dirac cone. The population dynamics of $Sb_2Te_2S$ have been analyzed. The femtosecond lifetimes of the first and second image-potential states show an $n^3$ dependence. The Dirac cone is populated by indirect filling via the conduction band. The relaxation of the Dirac cone happens on a picosecond timescale.

O 80.9 Thu 18:00 GER 38

**How far-from-equilibrium dynamics drive the ultrafast melting of a charge-density wave in $TiSe_2$** — •S. Eich[1], J. Urbancic[1], A. V. Carr[2], A. Stange[3], T. Popmintchev[2], T. Rohwer[3], M. Wiesenmayer[1], A. Ruffing[1], S. Jakobs[1], S. Hellmann[3], P. Matyba[2], C. Chen[2], L. Kipp[3], M. Bauer[3], M. M. Murnane[2], K. Rossnagel[3], H. C. Kapteyn[2], S. Mathias[1,2], and M. Aeschlimann[1] — [1]TU Kaiserslautern and Research Center OPTIMAS, Germany — [2]JILA, Boulder, Co, USA — [3]IEAP, Kiel, Germany

We present fs XUV ARPES with sub 150 meV energy- and sub 30 fs time-resolution of the prototypical semiconductor-to-metal photo-induced phase transition in the charge-density wave compound 1T-$TiSe_2$ [1]. We elucidate the role of far-from-equilibrium dynamics in the ultrafast melting of the charge-density wave in $TiSe_2$, and show that photo-induced transient non-equilibrium states are indispensible for the ultrafast response of the system. We find that hot carrier multiplication, which is only present during the first 200 fs, is the main driver of the ultrafast phase transition.

[1] Rohwer et al., Nature 471,490 (2011)

O 80.10 Thu 18:15 GER 38

**Ultrafast hot electron dynamics at the $SrTiO_3$-vacuum interface** — •Marc Herzog, Daniel Wegkamp, Julia Stähler, and Martin Wolf — Abteilung Physikalische Chemie, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

In the last decade many surprising properties have been observed at $SrTiO_3$-related oxide interfaces (e.g. metal-insulator transitions, superconductivity, large magnetoresistance) which originate from metallic states at the STO interface also referred to as quasi two-dimensional electron gas (2DEG). Due to the various exotic properties $SrTiO_3$ (STO) promises many applications in future oxide electronics. Recently, a 2DEG has been discovered even at the vacuum-cleaved surface of STO.

In order to gain insight into the role of electron interaction/correlation in the 2DEG we have studied the surface-confined electrons in STO by means of time- and angle-resolved photoemission spectroscopy (trARPES) and two-photon photoemission (2PPE) mapping the photoinduced dynamics of occupied and unoccupied electronic states, respectively. The ultrafast response of the 2DEG to below- and above-bandgap laser-pulse excitation reveals energy-dependent electron lifetimes below 60 fs which is much shorter than in 3D metals (e.g. Cu, Ag). These results suggest that electron screening may be strongly suppressed in the 2DEG. Moreover, we discuss the effect of transient surface photovoltage.

O 80.11 Thu 18:30 GER 38

**Ultrafast electron dynamics around the antinode in optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$** — •Kerstin Hanff, Lexian Yang, Gerald Rohde, Ankatrin Stange, Petra Hein, Lutz Kipp, Michael Bauer, and Kai Rossnagel — Institute of Experimental and Applied Physics, University of Kiel, Germany

Angle-resolved photoemission spectroscopy (ARPES) has added tremendously to our understanding of the electronic and superconducting properties of the cuprates, through direct measurement of the momentum-dependent electronic structure, spectral function, and order parameter. The technique is now also frequently used in pump-probe schemes and has thus added important insights on the momentum-dependent dynamics of quasiparticles and Cooper pairs. However, due to the use of ultraviolet (UV) probe pulses only, time-resolved ARPES studies on the cuprates have so far been limited in momentum space to the nodal region of the Fermi surface. Here, we report the results of time-resolved ARPES on optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ using extreme ultraviolet radiation delivered by a high-harmonic-generation source. The higher probe photon energy of 22 eV has allowed us to study the quasiparticle relaxation dynamics in momentum-space cuts that cover the complete region from the node to the antinode. Our results reveal bi-exponential decay dynamics with distinct temperature- and momentum-dependent time constants.

O 80.12 Thu 18:45 GER 38

**Pump-laser-induced space-charge effects in time-resolved photoelectron spectroscopy** — •Lars-Philip Oloff, Ankatrin Stange, Kerstin Hanff, Lutz Kipp, Michael Bauer, and Kai Rossnagel — Institute of Experimental and Applied Physics, University of Kiel, Germany

The development of ultrashort-pulsed extreme ultraviolet sources, such as high-harmonic generation sources (HHG) and free-electron lasers, has opened up a new field of physics by means of time-resolved pump-probe photoelectron spectroscopy experiments. The effects of these sources' high brilliance on photoemission spectra, i.e., intensity-dependent broadenings and shifts towards higher kinetic energies ("space-charge effects"), have been extensively studied by experiments and simulations [1,2] and are now rather well understood. However, in time-resolved photoelectron spectroscopy a further effect can be recognized in the high-pump-intensity regime: pump-induced space-charge effects due to nonlinear multiphoton photoemission. We have systematically studied these effects as a function of various experimental parameters (pump-probe delay, pump energy, pump intensity, work function of the sample) at our HHG-based photoemission setup (22 eV probing, 390 nm/780 nm pumping). The obtained experimental results are compared with the results of self-consistent $N$-body numerical simulations.

[1] S. Hellmann *et al.*, Phys. Rev. B **79**, 035402 (2009)
[2] S. Hellmann *et al.*, Phys. Rev. B **85**, 075109 (2012)

# O 81: Oxide and Insulator Surfaces III

Time: Thursday 16:00–19:00 Location: PHY C 213

O 81.1 Thu 16:00 PHY C 213

**Surface core-level shifts of zinc oxide** — •Navid Abedi Khaledi and Georg Heimel — Institut für Physik, Humboldt Universität zu Berlin, Brook-Taylor-Straße 6, 12489 Berlin, Germany

X-ray photo-emission spectroscopy (XPS) is an extremely useful tool for understanding the chemical composition of any surface. However, interpretation of experimental results is not always straightforward. To this aim, we perform density functional theory (DFT) based calculations of the most probable structures of Zinc oxide's complex (0001), (000-1) and (10-10) surfaces. Chemical core-level shifts are then obtained from total-energy differences and Slater's transition-state theorem. XPS intensities are estimated from tabulated values for electron mean free paths. In the end, we produce peak shapes with a combination of Lorentzian and Gaussian functions, allowing direct comparison with experimental spectra.

O 81.2 Thu 16:15 PHY C 213

**Tuning amorphous network structures** — •Christin Büchner, Stefanie Stuckenholz, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

A bilayer silica film system has been presented, exhibiting amorphous and ordered regions [1]. Noncontact atomic force microscopy (nc-AFM) and scanning tunneling microscopy (STM) with atomic resolution reveal a network of different ring sizes. The structure can be described in terms of ring size occurrence, neighborhoods and pair distance histograms, which are directly derived from atomic coordinates. In the study of the ring size arrangements of the amorphous region, valuable insights can be gained concerning formation principles of vitreous or amorphous structures. On the basis of knowing these structural properties, tuning the network structures is endeavored. Introducing Al as a dopant, combined with subsequent annealing, results in film structures with new characteristics [2]. Ring size distribution and film growth properties in particular are influenced by the element composition. A study of different networks is presented, focusing on the network features studied with SPM.

[1]L. Lichtenstein, C. Büchner, B. Yang, S. Shaikhutdinov, M. Heyde, M. Sierka, R. Włodarczyk, J. Sauer and H.-J. Freund, Angewandte Chemie International Edition 51 (2012) 404

[2]J. A. Boscoboinik, X. Yu, B. Yang, F. D. Fischer, R. Włodarczyk, M. Sierka, S. Shaikhutdinov, J. Sauer and H.-J. Freund, Angewandte Chemie International Edition 51 (2012) 6005

O 81.3 Thu 16:30 PHY C 213

**Importance of Space-Charge effects for the Concentration of Defects at Metal-Oxide Surfaces** — Norina A. Richter[1], Sabrina Sicolo[2], •Sergey V. Levchenko[1], Joachim Sauer[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft — [2]Humboldt Universität zu Berlin

We consider the charge-carrier conductivity induced by doping as a thermodynamic factor in the context of defect formation. As a technologically relevant example, we study surface oxygen vacancies (F centers) in MgO. Defect formation energies are determined using *ab initio* atomistic thermodynamics in combination with hybrid density-functional theory (DFT), with parameters of the exchange-correlation functional optimized according to a condition on DFT ionization energies. Formation energies for neutral defects are validated by coupled-cluster CCSD(T) calculations for embedded clusters. The virtual-crystal approximation [1] is used for a realistic modeling of doping. We find that at catalytically relevant conditions charge transfer between surface defects and dopants in deeper layers leads to formation of a macroscopically extended space-charge region. The concentration of $F_s^{2+}$ centers at the (100) terrace of *p*-type MgO can be as high as 1%, while $F_s^{+}$ and $F_s^{0}$ concentrations are negligible in both *p*-type and *n*-type MgO [2].—[1] L. Vegard, Z. Phys. **5**, 17 (1921); M. Scheffler, Physica B+C, **146**, 176 (1987); [2] N.A. Richter, *et al.*, Phys. Rev. Lett. **111**, 045502 (2013).

O 81.4 Thu 16:45 PHY C 213

**Metal nucleation and clusters on ultrathin $ZrO_2$ films** — Joong-Il J. Choi[1], Ilaria Valenti[2], Wernfried Mayr-Schmölzer[1], Florian Mittendorfer[1], Josef Redinger[1], Ulrike Diebold[1], and •Michael Schmid[1] — [1]Institut f. Angewandte Physik, TU Wien, Austria — [2]Università degli Studi di Modena e Reggio Emilia, Modena, Italia

Zirconia ($ZrO_2$) is used as a catalyst support and solid-state electrolyte in gas sensors and solid-oxide fuel cells. Nevertheless, its surface properties are insufficiently understood, mainly due to its insulating nature. To overcome this problem, we use ultrathin $ZrO_2$ films [1,2], which are accessible to scanning tunneling microscopy (STM). We have studied nucleation and growth of Ag, Au and Pd on these $ZrO_2$ films at room temperature. Compared to other ultrathin oxides like alumina or FeO, we find a high density of metal clusters or even single metal adatoms. Comparison between $ZrO_2$ grown on $Pd_3Zr(0001)$ and $Pt_3Zr(0001)$ indicates that the buckling of the Zr atoms in these oxide films plays an important role, which means that metal atoms can easily bind to Zr in the oxide, as already suggested in Ref. [1]. This explains the high nucleation density and also suggests that the various crystallographic phases of bulk $ZrO_2$ differ significantly in their surface properties.

[1] M. Antlanger et al., Phys. Rev. B 86, 035451 (2012)

[2] J.I.J Choi et al., submitted (2013)

O 81.5 Thu 17:00 PHY C 213

**Ultra-thin zirconia films on Zr-alloys** — •Joong Il Jake Choi[1], Wernfried Mayr-Schmölzer[1], Hao Li[2], Günther Rupprechter[2], Florian Mittendorfer[1], Josef Redinger[1], Ulrike Diebold[1], and Michael Schmid[1] — [1]Institute of Applied Physics, Vienna University of Technology, Austria — [2]Institute of Materials Chemistry, Vienna University of Technology, Austria

Zirconia ultra-thin films have been prepared by oxidation of $Pt_3Zr(0001)$ and showed a structure equivalent to (111) of cubic zirconia[1]. Following previous work, we have prepared ultra-thin zirconia by oxidation of a different alloy, $Pd_3Zr(0001)$, which resulted in a similar structure with a slightly different lattice parameter, $351.2\pm0.4$ pm. Unlike the oxide on $Pt_3Zr$, where Zr of the oxide binds to Pt in the substrate, here the oxide binds to substrate Zr via oxygen. This causes stronger distortion of the oxide structure, *i.e.* a stronger buckling of Zr in the oxide. After additional oxidation of $ZrO_2/Pt_3Zr$, a different ultra-thin zirconia phase is observed. A preliminary structure model for this film is based on (113)-oriented cubic zirconia. 3D oxide clusters are also present after growing ultra-thin zirconia films. They occur at the step edges, and the density is higher on $Pd_3Zr$. These clusters also appear on terraces after additional oxidation. XPS reveals different core level shifts of the oxide films, bulk, and oxide clusters.

[1] M. Antlanger, *et. al.*, Phys. Rev. B 86, 035451 (2012)

O 81.6 Thu 17:15 PHY C 213

**Ordered Phases of Reduced Ceria as Epitaxial Films on Cu(111)** — Tomáš Duchoň, Filip Dvořák, Marie Aulická, Vitalii Stetsovych, Mykhailo Vorokhta, Daniel Mazur, Kateřina Veltruská, Tomáš Skála, •Josef Mysliveček, Iva Matolínová, and Vladimír Matolín — Charles University in Prague, Faculty of Mathematics and Physics, Department of Surface and Plasma Physics, V Holešovičkách 2, 18000 Praha 8, Czech Republic

We study the relationship between the stoichiometry and the structure in thin epitaxial films of reduced ceria, $CeO_x$, $1.5\leq x\leq 2$, prepared via an interface reaction between a thin ceria film on Cu(111) and a Ce metal deposit. We show that the transition between the limiting stoichiometries $CeO_2$ and $Ce_2O_3$ is realized by equilibration of mobile oxygen vacancies near the surface of the film, while the fluorite lattice of cerium atoms remains unchanged during the process. We identify three surface reconstructions representing distinct oxygen vacancy ordering during the transition, $\sqrt{7}\times\sqrt{7}R19.1°$, $3\times3$, and $4\times4$ corresponding to bulk phases of ceria $\iota$-$Ce_7O_{12}$, $CeO_{1.67}$, and c-$Ce_2O_3$ [1], respectively. Due to the special property to yield ordered phases of reduced ceria the interface reaction between Ce and thin film ceria represents a unique tool for oxygen vacancy engineering. The perspective applications include advanced model catalyst studies with both the concentration and the coordination of oxygen vacancies precisely under control.

[1] Stetsovych, V.; *et al.*, Epitaxial Cubic $Ce_2O_3$ Films via Ce-$CeO_2$ Interfacial Reaction. *J. Phys. Chem. Lett.* **2013**, *4*, 866-871.

O 81.7 Thu 17:30 PHY C 213

**Surface phonons of titanium oxide ultrathin films on Pt(100)** — •Florian Schumann[1], Klaus Meinel[1], Johannes Lotze[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck Institut für Mikrostrukturphysik, Halle, Germany

Phonons and their softening are key elements for the understanding of the long-range coupling in ferroelectric and multiferroic materials. Titanium oxide is a relevant part and one possible termination in many perovskites like $BaTiO_3$ and $SrTiO_3$. In thin films, structure and lattice dynamics can be modified due to the interaction at the interfaces. Here we study the surface phonons of ultrathin titanium oxides grown by MBE on Pt(100). Three different well-ordered $TiO_x$ phases have been identified as (4×13), (3×5) and $(2\sqrt{2}\times2\sqrt{2})R45°$ structures based on their LEED pattern [1,2]. The three phases can be distinguished by their charakteristic phonon frequencies at 1020, 755 and $625\,\mathrm{cm}^{-1}$, respectively. The stability of the three phases as function of termperature and oxygen pressure will be discussed based on the phonon spectroscopy.

[1] T. Matsumoto et al., Surf. Sci. 572: 127, 2004.
[2] T. Matsumoto et al., Surf. Sci. 572: 146, 2004.

### O 81.8 Thu 17:45 PHY C 213

**Development of a new Phase on $TiO_2$ (101) Anatase with Reduced Bandgap** — •Christian Dette[1], Christopher S. Kley[1], Miguel A. Perez[2], Paul Punke[1], Christopher Patrick[2], Feliciano Giustino[2], Soon J. Jung[1], and Klaus Kern[1,3] — [1]MPI for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]University of Oxford, 16 Parks Road, Oxford OX1 3PH, United Kingdom — [3]EPF Lausanne, IPMC, 1015 Lausanne, Switzerland

Nanosized $TiO_2$ photocatalytic water-splitting technology has great potential for low-cost, environmentally friendly solar-hydrogen production to support the future hydrogen economy. Presently, the solar-to-hydrogen energy conversion efficiency is too low for the technology to be economically sound. The main barriers are the poor activation of $TiO_2$ by visible light. Hence, our research is focused on the reduction of the band gap to increase the photocatalytic activity in the visible.

We have created a reduced band gap phase (phase II) on the standard surface (phase I) of a natural grown $TiO_2$ (101) Anatase crystal by a combination of standard cleaning processes. The creation processes are fully reversible. We have taken detailed topography and spectroscopy data at various positions of each phase by using scanning tunnelling microscopy (STM) and spectroscopy (STS). We found a similarity in the electronic configuration between phase II and the [-111] oriented edge of phase I, since both show a reduced ban gap due to a band gap state near the valence band maximum. We will present a structural model of phase II consistent with the experimental data and first-principle density functional theory based calculations.

### O 81.9 Thu 18:00 PHY C 213

**Small and Large Polarons in $TiO_2$ Rutile and Anatase** — •Martin Setvin[1], Cesare Franchini[2], Xianfeng Hao[1], Benjamin Daniel[1], Michael Schmid[1], Georg Kresse[2], and Ulrike Diebold[1] — [1]TU Wien, Vienna, Austria — [2]Universität Wien, Viena, Austria

$TiO_2$ is a prototypical metal oxide and used in photocatalysis, photoelectrochemical (Grätzel) solar cells, and transparent optical conductors. Industrially two forms of $TiO_2$ are used, rutile and anatase. The behavior of charge carriers is of key importance in virtually all applications of these materials. When excess electrons are added to the conduction band of an oxide, the electron-phonon interaction may result in electron trapping – the formation of either localized (small) or delocalized (large) polarons.

We used a combination of STM, STS and DFT+U to investigate the nature of electron polarons in rutile and anatase. The excess electrons in rutile can localize at any lattice Ti atom, forming a small polaron. The polarons in rutile can easily hop to neighboring sites. Electrons in a perfect anatase lattice prefer delocalized (band-like) solution, while small polarons can only be formed at defects. Large polarons were observed in Nb-doped anatase in vicinity of subsurface Nb dopants. Our results help to understand the different behavior of $TiO_2$ rutile and anatase in applications.

Work supported by ERC Advanced Research Grant Oxide Surfaces.

### O 81.10 Thu 18:15 PHY C 213

**In-situ characterization of ferroelectric domains of epitaxially $BaTiO_3$(100) ultrathin films on Pt(100) by STM and STS** — •Maik Christl[1], Klaus Meinel[1], Stefan Förster[1], and Wolf Widdra[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

The understanding of ferroelectric domain properties of ultrathin films is of fundamental interest with regard to interface effects and smallest domain dimensions [1]. To adress these issues the widely used piezoresponse force microscopy is not a suitable tool due to its limited resolution and the low mechanical stability of the ultrathin films. Alternatively, we apply scanning tunneling microscopy (STM) and spectroscopy (STS) for writing and reading of ferroelectric domains in $BaTiO_3$(100) thin films. The films were grown pseudomorphically on a Pt(100) substrate with compressive strain of 2% [2]. A voltage dependent contrast between positively and negatively poled areas appears in dI/dV maps. In particular a contrast inversion at 1 V between different domains is observed. This inversion results from a characteristic shift of the density of states between $c^+$ and $c^-$ domains as confirmed by dI/dV point spectra. For ultrathin films of 2 and 3 unit cell thickness, we find different ferroelectric switching behaviors.
[1] J. F. Scott, *J. Phys.: Condens. Matter 18*, **2006**
[2] S. Förster et al., *J. Chem. Phys. 135*, 104701 **2011**

### O 81.11 Thu 18:30 PHY C 213

**Stress measurements during PLD growth of $BaTiO_3$ and $SrTiO_3$ films on single crystal metal substrates** — •Jörg Premper[1], Dirk Sander[1], and Jürgen Kirschner[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — [2]Institut für Physik, Martin-Luther-Universität, Halle, Germany

The in situ measurement of film stress by the optical 2-beam cantilever deflection technique [1] is used to study the correlation between stress and strain in $BaTiO_3$ and $SrTiO_3$ monolayers on Fe, Pd and Pt single crystal surfaces of different orientations. These films are grown by pulsed laser deposition (PLD). We find that the deposition of 18 uc (unit cells) $BaTiO_3$ on Pt(001) (misfit = −2.3%) leads to a compressive film stress of −4.2 GPa, whereas the deposition of $SrTiO_3$ (misfit = +0.4%) induces a tensile stress of +1.5 GPa. On Pd(001) the measured film stress for $BaTiO_3$/Pd(001) is −2.6 GPa (misfit = −3.0%) and for $SrTiO_3$/Pd(001) −2.0 GPa (misfit = −0.4%). The comparison between measured stress and calculated misfit-induced stress in the framework of continuum elasticity, considering elastic anisotropy, reveals a qualitative agreement between experiment and stress calculations. This identifies epitaxial misfit as one decisive contribution to film stress in $BaTiO_3$ and $SrTiO_3$ atomic layers. In contrast, no epitaxial order of $BaTiO_3$ and $SrTiO_3$ films on Fe(001) was observed for PLD at 420°C by LEED. Still film stress of +2.1 GPa and +3.8 GPa is measured. The results are discussed in view of substrate-mediated strain and the influence of growth conditions.

[1] J. Premper, D. Sander, and J. Kirschner, RSI **83**, (2012), 073904

### O 81.12 Thu 18:45 PHY C 213

**Structure, stress and magnetism of CoO(111) monolayers on Ir(001)** — •Sumalay Roy[1], Holger Meyerheim[1], Katayoon Mohseni[1], Zehn Tian[1], Dirk Sander[1], Arthur Ernst[1,2], Martin Hoffmann[1,3], Waheed Adeagbo[3], Wolfram Hergert[3], Roberto Felici[4], and Jürgen Kirschner[1,3] — [1]Max-Planck-Institute of Microstructure Physics, Halle, Germany — [2]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Leipzig, Germany — [3]Martin-Luther-University Halle-Wittenberg, Halle, Germany — [4]European Synchrotron Radiation Facility, Grenoble, France

To investigate the structural depolarization [1] and its correlation with magnetic properties [2] in ultrathin (111) oriented CoO films, 1.6 and 2 monolayers of CoO were deposited on Ir(001) using molecular beam epitaxy of Co followed by subsequent annealing in ambient oxygen. An in-situ Surface X-ray diffraction (SXRD) measurement and analysis of the so prepared CoO(111) films reveals the coexistence of wurtzite and rocksalt structure involving strong vertical relaxations, which is attributed to the reduction of the dipole moment in the polar CoO (111) film which in the bulk renders the structure unstable. The measured stress change (+2.1 N/m) during epitaxial growth can be attributed to the epitaxial misfit between the c-(10×2) CoO(111) film and the Ir(001) substrate. Ab-initio calculations using the SXRD structure parameters as input reveal an anti-ferromagnetic order (below 150K) in the CoO film. [1] P. W. Tasker J. Phys. C: Solid State Phys. 12, 4977 (1979). [2] F. Mittendorfer et. al., Phys. Rev. Lett. 109, 015501 (2012).

# O 82: Metal Substrates II

Time: Thursday 16:00–19:00 Location: WIL A317

O 82.1 Thu 16:00 WIL A317

**Measuring the mode-selective e-ph interaction constant on Sb(111) using Helium atom scattering** — •Patrick Kraus[1], Michael Mayrhofer-R.[1], Florian Apolloner[1], Christian Gösweiner[1], Giorgio Benedek[2], Salvador Miret-Artés[3], and Wolfgang E. Ernst[1] — [1]IEP, University of Technology, Graz, Austria — [2]DIPC, San Sebastián, Spain — [3]C.S.I.C, Madrid, Spain

As one of the essential components in the recently discovered group of topological insulators [1], the semimetal antimony (Sb) is an attractive candidate for studying the properties of its surface. Quite recently the surface phonon dispersion curve of Sb(111) as well as the influences of e-ph interaction were calculated using DFPT [2]. Helium Atom Scattering allows to investigate elastic as well as inelastic phenomena associated with structure and dynamics of the electronic corrugation slightly above the Sb(111) surface. Using exact approaches such as the Close-Coupling-Method, a fundamental analysis of the surface corrugation is possible. Furthermore, this approach can be extended to include inelastic interactions [3,4], rendering the measurement of the mode-selective electron-phonon interaction constant possible. The complete procedure, beginning with the determination of the three dimensional static interaction potential to the evaluation of the mode-selected electron-phonon interaction, will be presented. [1] H. Zhang et al., Nature Physics 5 (2009) 438-442 [2] D. Campi et al., Phys. Rev. B. 86 (2012) 075446 [3] A.S. Sanz and S. Miret-Artés, Phys. Rep. 451 (2007), 37-154 [4] M. Mayrhofer-R. et. al., Phys. Rev. B. 88 (2013), 205425

O 82.2 Thu 16:15 WIL A317

**Reinvestigation of the Acoustic Surface Plasmon Dispersion on Cu(111) by HREELS** — •Jan Pischel, Emanuel Welsch, Olaf Skibbe, and Annemarie Pucci — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg

During the past decade, the existence of the acoustic surface plasmon (ASP, [1]) on various single crystal metal surfaces has been established experimentally, see e. g. [2]. Its low energy in the meV range and a linear dispersion near $\bar{\Gamma}$ make it interesting for a wide range of phenomena and applications reaching from superconductivity to nano-optics. Only recently, it was reported that the ASP on Au(111) disperses into the electron-hole (e-h) pair continuum [3], which is in contrast to the theoretical prediction [1]. This unexpected behaviour could be traced back to the fact that the majority of bulk electrons around the Fermi level move slower than the electrons of the Shockley surface state and are hence screened by the latter rather than the other way around.

We used HREELS with low impact energies down to 2eV and an angular resolution of 1.4° to reinvestigate the situation on Cu(111). As shown here, the ASP turned out to be only one of multiple contributions to the broad excitation feature that was earlier exclusively ascribed to the ASP [2] and to disperse into the e-h pair continuum. These results suggest that a situation similar to the Au(111) case must be present on the Cu(111) surface, too.

[1] Silkin et al., Europhys. Lett. **66**(2):260–264, 2004.
[2] Pohl et al., Europhys. Lett. **90**:57006, 2010.
[3] Vattuone et al., Phys. Rev. Lett. **110**:127405, 2013.

O 82.3 Thu 16:30 WIL A317

**Probing Two-Band Superconductivity by Scanning Tunneling Spectroscopy** — •Michael Ruby[1], Benjamin W. Heinrich[1], Jose I. Pascual[1,2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]CIC nanoGUNE and Ikerbasque, Basque Foundation for Science, Tolosa Hiribidea 78, Donostia-San Sebastian 20018, Spain

Recent DFT simulations have shown that the two separated Fermi-surfaces of the strong-coupling s-wave BCS superconductor lead (Pb) exhibit different character in momentum space, namely s-p- and p-d-like [1]. The two Fermi-surfaces make Pb a two-band superconductor with different gap parameter for each band. Using scanning tunneling spectroscopy (STS) we observe an energy difference of the gap parameters of $\approx 150\ \mu$V, and different intensity for each of the BCS resonances. We use the high spacial resolution of STS measurements to further investigate the influence of surface defects, adsorbates, and impurities on the density of states of the two-band superconductor.

[1] A. Floris *et al.*, *Phys. Rev. B* **75**, 054508, (2007)

O 82.4 Thu 16:45 WIL A317

**Electromechanical coupling coefficients of sp-bonded metals from first principles** — •Anja Michl[1,2], Sandra Hoppe[2], Chandramouli Nyshadham[2], Jörg Weissmüller[1,3], and Stefan Müller[2] — [1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Germany — [2]Institute of Advanced Ceramics, Hamburg University of Technology, Germany — [3]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany

The coupling between mechanical stress or strain of a surface and its electronic properties is relevant for various applications ranging from sensors and actuators to catalysis. In experiment, coupling coefficients are determined via electrochemical experiments, e.g. by measuring the variation of the electrode potential upon applying tangential strain $e$ to the electrode surface. Theoretically, this coupling strength is accessible as the response of the electronic work function $W$ to strain. Using density functional theory, we calculate such strain response parameters $\mathrm{d}W/\mathrm{d}e$ for sp-bonded metals. While for Al we find an abnormal positive sign for the coupling coefficient [1], all other investigated metals show the usual negative response parameter (in their natural crystal structure). We analyze trends of the coupling coefficients with respect to valence electron density, crystal structure and work function of the unstrained surface and discuss the identified correlations.
[1] A. Michl, J. Weissmüller and S. Müller, J. Phys.: Condens. Matter **25**, 445012 (2013)

O 82.5 Thu 17:00 WIL A317

**Ground-state structures for oxygen adsorption on Ir(100)-(1×1) investigated via the cluster-expansion method** — •Anja Michl[1,2], Pascal Ferstl[3], Lutz Hammer[3], M. Alexander Schneider[3], and Stefan Müller[2] — [1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Germany — [2]Institute of Advanced Ceramics, Hamburg University of Technology, Germany — [3]LS f. Festkörperphysik, Universität Erlangen-Nürnberg, Germany

The interaction of oxygen with transition metal surfaces is of fundamental importance for a variety of processes in heterogeneous catalysis. In the case of iridium, oxygen exposure lifts the (5×1)-hex reconstruction of the (100) surface leading to a (1×1) structure.

We performed an exhaustive ground-state search for the O/Ir(100)-(1×1) system by using the cluster-expansion formalism in conjunction with first-principles calculations. Our study reveals $(n\times1)$-$m$O superstructures as the dominant structural motif of energetically favorable structures, where the periodicity $n$ and the number of oxygen atoms in the unit cell $m$ vary with the coverage. Bridge site occupation is preferred and the most pronounced ground state ist the well-known (2×1)-br superstructure. At low coverage, structures formed by an alternation of (2×1)-br stripes and a shifted row reconstruction have lower formation energies than the corresponding structures on a merely (1×1) ordered substrate. Our findings are in agreement with experimental data obtained by STM and LEED.

O 82.6 Thu 17:15 WIL A317

**Origin of unexpected attractive adsorbate-adsorbate interactions between negatively charged ions on Mg(0001) surfaces** — Su-Ting Cheng, •Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf

Electrostatic repulsion usually leads to an increase in work function and a decrease in binding energy when the coverage of electronegative elements adsorbed on a metal surface is increased. Using density-functional theory we investigate the adsorption of {N,O,F,Cl} on Mg(0001) and find that only Cl complies with this expectations. All the considered 2nd row elements cause a decrease in work-function and an increase in binding energy with increasing coverage. We show that these counter-intuitive phenomena can be understood in terms of an efficient embedding of the adsorbate atoms into the unusually large electronic surface spill-out of Mg(0001). The described mechanism is based on purely electrostatic arguments and thus expected to be a generic feature on surfaces consisting of highly electropositive elements.

O 82.7 Thu 17:30 WIL A317

**Local Adsorption Sites of Oxygen and Hydrogen on the Ir(100) surface** — •Pascal Ferstl[1], Lutz Hammer[1], M. Alexander Schneider[1], Florian Mittendorfer[2], Md. Alif Arman[3], Edvin Lundgren[3], and Jan Knudsen[3] — [1]Lst f. Festkörperphysik, FAU Erlangen-Nürnberg, Germany — [2]Inst. f. Angewandte Physik & CMS, TU Wien, Austria — [3]Synchrotron Radiation Research, Lund, Sweden

The adsorption behavior of oxygen and hydrogen on transition metal surfaces is of fundamental importance for heterogeneous catalysis. In this high-resolution X-ray photoelectron spectroscopy study we investigated their adsorption on the Ir(100) surface in the whole accessible coverage range $\Theta = 0 - 1.0$. The investigation is complemented by LEED, STM and TDS measurements, as well as by DFT calculations, allowing the clear identification of different components in the XP-spectra of the various phases.

A detailed investigation of the Ir $4f_{7/2}$ line reveals that on the unreconstructed Ir(100)-1×1 surface both adsorbates are found to occupy exclusively bridge sites of the substrate. For the maximum coverage $\Theta = 1.0$ – in case of oxygen this can only be achieved by offering atomic species – every Ir surface atom is connected to two adsorbate atoms while for $\Theta = 0.5$ every two substrate atoms have to share one adsorbate. This leads to clear shifts in the Ir $4f_{7/2}$ core level energies. Series of spectra taken for various coverages achieved via successive thermal desorption can be explained by a superposition of spectra of these limiting structures and that for the finally reached clean, reconstructed 5×1 phase discarding any further local binding configuration.

O 82.8 Thu 17:45 WIL A317

**Au-Ag(110) Alloy Surfaces: Surface Restructuring and Oxygen Chemistry** — •Martin Schmid, Joshua Klobas, Robert J. Madix, and Cynthia M. Friend — Department of Chemistry and Chemical Biology, Harvard University, Cambridge MA, USA

We investigated the morphology and oxygen chemistry of thin film Au-Ag(110) alloy surfaces. The alloys were prepared by deposition of Au onto an Ag(110) single crystal under UHV conditions. The initial deposition was followed by several steps of moderate annealing in order to fabricate a thin, homogeneous surface alloy. Examination of the Au-Ag(110) surfaces with Scanning Tunneling Microscopy (STM) showed a substantial surface restructuring on the submicrometer scale, which is associated with the onset of gold diffusion into the Ag(110) bulk, starting at 400K. After repeated moderate annealing steps to 630K, an apparently constant thin film composition could be established, as confirmed with angle resolved X-ray Photoelectron Spectroscopy (XPS). The oxygen chemistry of the thin film alloys was monitored with Temperature Programmed Desorption (TPD) experiments. Exposing the thin film alloys to $O_2$ (pressure range of $1x10^{-6}$ mbar) showed a linear dependence between the oxygen uptake of the thin film at 300K and its gold content. Furthermore, probing the adsorption sites of chemisorbed $O_2$ at low temperatures (125K) showed strong indications that gold atoms, while being unreactive themselves, control the oxygen uptake by shaping the size, amount, and distribution of reactive Ag sites.

O 82.9 Thu 18:00 WIL A317

**Investigation of ice on Ag(111) via scanning tunneling microscopy: Kinetics and thermodynamics** — •Cord Bertram, Karsten Lucht, and Karina Morgenstern — Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum

As a member of the dipolar liquids and a well-known solvent, water is a very important component in electro-catalysis. For a further understanding of the microscopic processes taking part in electrocatalytic reactions, the local rearrangement of molecules in frozen water on Cu(111) in presence of an electrical field has recently been studied by scanning tunneling microscopy[1]. However, the local rearrangement depends highly on the coordination of the water molecules within the ice structure, which largely influences its ability to solvate ions or electrons. Therefore water structures on Cu(111) and on Ag(111) are studied. These surfaces with a difference in adsorption energy show substrate-mediated structure formation due to lattice mismatch effects. Additionally different preparation procedures result in structural differences, which can be explained by kinetic and thermodynamic processes. The consideration of these effects leads to new candidates for the microscopic observation of ion solvation.

[1] Mehlhorn et al.: Chem Electro Chem (2013) *in print*

O 82.10 Thu 18:15 WIL A317

**The CO adsorption on Ru(0001) and bimetallic PtRu/Ru(0001) surfaces at elevated pressures (from $10^{-3}$ to 100 mbar)** — •Thomas Diemant, Joachim Bansmann, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

PtRu catalysts are, due to their superior CO tolerance, a promising material for the anodic hydrogen oxidation reaction in low-temperature polymer electrolyte fuel cells in the presence of small amounts of CO. After studying the adsorption of CO and hydrogen on structurally well-defined PtRu/Ru(0001) surfaces under UHV conditions, we extended our studies to catalytically relevant conditions (atmospheric pressure and RT), investigating the CO adsorption on Ru(0001) and bimetallic surfaces at elevated CO pressure, using polarization-modulated IR reflection absorption spectroscopy (PM-IRAS).

On unmodified Ru(0001), we find a gradual blue-shift of the peak position with increasing pressure, which stops at a wave number higher than the value found for UHV CO saturation. In agreement with a recent XPS study on this topic [1], we explain this finding by a higher CO saturation coverage than obtained under UHV conditions. For CO adsorption on a Pt/Ru(0001), we find a comparable wave number. In this case, however, it resembles the value obtained for UHV adsorption at 150 K, supporting our previous model of a kinetic barrier for direct CO adsorption on Ru(0001) at high CO coverages, which can be circumvented by spillover from Pt monolayer islands.

[1] D. E. Starr, H. Bluhm, Surf. Sci. 608 (2013) 241.

O 82.11 Thu 18:30 WIL A317

**Spontaneous step creation during NO reduction on Pt surfaces: a high-pressure STM study** — •Matthijs van Spronsen, Qian Liu, and Joost Frenken — Kamerlingh Onnes Laboratory, Leiden University, Leiden, P.O. Box 9504, 2300 RA, The Netherlands

When atoms and molecules adsorb on surfaces, they can introduce significant changes in the surface stress, for example when an overlayer is formed of dipolar molecules that strongly repel each other. This may have dramatic consequences for the structure of catalysts that have dense overlayers due the to high gas pressures. We have used a scanning tunneling microscope (STM), dedicated for atomic-scale, high-pressure, high-temperature observations of active catalysts, to investigate the structural changes that occur on a Pt(110) surface when this is active as a catalyst for NO reduction by H2. To our surprise we find that atmospheric pressures of (NO,H2) gas mixtures lead to the spontaneous creation of regular step arrays on the initially flat surface. We propose that the step creation is a pathway for the surface to relax part of the high, adsorption-induced stress. This interpretation finds support in DFT calculations.

O 82.12 Thu 18:45 WIL A317

**Pt-coverage dependence and adsorption kinetics of the coadsorption of CO and deuterium on bimetallic Pt/Ru(0001) surfaces** — Heinrich Hartmann, •Joachim Bansmann, Thomas Diemant, and R. Jürgen Behm — Institut for Surface Chemistry and Catalysis, Ulm University, D-89081 Ulm

The interaction of hydrogen and CO with bimetallic PtRu surfaces as technological promising materials is of high interest for the understanding of the chemistry in low temperature Polymer Electrolyte (PE) fuel cells. In the present TPD and IR study we investigated the coadsorption of CO and deuterium at 100 K (subsequently exposed) on sub-monolayer Pt films on Ru(0001) as model systems.

The total coverage of adsorbates ($CO_{ad}$ and $D_{ad}$) on the bimetallic Pt/Ru(0001) surface depends not only on the amount of Pt on the surface, but also strongly on the sequence in the coadsorption process. Deuterium adsorption followed by high CO exposures results in very high coverages, whereas, in the opposite case, no further $D_2$ adsorption is possible on a saturated CO layer and the total coverages are smaller. Here, we will additionally analyze the influence of pre-adsorbed $D_{ad}$ species on the CO adsorption kinetics and the total adsorbate coverage compared to pure CO and deuterium adsorption on bimetallic Pt/Ru(0001) [1] and PtRu/Ru(0001) surfaces alloys [2].

[1] H. Hartmann et al., Phys. Chem. Chem. Phys. 14 (2012) 10919.
[2] T. Diemant et al., Chem. Phys. Chem. 11 (2010) 1482.

# O 83: Graphene: Adsorption, Intercalation, Doping (O jointly with DS, HL, MA, TT)

Time: Thursday 16:00–18:45 Location: WIL C107

O 83.1 Thu 16:00 WIL C107

**Covalent binding of single iron phtalocyanine molecules to graphene on Ir(111)** — •Simon J. Altenburg[1], Shiri R. Burema[2], Bin Wang[3], Richard Berndt[1], and Marie-Laure Bocquet[2,4] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Université de Lyon, Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, CNRS, F69007 Lyon, France — [3]Department of Physics & Astronomy, Vanderbilt University, Nashville, TN 37235 — [4]Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139

Single iron phtalocyanine (FePc) molecules on graphene on Ir(111) are studied by low temperature scanning tunneling microscopy. The molecules are either unperturbed and weakly coupled to the substrate or bound to graphene by a lobe in a specific region of the moiré unit cell. Concomittant density functional calculations reveal that the binding between the FePc lobe and graphene is the result of a new kind of cyclization reaction. This reaction is activated in certain regions of the moiré unit cell by the presence of the iridium substrate.

O 83.2 Thu 16:15 WIL C107

**Adsorption of Pentacene on Epitaxial Graphene and BN** — •Alexei Nefedov[1], Wenua Zhang[1,2], Hikmet Sezen[1], Alexandr Fedorov[3], Nikolay Verbitskiy[4], Alexander Grüneis[3,4], and Christof Woell[1] — [1]Institute of Funcional Interfaces, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [2]NSRL, Hefei, China — [3]IFW, Dresden, Germany — [4]University of Vienna, Vienna, Austria

Smooth interfaces are a prerequisite for future high-performance and low-cost organic electronic devices based on small conjugated molecules. Since all important charge transport processes are confined to the first several monolayers, the quality of the first layer plays a key role on device performance. Pentacene stands out as a model molecule among organic semiconductors due to its ability to form well-ordered films showing a high field effect mobility. Moreover, the morphology of the first layer of a thin Pn film is known to be strongly influenced by the substrate termination, which further decisively affects the interfacial charge transport properties. Thus, information on the molecular orientation of pentacene in a case of (sub)monolayer coverages can provide a key information on improvement of device performance. In this study the adsorption of pentacene on a single layer of graphene or boron nitride (BN) has been investigated by means of XPS and NEXAFS spectroscopy. The experiments were performed on the HE-SGM beamline at BESSY II in Berlin. It was found that pentacene molecules demonstrate a dependence of their orientation and electronic structure on the coverage.

O 83.3 Thu 16:30 WIL C107

**Wetting properties of parahexaphenyl on exfoliated graphene** — •Markus Kratzer[1], Stefan Klima[1], Borislav Vasić[1], Aleksandar Matković[2], Marijana Milićević[2], Rados Gajić[2], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversität Leoben,Franz Josef Straße 18, 8700 Leoben, Austria — [2]Institute of Physics, University of Belgrade, Pregrevica 118 P.O. Box 68, 11080 Belgrade, Serbia

Graphene (Gr) bears potential to serve as transparent and flexible electrode material in organic electronics. Therefore, understanding of the growth of organic thin films on it is essential. Here, we investigated the growth morphology of films formed by the rodlike para-hexaphenyl (6P) molecule on Gr as a model system. As substrates exfoliated graphene transferred onto a silicon oxide support were used. Submonolayer amounts of 6P were deposited by means of hot-wall epitaxy between 333 K and 393K. The evolving film morphologies, investigated by atomic-force microscopy (AFM), exhibited a strong dependence on temperature and number of supporting Gr layers. At 333 K, needle like structures - which are known to be composed of flat lying molecules [1]- and islands composed of upright standing molecules coexist on the Gr. For the higher temperatures solely needles, forming networks, are found. The needles forming at 363 K exhibit an increasing dewetting with increasing number of Gr layers which is attributed to Gr layer dependent changes in surface energy, diffusion properties and preferential adsorption sites.

[1] C. Teichert et al. Appl. Phys. A 82 (2006) 665.

O 83.4 Thu 16:45 WIL C107

**H-adsorption and $H_2$-splitting on graphene/SiC(0001)** — •Gabriele Sclauzero and Alfredo Pasquarello — École Polytechnique Fédérale de Lausanne (EPFL), Lausanne (Switzerland)

High-quality graphene grown epitaxially on SiC(0001) can be regarded as a convenient template for the realization of graphene-based electronics. However, the presence of a carbon “buffer” layer buried at the interface between the SiC surface and the epitaxial graphene is detrimental to the electronic transport properties of graphene. Hydrogen intercalation at high temperatures can be used to convert the buffer layer into a quasi-free standing graphene lying directly above a H-saturated SiC(0001) surface, which provides a much more effective decoupling from the substrate.

Here, the processes of H-adsorption and $H_2$-splitting at the graphene/SiC(0001) interface is addressed through first-principles atomistic simulations based on realistic interface models, including the experimentally observed $6\sqrt(3)\times 6\sqrt(3)R30^\circ$ reconstruction. Our main finding is a great enhancement of the chemical reactivity of the carbon buffer layer with respect to pristine graphene, as a result of the partial $sp^2$ to $sp^3$ rehybridization of the C atoms in the buffer. H-binding energies on threefold-coordinated C atoms of the buffer are three-to-four times larger than on graphene and $H_2$-splitting becomes an exothermic process, with activation barriers that can be up to four times smaller than on graphene. On favorable sites, energy barriers can become as low as 1 eV and are in agreement with the observation of atomic-H intercalation also when $H_2$ is used as hydrogen source.

O 83.5 Thu 17:00 WIL C107

**Deuterium adsorption on (and desorption from) SiC(0001)-(3x3), (R3xR3)R30°, (6R3x6R3)R30° and quasi-free-standing graphene obtained by hydrogen intercalation** — •Bocquet F.C.[1], Bisson R.[2], Themlin J.-M.[3], Layet J.-M.[2], and Angot T.[2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich - 52425 Jülich, Germany — [2]Aix-Marseille Université, PIIM, CNRS, UMR 7345, 13013 Marseille, France — [3]Aix-Marseille Université, IM2NP, 13397, Marseille, France and CNRS, UMR 7334, 13397, Marseille - Toulon, France

I present a comparative High-Resolution Electron Energy-Loss Spectroscopy (HREELS) study on the interaction of atomic hydrogen and deuterium with various reconstructions of SiC(0001). We show that deuterium passivation of the (3x3) is only reversible when exposed to atomic deuterium at a surface temperature of 700 K since tri- and dideuterides, necessary precursors for silicon etching, are not stable at this temperature. On the other hand, we show that the deuteration of the (R3xR3)R30° is always reversible because precursors to silicon etching are scarce on the surface [1]. Further, the comparison of the deuterium binding in the intercalation layer of quasi-free-standing graphene with the deuterated (R3xR3)R30° surface provides some indication on the bonding structure at the substrate intercalation layer [1,2].

[1] F.C. Bocquet et al. J. Phys. D: Appl. Phys. (2014) in press

[2] F.C. Bocquet et al. Phys. Rev. B. 85 (2012) 201401

O 83.6 Thu 17:15 WIL C107

**Charge doping induced phase transitions in hydrogenated and fluorinated graphene** — •Tim Wehling[1,2], Bernhard Grundkötter-Stock[2], Bálint Aradi[2], Thomas Niehaus[3], and Thomas Frauenheim[2] — [1]Institute for Theoretical Physics, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]Bremen Center for Computational Material Science, Universität Bremen, Am Fallturm 1, 28359 Bremen, Germany — [3]Department of Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We show that charge doping can induce transitions between three distinct adsorbate phases in hydrogenated and fluorinated graphene. By combining ab initio, approximate density functional theory and tight binding calculations we identify a transition from islands of $C_8H_2$ and $C_8F_2$ to random adsorbate distributions around a doping level of ±0.05 e/C-atom. Furthermore, in situations with random adsorbate coverage, charge doping is shown to trigger an ordering transition where the sublattice symmetry is spontaneously broken when the doping level exceeds the adsorbate concentration. Rehybridization and lattice distortion energies make graphene which is covalently functionalized from one side only most susceptible to these two kinds of phase transitions. The energy gains associated with the clustering and ordering transitions exceed room temperature thermal energies.

O 83.7 Thu 17:30 WIL C107

**Graphene Oxide Formation by Adsorption and Photolysis of NO$_2$ and SO$_2$ on Graphene/Ir(111)** — •Stefan Böttcher, Hendrik Vita, and Karsten Horn — Fritz-Haber Institute of the Max-Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

Graphene oxide is a widely discussed precursor for the technological application of graphene-based systems; for example, its controlled reduction into graphene may lead to a tunable band gap. We report on the formation of oxidized graphene layers on Ir(111) by adsorption and photodissociation of NO$_2$ and SO$_2$ at low temperatures. Both adsorbates induce atomic oxygen on the surface when irradiated with intense UV light, leading to an oxidation of the graphene layer. The method presented here is expected to be less intrusive compared for example to oxygen bombardment methods. We also believe the photon induced oxidation to be more selective compared to other physical or wet chemical methods. A band gap opening at room temperature is observed, showing that the graphene oxide phase is also stable above 100 K. High quality graphene can be recovered after annealing, judged by the reappearance of its core and valence level spectral features. Apart from the selective formation of the epoxidic phase, the reaction can also be driven towards a metastable oxide phase from NO$_2$ using low photon flux. SO$_2$ on the other hand produces fragments upon dissociation, which have a strong influence on the hybridization state of the graphene backbone.

O 83.8 Thu 17:45 WIL C107

**Tuning the van der Waals Interaction of Graphene with Molecules by Doping** — •Felix Huttmann[1], Antonio Javier Martinez-Galera[1], Nicolae Atodiresei[2], Vasile Caciuc[2], Stefan Blügel[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

Strong n-doping of graphene on its epitaxial substrate can be introduced via intercalation of highly electropositive elements such as Cs and Eu, and has recently been shown to lead to reduced binding energy for electropositive, ionic adsorbates [1].

Here, we explore tuning of graphene's van der Waals (vdW) interaction with adsorbates via doping. Employing an all in-situ surface science approach, we find by scanning tunneling microscopy and thermal desorption spectroscopy a significantly higher binding energy on n-doped as opposed to undoped graphene for the vdW-bonded molecules benzene and naphthalene. This is just opposite to the case of electropositive, ionic adsorbates. Based on the model character of these simple pi-conjugated molecules [2], we propose that the strength of the van der Waals interaction is modified by doping. The experimental results are compared to density functional calculations, including van der Waals interactions.

References:

[1] S. Schumacher et al., Nano Lett. 13, 5013 (2013)

[2] S. D. Chakarova-Käck et al., Phys. Rev. Lett. 96, 146107 (2006)

O 83.9 Thu 18:00 WIL C107

**Li intercalation at the graphene/Cu interface: An electronic structure view of synchrotron-based spectroscopy** — •Liang Zhang[1,2], Jinghua Guo[2], and Junfa Zhu[1] — [1]National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, 230029, China — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA

The synthesis of graphene on metal surfaces (such as Ni, Pd, Ru or Cu) by chemical vapor deposition (CVD) is one of the most promising, inexpensive and readily accessible methods to prepare single-layer graphene, which is a prerequisite for the fabrication of graphene-based electronic devices. In particular, graphene grown on Cu foils over large areas has allowed access to high quality of this material.

In this presentation, we report our recent studies on the electronic structure of graphene/Cu and Li-intercalated graphene/Cu by synchrotron-based spectroscopy. The results indicate a high degree of alignment and a slight corrugation/rippling of the graphene layer on Cu. The deposition of Li atoms on graphene surface under ultrahigh vacuum condition at room temperature results in a charge transfer from the adsorbed Li atoms to graphene. After annealing the as-deposited Li/graphene/Cu sample at 300 °C for 10 min, the Li atoms intercalate into the interface of graphene/Cu. These interfacial Li atoms show a strong passivation from oxidation environment due to the protection of graphene layer.

O 83.10 Thu 18:15 WIL C107

**Progressive nitrogen-doping of graphene on SiC(0001)** — •Mykola Telychko, Pingo Mutombo, Martin Ondráček, Prokop Hapala, Jan Berger, Pavel Jelinek, and Martin Švec — Institute of Physics ASCR, Cukrovarnická 10, Praha, Czech republic

Doping of epitaxial graphene on SiC substrates was achieved by direct nitrogen ion implantation and stabilization at temperatures above 1300K. Scanning tunneling microscopy reveals very well-defined single substitutional defects on single and bilayer graphene. Repeated nitrogen implantation and stabilization leads to formation of double defects, which comprise of two nitrogen defects in a second-nearest-neighbour (meta) configuration. DFT calculations and scanning tunneling microscopy simulations are used to evaluate the electronic properties and to explain varying contrast of these defects in the atomically-resolved images, depending on the probe type. A mechanism of defect formation is proposed.

O 83.11 Thu 18:30 WIL C107

**Electronic and magnetic properties of cobalt interaction with graphene on Ir(111)** — Hendrik Vita, Stefan Böttcher, and •Karsten Horn — Fritz-Haber-Institut of the Max-Planck-Society, Faradayweg 4-6, 14195 Berlin, Germany

The interaction of graphene with transition metal surfaces has attracted much interest because these are ideal templates for the growth of high quality films. Ferromagnetic substrates such as Ni(111) and Co(0001) are interesting since graphene grown on these surfaces can act as a spin filter. We have earlier found that the proximity of graphene to the ferromagnetic Ni(111) substrate induces a sizeable magnetic moment in the carbon $\pi$ -states as determined from carbon K edge XMCD. Here we study the influence of thin layers of ferromagnetic Co sandwiched between Ir(111) and graphene with consequences for the magnetic properties expected. We find that the cobalt films show ferromagnetic behavior even for very low thicknesses. In order to study the behavior of magnetic heterostructures utilizing graphene as an interlayer we examine sandwich systems consisting of a thin layer of cobalt on top graphene/Ni(111). Using element-specific XMCD and hysteresis measurements it is possible to gain insight into the magnetic coupling across this magnetic heterostructure.

# O 84: Nanotribology

Time: Thursday 16:00–17:30 Location: WIL B321

O 84.1 Thu 16:00 WIL B321

**Theory of charge-density-wave noncontact phase slip nanofriction** — •Franco Pellegrini[1,2], Giuseppe E. Santoro[1,2,3], and Erio Tosatti[1,2,3] — [1]SISSA, Via Bonomea 265, I-34136 Trieste, Italy — [2]CNR-IOM Democritos National Simulation Center, Via Bonomea 265, I-34136 Trieste, Italy — [3]nternational Centre for Theoretical Physics (ICTP), P.O. Box 586, I-34014 Trieste, Italy

Bulk dissipation caused by charge-density-wave (CDW) voltage-induced depinning and sliding is a classic subject. We present a local, nanoscale mechanism describing the occurrence of distance-dependent dissipation in the dynamics of an atomic force microscope tip oscillating over the surface of a CDW material. A mechanical tip hysteresis is predicted in correspondence to localized $2\pi$ slips of the CDW phase, giving rise to large tip dissipation peaks at selected distances. Results of static and dynamic numerical simulations of the tip-surface interaction are believed to be relevant to recent experiments on the layered compound $NbSe_2$.

O 84.2 Thu 16:15 WIL B321

**Self-Assembled Monolayers under Mechanical Stress** — Christian Meltzer, Jonas Paul, Wolfgang Peukert, and •Björn Braunschweig — University of Erlangen-Nuremberg; Institute of Particle Technology (LFG), Cauerstrasse 4, 91058 Erlangen

The molecular structure of mechanically compressed octadecylphosphonic acid self-assembled monolayers (ODPA SAMs) on $\alpha$-$Al_2O_3$ is studied with co-localized vibrational sum-frequency generation (SFG). The excellent stability of our custom-built manipulation device and SFG spectrometer has allowed us to apply defined normal forces and to probe the contact area in-situ with SFG over hours without significant drift which has also facilitated time resolved studies of compressed SAMs. Normal pressures up to 208 MPa are applied and load dependent SFG spectra are recorded as a function of pressure and lateral position relative to the center of contact. These co-localized SFG spectra allow for a comparison of measured contact areas with theoretical predictions from Hertzian theory. A detailed analysis of vibrational SFG spectra shows that both intensity and relative contributions of methylene and methyl vibrational bands to the SFG intensity are excellent indicators for pressure dependent changes in the molecular structure of ODPA SAMs. Analysis of SFG spectra provides strong evidence for the formation of gauche defects. In fact, after load release healing of defects occurs on two different time scales - a fast recovery and a slow process over a time period of several hours. The former is indicative for healing of shallow defects close to the head group while the latter is dominated by high energy barrier defects close to the anchor group.

O 84.3 Thu 16:30 WIL B321

**Ab-initio modelling of energy dissipation in nanotribological systems. A DFT study of fcc Cu(111).** — •Michael Wolloch[1,2], Gregor Feldbauer[1,2], Josef Redinger[1], Peter Mohn[1], and András Vernes[1,2] — [1]Institute of Applied Physics, Vienna University of Technology, Gußhausstraße 25-25a, 1040 Vienna, Austria — [2]Austrian Center of Competence for Tribology, Viktor-Kaplan-Straße 2, 2700 Wiener Neustadt, Austria

Accurate modelling of the energy dissipation in sliding friction with *ab-initio* methods in nanotribological systems poses a fundamental challenge in modern tribology. Here we present a quasi-static model to obtain the nanofrictional response of dry, wearless systems based on quantum mechanical all electron calculations. We propose a mechanism for energy dissipation, which relies on the atomic relaxations during sliding. Since our approach does not impose any limits on lengths and directions of the sliding paths, we investigate two different ways of calculating the mean nanofriction force, both leading to an exponential friction versus load behaviour for all sliding directions. We investigate arbitrary sliding directions for an fcc Cu(111) interface and detect two periodic paths which form the upper and lower bound of nanofriction. For long aperiodic paths the friction force convergences to a value in between these limits. For low loads we retrieve the Derjaguin generalization of Amontons-Coulomb kinetic friction law which appears to be valid all the way down to the nanoscale. We observe a non-vanishing Derjaguin-offset even for atomically flat surfaces in dry contact.

O 84.4 Thu 16:45 WIL B321

**Plasticity during Contact of Rough Solids** — •Tristan A. Sharp[1], Lars Pastewka[2], and Mark O. Robbins[1] — [1]Johns Hopkins University, Baltimore, USA — [2]Fraunhofer-IWM, Freiburg, Deutschland

Surfaces of many solids exhibit multiscale roughness which has important consequences for contact area, contact stiffness, and friction. Continuum theories and simulations typically can not treat certain atomic-level features despite indications of their importance. For example, the atomic steps on the surface of crystalline solids can alter the contacting area predicted by continuum. Similarly, an appropriate model of yielding is necessary to capture the spatial distribution of surface pressure in the contact. Here, we use large-scale molecular dynamics simulation to study elastoplastic contact between self-affine rough solids. We observe that the elastic continuum result of linearity between contact area and load at small loads is preserved, but with a larger proportionality constant due to yielding. The spatial distribution of contact area is modified only at short length scales. Atomic steps concentrate the stress, increasing the amount of plasticity and contact area. The mean pressure of contacting regions is then given as a decreasing function of atomic step density.

O 84.5 Thu 17:00 WIL B321

**Scaling laws of friction: Area, time and temperature** — •Dirk Dietzel, Michael Feldmann, and Andrè Schirmeisen — Institute of Applied Physics, Justus Liebig University Giessen, Germany

The investigation of friction by AFM assisted nanoparticle manipulation has presented itself as a very useful approach to gain insight into tribological processes of extended nano- and mesocontacts. Currently, this approach is utilized to analyze the significance of dynamic processes at the interface formed between particles and substrates. Our studies reveal that some experiments, like the contact area dependence of friction, can be explained by purely structural considerations of rigid interfaces, whereas other experiments, like the combined velocity and temperature dependence of interfacial friction, highlight the importance of dynamic interface processes, i.e. contact ageing and thermal activation. Comparing these experiments thus sheds a light on the validity of assuming rigid interfaces, with possible ramifications on the concept of structural lubricity. Additionally, we will show how measuring stick slip during nanoparticle sliding can be viable route to further analyze interface processes.

O 84.6 Thu 17:15 WIL B321

**Adhesion and material transfer between contacting Al and TiN surfaces from first principles** — •Gregor Feldbauer[1,2], Michael Wolloch[1,2], Peter Mohn[1], Josef Redinger[1], and Andras Vernes[1,2] — [1]Vienna University of Technology, Gusshausstrasse 25-25a/134, 1040 Vienna, Austria — [2]Austrian Center of Competence for Tribology, 2700 Wiener Neustadt, Austria

Contacts of surfaces at the atomic length scale are of fundamental interest for a better understanding of nanotribological processes, which are crucial in modern applications from nanoindentation or AFM/FFM to nanotechnologies applied in NEMS/MEMS.

A series of density functional theory (DFT) simulations was performed to investigate the approaching, contact and subsequent separation of two atomically flat surfaces consisting of various materials. Here, aluminum (Al) and titanium-nitride (TiN) slabs were chosen as a model system representing the interaction between soft and hard materials. The approaching and separation were simulated by moving one slab in discrete steps and allowing for electronic and ionic relaxations after each step. Various configurations of the interface were analyzed by considering (001), (011) and (111) surface orientations as well as several alignments of surfaces. The performed simulations revealed the influences of these aspects on the adhesion, equilibrium distance, charge distribution and material transfer. Material transfer in particular was observed for configurations where the interface is stronger than the softer material in the system, in the sense that the adhesion energy was found larger than the energy cost to remove surface atoms.

# O 85: Molecular Simulations

Time: Thursday 17:45–19:00 Location: WIL B321

O 85.1 Thu 17:45 WIL B321

**Representing Complex Potential Energy Surfaces by Artificial Neural Networks** — •Christopher Handley and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Computer simulations of large systems are computationally costly,and in many cases intractable, when using ab initio models. More efficient potentials are typically based on approximations representative of particular atomic interactions, and the fitting of these potentials is not straightforward. Neural Networks (NNs) recently have been shown to provide interatomic potentials that are comparable to the accuracy of quantum mechanical calculations[1,2]. They are flexible enough to fit complex functions,to quantum mechancial training data, accurate energies and forces. Here, we present the first steps towards a more transferable NN based upon electronic structure methods.

[1] C. M. Handley and P. L. A. Poplier, J. Phys. Chem. A,114,3371-3383, (2010).

[2] J. Behler, PCCP, 13, 17901-18232 (2011).

O 85.2 Thu 18:00 WIL B321

**Accelerating *ab initio* molecular dynamics simulations of water by artificial neural networks** — •Tobias Morawietz[1], Andreas Singraber[2], Christoph Dellago[2], and Jörg Behler[1] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria

*Ab initio* molecular dynamics (AIMD) simulations based on density-functional theory (DFT) are a valuable tool to study processes involving water at the atomic level. However, many important properties of *ab initio* water are unknown because the costly evaluation of the forces restricts the simulation time. Artificial neural network (NNs) trained to DFT calculations provide an unbiased way to construct accurate and efficient interatomic potentials [1]. Here, we show that NN potentials closely reproduce the DFT potential-energy surface of water under a wide range of conditions, thus enabling us to study properties of water so far not accessible to AIMD simulations [2].

[1] J. Behler, PCCP **13**, 17930 (2011).

[2] T. Morawietz, A. Singraber, C. Dellago, and J. Behler, in preparation.

O 85.3 Thu 18:15 WIL B321

**The dissociation constant of water at extreme conditions** — •Otto E Gonzalez Vazquez[1], Sandro Scandolo[1], and Luigi Giacomazzi[1,2] — [1]Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy — [2]International School for Advanced Studies (SISSA), Trieste, Italy

Only one out of 10ˆ7 water molecules is dissociated in liquid water at ambient conditions, but the concentration of dissociated molecules increases with pressure ad temperature, and water eventually reaches a fully dissociated state when pressure exceeds 50-100 GPa and temperature reaches a few thousand Kelvin. The behavior of the dissociation constant of water (pKa) at conditions intermediate between ambient and the fully dissociated state is poorly known. Yet, the water pKa is a parameter of primary importance in the aqueous geochemistry as it controls the solubility of ions in geological fluids. We present results of molecular dynamics calculations of the pKa water at extreme conditions. Free-energy differences between the undissociated and the dissociated state are calculated by thermodynamic integration along the dissociation path. The calculations are based on a recently developed all-atom polarizable force-field for water, parametrized on density-functional theory calculations.

O 85.4 Thu 18:30 WIL B321

**Simulating the non-equilibrium growth of complex molecules: the influence of anisotropy** — •Nicola Kleppmann and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

In the last decade complex organic molecules have become of increasing importance. Their large charge carrier densities and tuneable resonance energies make them ideal candidates for applications in semiconductor devices. However the efficiency of such devices strongly depends on the structure formed by the adsorbed molecules, which depends on a complex interplay of growth conditions and molecular properties.

Recent ab initio calculations and experiments [1] inspire us to examine the growth of sexiphenyl (6P) on ZnO(10-10) as a model system to understand the influence of molecular anisotropy on structure formation during growth. We use kinetic Monte Carlo simulations to examine the real-space surface and single-particle dynamics as a function of time. The interaction hamiltonian of 6P molecules is modelled using a Gay-Berne potential and a linear quadrupole interaction term with additional substrate influence. Thus, we examine the influence of the molecular anisotropy on growth and on the self-assembled structures formed during growth, based on our previous studies of C60 epitaxy [2]. This system has macroscopic structures characterized by morphological quantities such as island density and layer coverage, but also microscopic ordering of molecules within the islands.

[1] F. Della Sala et al., PRL 107, 146401 (2011)

[2] S. Bommel, N. Kleppmann et al., submitted to PRL

O 85.5 Thu 18:45 WIL B321

**Free energy surface reconstruction from umbrella samples using Gaussian process regression** — •Thomas Stecher[1,2], Noam Bernstein[3], and Gábor Csányi[1] — [1]Department Chemie, TU München, Garching, Deutschland — [2]Department of Engineering, University of Cambridge, Cambridge, UK — [3]Naval Research Laboratory, Center for Computational Materials Science, Washington, DC, USA

We demonstrate how a prior assumption of smoothness can be used to enhance the reconstruction of free energy profiles from multiple umbrella sampling simulations using the Bayesian Gaussian process regression approach. The method we derive allows the concurrent use of histograms and free energy gradients and can easily be extended to include further data. In a system with one collective variable we demonstrate improved performance with respect to the weighted histogram analysis method and obtain meaningful error bars without any significant additional computation. In the case of multiple collective variables we compare to a reconstruction using least squares fitting of radial basis functions and find substantial improvements in the regimes of spatially sparse data or short sampling trajectories.

## O 86: Organic Electronics and Photovoltaics VI (DS jointly with CPP, HL, O)

Time: Thursday 17:45–19:45 Location: CHE 91

O 86.1 Thu 17:45 CHE 91

**The role of residual additives on the stability of polymer blend materials for organic photovoltaic applications.** — •Aurélien Tournebize[1,2], Agnès Rivaton[2], Heiko Peisert[1], and Thomas Chassé[1] — [1]Institute of Physical and Theoretical Chemistry, Tübingen, Germany — [2]Institut de Chimie de Clermont-Ferrand, France

Processing additives for improved the morphology of the bulk heterojunction (BHJ) materials used in organic solar cells (OSCs) is now very popular. Thus, by optimizing the donor and acceptor nano domains, the efficiency of OSCs devices could be significantly increased. [1] The impact of those additives on the performances has been widely explored recently but nothing in terms of stability. And yet, a part of the additives stays trapped in the thin film [2] and could participate in the complex photodegradation of the polymer blend materials.

In the present work, we have investigated the impact of residual additives on the polymer blend photostability. By using essentially spectroscopic technics, we have observed an acceleration of the polymer blend photodegradation in presence of additives. In this context, the use of new additives providing a better morphology and by the way a better stability was also explored.

[1] J.K. Lee, W.L. Ma, C.J. Brabec, J. Yuen, J.S. Moon, J.Y. Kim, K. Lee, G.C. Bazan, and A.J. Heeger JACS. 2008, 130, 3619-3623 [2] L. Ye, Y. Jing, X. Guo, H. Sun, S. Zhang, M. Zhang, L. Huo, and J. Hou J. Phys. Chem. C 2013, 117, 14920-14928

O 86.2 Thu 18:00 CHE 91

**Electronic States and Electrochemical Properties of Polymeric Phthalocyanine Sheets** — •Clemens Geis and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Phthalocyanines are forming organic semiconducting thin films applicable in field-effect transistors, organic solar cells and as heterogeneous chemical catalysts. They consist of a planar organic aromatic ligand around a central metal atom like *Cu*, *Fe* or *Co*. In a chemical vapour deposition reaction (CVD) phthalocyanines with polymerized ligands were synthesized by reactions of bifunctional 1,2,4,5-tetracyanobenzene with thin metal films. By these means a high concentration of the catalytically active metal-sites on the substrate is established, they are electronically coupled and a molecular network is formed by such sheet polymers. Photoelectron spectroscopy was used to characterize the electronic states of the metals and ligands. Metal ions in the complexes as well as neutral metal clusters were detected in the films. Optical transmission spectroscopy was used to discuss the uniformity of the electronic excitation energy and its dependence on preparation conditions. The films were electrochemically reduced and oxidized to further study their accessible electronic states, study consequences for their optical absorbance and to test the polymeric phthalocyanines as electrocatalysts for water oxidation to oxygen and reduction to hydrogen, reactions of highest interest for the chemical storage of electrical energy from fluctuating renewable sources.

O 86.3 Thu 18:15 CHE 91

**Asymmetry of mixing length scales and kinetics of phase-separation in co-evaporated donor-acceptor organic thin film blends** — •Rupak Banerjee, Christopher Lorch, Alexander Gerlach, Jiří Novák, Christian Frank, Johannes Dieterle, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Small molecular organic semiconductors have found widespread usage in organic photovoltaics (OPV) due to their attractive optical, structural and electronic properties [1]. One of the many ways to tune the efficiency of an OPV is by mixing donor (D) and acceptor (A) materials [1] since the efficiency depends on the interplay of the diffusion lengths of the excitons generated by the absorption of light and the structural length scales of the D:A mixture. Controlling the structural length scales in D:A mixtures is thus of paramount importance [2]. We discuss *in situ* and real-time x-ray scattering studies on the structure of mixed D:A films as a function of mixing ratio which reveal the kinetics and thickness dependence of phase separation and in particular the asymmetry between top and bottom interfaces [3]. We further discuss the influence of interrupted growth on the phase-separation kinetics of such systems.

[1] W. Brütting and C. Adachi, Physics of Organic Semiconductors, Wiley-VCH, Weinheim (2012).

[2] A. Opitz *et al.*, IEEE J. Sel. Top. Quant. **16**, 1707 (2010).

[3] R. Banerjee, J. Novák, C. Frank, C. Lorch, A. Hinderhofer, A. Gerlach, and F. Schreiber, Phys. Rev. Lett. **110**, 185506 (2013).

O 86.4 Thu 18:30 CHE 91

**UPS studies on different air-stable molecular n-dopants** — •Martin Schwarze[1], Max L. Tietze[1], Paul Pahner[1], Ben Naab[2], Zhenan Bao[2], Björn Lüssen[1], Daniel Kasemann[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Chemical Engineering, Stanford University, Stanford, California 94305, United States

Understanding the working mechanism of electrical doping in organic semiconductors is essential for the optimization of organic semiconductor devices. A defined doping level allows for the control of the Fermi level position and the conductivity of transport layers. In comparison to molecular p-doping of organic semiconductors, n-doping has the additional problem of air instability. To successfully transfer an electron to the lowest unoccupied molecular orbital (LUMO) of the matrix material, dopants exhibiting shallow highest molecular orbitals (HOMO) are necessary, rendering them prone to reactions with e.g. oxygen. In this study, three different types of n-dopants are compared, an air stable cationic DMBI and DMBI dimer with the air sensitive W2(hpp)4. Doping efficiency, Fermi-level shift, air stability, and conductivity at different doping concentrations are investigated by ultraviolet photoelectron spectroscopy (UPS) and electrical measurements.

O 86.5 Thu 18:45 CHE 91

**Fracture and corrosion protection for thin-film encapsulation - Fine-tuning the electrical calcium corrosion test for water vapor permeation measurements** — •Frederik Nehm, Hannes Klumbies, Lars Müller-Meskamp, and Karl Leo — Institut für Angewandte Photophysik, TU Dresden, Dresden, Deutschland

In recent years, the demand for ultra-high moisture barriers has strongly increased due to the ongoing development of organic electronics. Thus, the ability to measure water vapor transmission rates (WVTRs) below $10^{-5}\,\frac{g(H_2O)}{m^2 d}$ - less than a monolayer in 10 days - is crucial for barrier development. The electrical calcium corrosion test - monitoring the decreasing conductivity of a thin calcium film turning into calcium hydroxide - is a sensitive, cost-efficient method to measure such low WVTRs. However, poor design can cause a high background rate or test breakdown. We show that calcium corrosion causes barrier breaking by both expansion and hydrogen emission. As a countermeasure, we introduce organic ($C_{60}$) buffer layers for decoupling on both sides of the calcium film. Further investigations show elevated calcium corrosion at the calcium-electrode-interface which can be prevented by a proper choice of the electrode material. Finally, the massive corrosion of barrier thin films is shown to be prevented by glueing a polymer foil onto the barrier under testing. With these precautions, we show atomic layer deposited alumina barriers measured in thin film encapsulation structure close to an actual device architecture. At 30°C, 90% rh, WVTRs of below $5 \cdot 10^{-5}\,\frac{g(H_2O)}{m^2 d}$ were obtained.

O 86.6 Thu 19:00 CHE 91

**Commensurability as the determining factor for molecular tilt and multilayer growth: In-situ and real-time growth study of the nanographene HBC on $SiO_2$ and HOPG** — •Paul Beyer[1], Tobias Breuer[2], Saliou Ndiaye[2], Anton Zykov[1], Andreas Viertel[1], Manuel Gensler[1], Jürgen P. Rabe[1], Stefan Hecht[1], Gregor Witte[2], and Stefan Kowarik[1] — [1]HU Berlin, 12489 Berlin — [2]Philipps-Universität Marburg, 35032 Marburg

We investigate the influence of symmetries and the substrate-molecule commensurability on the structure and growth kinetics of the nanographene hexa-*peri*-hexabenzocoronene (HBC). We study organic molecular beam deposited ultrathin HBC films on $SiO_2$, pristine and sputtered HOPG because of the similar surface energies, singling out the influence of the lattice-matching between HBC and graphite. Using real-time and *in situ* x-ray growth oscillations we find the first ad-layer to grow lying down on both substrates. On pristine HOPG we find a superstructure of hexagonally arranged, recumbent molecules in a new polymorph using GIXD, XRR and NEXAFS. The loss of commensurability in the sputtered HOPG leads to mainly upright molecules. Equally, we find a transition to upright molecules on amorphous $SiO_2$ surfaces. On $SiO_2$ micro-crystallites in the bulk structure that completely cover the substrate are found, while the strong ordering on HOPG leads to island growth of the new polymorph as observed by AFM. Our results demonstrate that the (lack of) symmetry- and lattice-matching critically determines the molecular orientation and occurrence of surface induced polymorphs.

O 86.7 Thu 19:15 CHE 91

**Spray coating process for highly conductive silver nanowire networks as transparent top electrode for small molecule organic photovoltaics** — •Franz Selzer[1], Nelli Weiss[2], David Kneppe[1], Ludwig Bormann[1], Christoph Sachse[1], Nikolai Gaponik[2], Lars Müller-Meskamp[1], Alexander Eychmüller[2], and Karl Leo[1] — [1]IAPP, TU Dresden — [2]Phy. Chem., TU Dresden

Organic photovoltaics are a promising technology for fabrication in high throughput R2R-coating machines. Therefore, flexible and highly conducting transparent electrodes on temperature sensible polymer films are required. Percolative networks made of silver nanowires (AgNWs) are a flexible alternative, showing an opto-electrical performance comparable to ITO. Usually, they are deposited from solution, followed by post-annealing (200°C). The solvents involved in the deposition limit the versatility of this type of electrode and do not allow the direct deposition as top contact onto evaporated small molecule devices. Here, we present a novel spray-coated AgNW mesh, showing excellent opto-electrical performance although processed below 80°C. We investigate different types of wire functionalization and the consequences on typical network parameters of AgNWs. By comparing all investigated materials for different parameters like varying concentration and by scanning electron microscopy, the basics of the sheet resistance reduction mechanism are extracted and AgNW electrodes (<50Ohm/sq@>80%) are processed at 30°C. Finally, the successful implementation as transparent top electrode for high-performance organic p-i-n type solar cells is demonstrated.

O 86.8 Thu 19:30 CHE 91

**Tuning the energy levels of carbon nanotubes by functionalization** — •Gerhard Lackner[1], Wei Xia[2], Vladimir Shvartsman[1], Martin Muhler[2], and Doru C. Lupascu[1] — [1]Institute for Materials Science, University of Duisburg-Essen, 45141 Essen, Germany — [2]Laboratory of Industrial Chemistry, Ruhr-University Bochum, 44801 Bochum, Germany

Carbon nanotubes (CNT) are a promising material for electrical applications due to their extraordinary properties. Nevertheless, a defined tuning of the energy levels of this material has not been reported so far. We show a possible route to set the energy levels of CNT by functionalization. The energy levels before and after the functionalization are analysed by Kelvin Probe measurements. Additionally, the functionalized and non-functionalized CNT are applied in organic solar cells and a comparative study about the solar cell performances is given.

## O 87: Poster: Topological Insulators (HL jointly with MA, O)

Time: Thursday 17:00–20:00 Location: P1

O 87.1 Thu 17:00 P1

**Theoretical description of scanning gate microscopy on quantum Hall point contacts** — •Martin Treffkorn and Bernd Rosenow — Institut für theoretische Physik, Universität Leipzig, Germany

In the integer quantum Hall regime, the concept of edge states allows to describe dissipationless, one-dimensional transport along the boundary of a sample. Recent experimental progress in the application of low-temperature scan-gate microscopy has allowed to image the spatial structure of edge states with high resolution [1]. To this end, a negatively charged scanning tip approaches a quantum point contact (QPC), such that changes in the spatial edge structure can be measured in the differential resistance of the QPC. The resistance only change when the tip induced change in electron density prevents an edge channel from passing through the point contact, since electrons may only travel along the quasi one dimensional channels at the edge. From the differential change of resistance versus the tip position one obtains a picture of the edge channels that are present in the system. We use a recursive Greens function algorithm to calculate the conductance of a QPC in the presence of a scanning tip. In our calculations we consider the existence of alternating compressible and incompressible strips across the system, paying particular attention to the influence of Coulomb interactions on the edge structure.

[1] N. Pascher, C. Rössler, T. Ihn, K. Ensslin, C. Reichl, and W. Wegscheider, arXiv:1309.4918 (2013).

O 87.2 Thu 17:00 P1

**Dirac and Weyl semimetal states in $Na_3Bi$ from first principles** — •Patrick Buhl, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recently, the three-dimensional Dirac semimetal state was theoretically predicted to exist [1] and experimentally observed [2] in bulk $Na_3Bi$. Using first principles methods in combination with the Wannier functions technique [3], we construct and analyze the topological phase diagram of $Na_3Bi$ as a function of spin-orbit strength and external exchange field. In particular we aim at realization of the Weyl semimetal phase in this material. The topological properties are characterized in terms of what computed from ab initio Chern and spin Chern numbers of the Berry curvature flux around the points of band degeneracy. Additionally, we consider finite slabs of $Na_3Bi$ and focus on the electronic structure of the surface states in correlation to the bulk topological phase diagram. Financial support by the HGF-YIG Programme VH-NG-513 is gratefully acknowledged.

[1] Z. Wang *et al.*, Phys. Rev. B **85**, 195320 (2012)
[2] Z.K. Liu *et al.*, arXiv:1310.0391 (2013)
[3] www.flapw.de

O 87.3 Thu 17:00 P1

**Dielectric Function of the Topological Surface States of $Bi_2Se_3$** — •Markus Heinemann, Christian Franz, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University, 35392 Giessen, Germany

We investigate the material system $Bi_2Se_3$ which recently has been discovered to belong to the new class of topological insulators (TI). In this TI, robust surface states located in the insulating band gap of the bulk are protected by time-reversal symmetry and consist of a single Dirac cone at the Γ-point [1]. We use density functional theory to investigate the electronic structure and dielectric function of $Bi_2Se_3$ by first principles. In our calculations we study the bulk material and the Se terminated surface of $Bi_2Se_3$ which we simulate by a slab model and examine the effect of the slab thickness, i.e. the number of atomic layers. The essential effect of spin-orbit-coupling for the topological state and thus on the electronic and dielectric properties is presented by comparing calculations with and without this feature.

[1] H. Zhang, C.-X. Liu, X.-L. Qi, X. Dai, Z. Fang, and S.-C. Zhang, Nature Phys. 5, 438 (2009)

O 87.4 Thu 17:00 P1

**Topological Insulator Nanowires by Chemical Vapour Deposition** — •Piet Schönherr and Thorsten Hesjedal — Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, OX1 3PU, United Kingdom

Topological insulators (TIs) are a new state of quantum matter which insulates in the bulk and conducts on the surface. The study of bulk TIs has been hindered by high conductivity inside the bulk, arising from crystalline defects. Such problems can be tackled through compositional engineering or the synthesis of TI nanomaterials. We combined both approaches in a systematic study of various growth parameters to achieve uniform, high purity nanowires with high substrate coverage.

The highlight of this study is the development of a new growth route for nanowires, based on a $TiO_2$ catalyst rather than the conventional Au. Comparative studies demonstrate that Au significantly contaminates the nanowires, whereas $TiO_2$ stays well separated. Details of the Au and $TiO_2$-catalysed growth mechanism were investigated. For Au it was found that the growth mechanism is vapour-liquid-solid. For $TiO_2$ nanoparticles, in contrast, the growth mechanism can be described in the vapour-solid scheme.

Nanowires of the doped compound $(Bi_{0.78}Sb_{0.22})_2Se_3$ were studied using synchrotron radiation. It was discovered that the material mainly adopts an orthorhombic phase known from $Sb_2Se_3$. The Raman spectrum is reported and matched with the structural information for the first time. Further, a method to control the length and diameter of $Bi_2Se_3$ nanowires through laser-cutting was developed.

O 87.5 Thu 17:00 P1

### Strained HgTe shell on CdTe nanowires grown by Au catalyst MBE

— •Maximilian Kessel, Rebekka Pfeuffer, Claus Schumacher, Hartmut Buhmann, and Laurens W. Molenkamp — Experimental Physics 3, University of Würzburg, Germany

The topological insulator properties of 2D and strained 3D HgTe layers have attracted strong attention over the past years. One interesting question that rose was how the TI state evolves in quasi-one dimensional geometry. Here, we present the first realization of a strained HgTe shell on CdTe nanowires.

Doped GaAs wafers are used as substrates for the nanowire growth in a multi-chamber ultra-high vacuum system. The CdTe growth is seeded by liquid Au/Ga eutectic droplets. For straight, uniform and smooth shaped CdTe wires, a special growth start is performed and the substrate temperature is hold within narrow limits. The wires have a diameter of 30 to 100 nm and grow along the [111]B direction up to a length of 3 $\mu$m. The ensemble of CdTe wires is used as substrate for HgTe molecular beam epitaxy. Shell and core of the nanowires are characterized by electron and X-ray diffraction. The radial heterostructures show strained crystalline structure. Transport characterization measurements on separated radial HgTe/CdTe heterostructures are done at low temperature.

O 87.6 Thu 17:00 P1

### Weak anti-localization in HgTe quantum wire arrays

— •Johannes Ziegler[1], Sabine Weishäupl[1], Christopher Ames[2], Christoph Brüne[2], Hartmut Buhmann[2], Laurens W. Molenkamp[2], and Dieter Weiss[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Physikalisches Institut (EP III), Universität Würzburg, Germany

We present our progress in fabricating quasi-1D quantum wire arrays in inverted HgTe quantum wells, being a 2D topological insulator. These quasi-1D quantum wire arrays were fabricated with widths between 120 nm and 250 nm. Our experiments focus on phase-coherent effects, like weak anti-localization and weak-localization, in both wire arrays and 15 and 40 $\mu$m wide Hall-bars. From these measurements we extract the phase-coherence length $l_\phi$ and the spin-relaxation length $l_{SO}$.

Our work is motivated by a proposal for all-electrical detection of the relative spin-orbit interaction strength $\alpha$ / $\beta$ [1,2], where $\alpha$ is the Rashba and $\beta$ the Dresselhaus spin-orbit parameter. A key requirement for this method is the transition from weak anti-localization (WAL) to weak localization (WL) through 1D confinement. The analysis of these characteristic lengths allows us to check when the suppression of WAL occurs.

[1] M. Scheid *et al.*, Phys. Rev. L **101**, 266401 (2008).

[1] M. Scheid *et al.*, Semicond. Sci. Technol. **24**, 064005 (2009).

O 87.7 Thu 17:00 P1

### Magnetotransport and ac conductivity in 2D and 3D topological insulators

— •Christian Michel and Ewelina M. Hankiewicz — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

We study theoretically Landau level structure and optical selection rules in 2D and 3D TIs. Our focus is to find the features which are specific to the Dirac physics. We show that the optical selection rules are different for the particle-hole symmetric Dirac model in comparison with the particle-hole asymmetric models. We explain the influence of dimensionality on the characteristic features of optical selection rules.

We acknowledge grant HA 5893/4-1 within SPP 1666.

O 87.8 Thu 17:00 P1

### Ferromagnetic contacts on topological insulators: Lithographic realization on strained 3-dimensional HgTe

— •Kalle Bendias, Erwann Bocquillon, Simon Hartinger, Christoph Brüne, Hartmut Buhmann, and Laurens Molenkamp — EP3, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg

Topological insulators are a new class of material with insulating bulk and conducting Dirac-like surface states. These states are associated with spin-momentum locking, which is supposed to lead to numerous applications in spintronics [1].

Here we report on lithographic ways to realize the concept of spin injection and detection into the Dirac-like surface states of the 3-dimensional topological insulator HgTe. We discuss fabrication challenges such as unstrained deposition of ferromagnetic material and the realization of a diffusion barrier on the high temperature-sensitive HgTe material system.

[1]C. Brüne, et. al, Phys. Rev. Lett. 106, 126803 (2011)

O 87.9 Thu 17:00 P1

### Transport properties of the high mobility topological insulator HgTe

— •Jonas Wiedenmann[1], Cornelius Thienel[1], Christopher Ames[1], Christopher Brüne[1], Steffen Wiedmann[2], Hartmut Buhmann[1], and Laurens Molenkamp[1] — [1]Universität Würzburg, Würzburg, Deutschland — [2]Radboud Universität Nijmegen, Nijmegen, Holland

It has been demonstrated recently, that the semimetal HgTe opens a band gap of approximately 20 meV when grown strained on a CdTe substrate and thus becomes a three dimensional topological insulator (3D TI)[1].

We show that it is possible to increase the mobility of the surface states by an order of magnitude, if HgTe is sandwiched between epitaxial layers of HgCdTe. The topological insulator is investigated in transport measurements at low temperatures and magnetic fields up to 30 T. Through the enhanced surface mobilites we are able to observe a Dirac specific quantum hall effect. The experimental data suggest, that it has to be discussed within a two surface model for Dirac fermions.

[1] C. Brüne et al., Phys. Rev. Lett. 106, 126803 (2011)

O 87.10 Thu 17:00 P1

### Heteroepitaxial $Li_2IrO_3$ Thin Films Grown by Pulsed Laser Deposition

— •Marcus Jenderka, Heiko Frenzel, Rüdiger Schmidt-Grund, Marius Grundmann, and Michael Lorenz — Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig. Germany

The layered perovskite oxides $A_2IrO_3$ (A = Na, Li) have been studied in recent years in terms of a physical realization of spin-liquid [1] and topological insulator [2] phases, desired within certain quantum computation proposals. We report on the pulsed laser deposition of heteroepitaxial $Li_2IrO_3$ films on $ZrO_2$:Y(001) single crystalline substrates. As in $Na_2IrO_3$ [3], X-ray diffraction confirms a preferential (001) out-of-plane crystalline orientation with a defined in-plane epitaxial relationship. Resistivity between 35 and 300 K is dominated by a three-dimensional variable range hopping mechanism. Infrared optical transmission from 0 to 1.85 eV, measured by Fourier transform infrared spectroscopy (FTIR), reveals a small optical gap $E_{go} \approx 300$ meV together with a splitting of the $5d$-$t_{2g}$ manifold caused by the interplay of spin-orbit coupling and electronic correlations. By means of infrared spectroscopic ellipsometry, the dielectric function (DF) is presented in the spectral range between 0.03 and 3.50 eV. The calculated absorption coefficient confirms the value for $E_{go}$.

[1] J. Chaloupka *et al.*, Physical Review Letters **105**, 027204 (2010).

[2] H.-S. Kim *et al.*, Physical Review B **87**, 165117 (2013).

[3] M. Jenderka *et al.*, Physical Review B **88**, 045111 (2013).

O 87.11 Thu 17:00 P1

### Epitaxial growth of $LaNiO_3$ and $LaAlO_3$ thin films and multilayers by PLD

— •Haoming Wei, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany

As predicted by recent theoretical study, the superlattices (SLs) consisting of paramagnetic metal $LaNiO_3$ (LNO) and band insulator $LaAlO_3$ (LAO) may exhibit exotic topological phases[1]. We have grown LNO, LAO films and LNO/LAO heterostructures by plused laser deposition (PLD). All the films show good out-of-plane and in-plane crystalline orientation and definite epitaxial relationship. The lattice constant and strain of LNO films could be controlled by adjusting growth conditions. The LNO films have an excellent metallic conductivity and the resistivity is related to strain. The low resistivity is about 300$\mu\Omega$·cm at 300 K, which is low enough for use as an electrode material. The LAO films obtained by interval PLD exhibit terraced surface even when grown at a low temperature. The height of the terraces is about 0.4 nm in accord with the calculated result from XRD pattern. Further, LNO/LAO multilayer structures were fabricated. Atomic force microscopy (AFM) together with reflection high-energy electron diffraction (RHEED) images show that the multilayers have a smooth surface with the root mean square roughness about 3.2 nm.

[1] K. Y. Yang, et al. Physical Review B 84, 201104(R) (2011).

O 87.12 Thu 17:00 P1

**Combined XMCD and STS study of transition metal adatoms adsorbed on the surface of prototypical 3D topological insulators** — •Jonas Warmuth[1], Martin Vondráček[2], Matteo Michiardi[3], Lucas Barreto[3], Cinthia Piamonteze[4], Andreas Eich[1], Alexander Khajetoorians[1], Jian-Li Mi[3], Bo Brummerstedt Iversen[3], Philip Hofmann[3], Jens Wiebe[1], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, Uni Hamburg, Germany — [2]Institute of Physics ASCR, Prague, Czech Republic — [3]iNano, Aarhus University, Denmark — [4]Laboratory of Condensed Matter Physics, PSI, Switzerland

The spin of Dirac electrons in topological surface states is rigidly locked to the direction of their momentum leading, e.g., to prohibited backscattering. Their interaction with magnetic impurities is currently a matter of debate, because it can destroy this effect, heavily depending on the magnetic properties of the impurities. Using x-ray magnetic circular dichroism techniques we investigated 3d transition metal adatoms adsorbed on the surface of different prototypical 3D topological insulators. We compare our results to crystal field multiplet calculations [1] of the 3d states. For some of the adatom species, we find a considerable magnetic anisotropy, which depends crucially on the coupling of their 3d states to the substrate electrons. Furthermore, we investigate the interaction of the adatoms and the Dirac electrons by Fourier-transform scanning tunneling spectroscopy [2], which reveals shifts of the linear dispersion due to surface doping effects.

[1] J. Honolka et al., PRL 108, 256811 (2012)

## O 88: Poster: Spintronics (HL jointly with MA, O)

Time: Thursday 17:00–20:00 Location: P1

O 88.1 Thu 17:00 P1

**Electrical detection of spin Hall effect in semiconductors** — •Markus Ehlert[1], Cheng Song[1,2], Mariusz Ciorga[1], Thomas Hupfauer[1], Martin Utz[1], Dieter Schuh[1], Dominique Bougeard[1], and Dieter Weiss[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [2]Key Laboratory of Advanced Materials, School of Material Science & Engineering, Tsinghua University, Beijing, China

We present different geometries which allow for the all-electrical detection of either direct spin Hall effect (DSHE) or inverse spin Hall effect (ISHE) in semiconductor microstructures. We describe our experimental methods and compare results to previous experiments and theory. In our DSHE experiments a spin-unpolarized charge current flows through a $n$-GaAs channel and induces, due to DSHE, a transverse spin current. Hence, spins accumulate at the boundaries of the channel and are detected by spin-sensitive Esaki diodes [1]. For ISHE experiments in $p$-GaAs we used spin-injecting contacts to generate a spin current, which, via ISHE, should lead to a measurable charge imbalance in a Hall bar geometry. Another ISHE device consists of the so-called H-bar geometry, where an electric current is driven in one leg of an H-shaped structure. This generates, due to DSHE, a transverse spin current, which flows along the connection between both legs of the "H". By means of ISHE a charge imbalance is then induced in the second leg of the "H" [2].

[1] M. Ehlert *et al.*, Phys. Rev. B **86**, 205204 (2012).

[2] M. Ehlert *et al.*, Phys. Status Solidi B (2013) (acc.).

O 88.2 Thu 17:00 P1

**Spin blockade effects in a GaMnAs double quantum dot system** — Stefan Geissler[1], •Sebastian Pfaller[2], Andrea Donarini[2], Milena Grifoni[2], and Dieter Weiss[1] — [1]Institute for Exp. and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Spin polarized transport measurements of a double quantum dot defined in a GaMnAs nano constriction are presented. In the experimental setup, the polarization of the leads as well as of the quantum dot system can be controlled by an external magnetic field. In presence of a magnetic field, differential conductance measurements show a gap opening in the charge stability diagrams, that can be explained by spin blockade effects. Transport calculations of metallic quantum double dots coupled to spin polarized leads show excellent agreement with experimental data.

O 88.3 Thu 17:00 P1

**Exciton dynamics in transition metal dichalcogenides** — •Igor Libman, Hendrik Kuhn, Jan G. Lonnemann, Julia Wiegand, Michael Oestreich, and Jens Hübner — Institute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

Among the newly emerging two-dimensional transition metal dichalcogenides molybdenum disulfide ($MoS_2$) has attracted an increasing attention as promising material for transport, optical and spintronic applications [1]. A contrasting key feature to the ubiquitous mono- and bilayer graphene is the easily accessible direct optical band gap of single layer $MoS_2$ [2]. Furthermore, the two-component nature breaks the inversion symmetry [3] and leads jointly with spin-orbit interaction to a copious number of spin-optoelectronic effects. Here, we present a scheme for the investigation of the complex dynamics of A and B excitons and their excited states (A' and B') in single layer $MoS_2$ [4] by ultrafast two-color time-resolved laser spectroscopy with focus on distinct impact of the electron-phonon interaction [5] onto the spectral shape of the s- and p-equivalent excitons states.

[1] Q. H. Wang *et al.*, Nature Nanotech. **7**, 11 (2012).

[2] Andrea Splendiani *et al.*, Nano Lett., **10**, 1271 (2010).

[3] G. Sallen *et al.*, Phys. Rev. B, **86**, 081301(R) (2012).

[4] Diana Y. *et al.*, Phys. Rev. Lett, **111**, 216805 (2013).

[5] A. Marini, Phys. Rev. Lett. **101**, 106405 (2008).

O 88.4 Thu 17:00 P1

**Spin dynamics in quantum wells under surface acoustic waves** — •Johannes Wanner[1], Cosimo Gorini[2], Peter Schwab[1], and Ulrich Eckern[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Service de Physique de l'Etat Condensé, CEA-Saclay, 91191 Gif sur Yvette, France

Various recent experiments have shown the flexibility of surface acoustic waves (SAW) as a mean for transporting charge and spin in quantum wells [1]. In particular, SAW have proven highly effective for the coherent transport of spin-polarized wave packets, suggesting their potential in spintronics applications. Motivated by these experimental observations we have theoretically studied the spin and charge dynamics in a quantum well under surface acoustic waves. Based on previous work by some of us [2], we show that the dynamics acquires a simple and transparent form in a reference frame co-moving with the SAW. The observed values for spin relaxation and precession length can thus be explained.

[1] H. Sanada et. al., Phys. Rev. Lett. **106**, 216602 (2011); O. Couto et. al., Phys. Rev. B **78**, 153305 (2008)

[2] P. Schwab et al., Phys. Rev. B **74**, 155316 (2006)

O 88.5 Thu 17:00 P1

**Electron spin control in Manganese doped GaAs/AlAs nanostructures** — •Markus Kuhnert[1], Ilya A. Akimov[1], Vladimir L. Korenev[2], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]2A.F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

The field of spintronics, which in contrast to electronics, uses the spin instead of charge as information carrier, presents many interesting possibilities. For proper implementation of spintronic devices, research of adequate materials and methods is required. Here we present the results of our research into Manganese doped GaAs/AlAs quantum wells, which might offer long lived spin coherence as well as spin manipulation mediated by the magnetic Manganese ions. We use pump-probe Kerr effect measurement techniques and time resolved photoluminescence measurements to investigate properties such as spin coherence and spin lifetime of the Mn doped nanostructures. The temperatures at the time of measurement range from 2K to 8K. Further studies are done on optically induced EPR of the Mn ions by applying a microwave modulation to the excitation laser beam. Exchange interaction between the Manganese ions and electrons in the quantum well might function as a channel for spin manipulation or conservation.

O 88.6 Thu 17:00 P1

**Coherence Properties of Nitrogen Vacancy Centers in Nano Diamond** — •Bernd Sontheimer, Niko Nikolay, Max Strauss, Andreas W. Schell, Janik Wolters, and Oliver Benson — Humbold Universität zu Berlin, Institut für Physik AG Nano-Optik, Newtonstr. 15, 12489 Berlin

The nitrogen vacancy (NV) center in diamond is a stable single photon emitter, combining optical transitions with a long-lived electronic spin with excellent coherence properties [1]. NV centers in nano diamonds are of special interest due to their integrability in photonic hybrid devices [2]. In our research we examine the coherence properties of nano diamonds based on optically detected magnetic resonance (ODMR) [3]. In particular the influence of surface treatments on the $T_2$ time is examined via spin-echo experiments [4]. Also a change of spectral diffusion is determined using correlation interferometry.

[1] G. Balasubramanian, et al., Ultralong spin coherence time in isotopically engineered diamond. Nat. Mater. 8, 383 (2009).

[2] J. Wolters, et al., Enhancement of the zero phonon line emission from a single nitrogen vacancy center in a nanodiamond via coupling to a photonic crystal cavity. Appl. Phys. Lett. 97, 141108 (2010).

[3] J. Wolters, et al., Measurement of the Ultrafast Spectral Diffusion of the Optical Transition of Nitrogen Vacancy Centers in Nano-Size Diamond Using Correlation Interferometry. Phys. Rev. Lett. 110, 027401 (2013).

[4] F. Jelezko, et al., Observation of Coherent Oscillations in a Single Electron Spin. Phys. Rev. Lett. 92, 076401 (2004).

O 88.7 Thu 17:00 P1

**Magnetic susceptibility of 2 dimensional electron gases with Rashba spin-orbit coupling** — •Christiane Scholl, Tobias Hartenstein, and Hans Christian Schneider — TU Kaiserslautern

The transverse spin-spin correlation, or dynamical magnetic susceptibility, is an important quantity both from the experimental and theoretcial point of view. It determines light-scattering and spin noise spectra, as well as the dispersions of elementary excitations of the magnetic type, such as magnons or magneto-magnons. Here, we consider a two-dimensional electron gas including Rashba spin-orbit coupling and Coulomb interaction. We use a decoupling scheme to derive the equations of motion for the relevant Green functions. Approximating the full Coulomb matrix element by a local interaction U, a closed expression for the dynamic transverse magnetic susceptibility results, which we analyze numerically. We find a complex interplay of internal effective Rashba fields with the external magnetic field. Further, the elementary "magnetic" excitations arise from resonances of the magnetic suscpetibility that are very different from plasmon resonances [1,2] with Rashba spin-orbit coupling or magneto-magnon [3] resonances.

[1] M. Pletyukhov, V. Gritsev, Phys. Rev. B 74, 045307 (2006).

[2] S. M. Badalyan, A. Matos-Abiague, G. Vignale, and J. Fabian, Phys. Rev. B 79, 205305 (2009.)

[3] D. M. Edwards, J. Phys. C. 2, 84 (1969).

## O 89: Annual General Meeting of the Surface Science Division

Time: Thursday 19:30–20:00 Location: TRE Phy

**Report of the Chairman; Election; Presentation of the Gerhard Ertl Young Investigator Award; Miscellaneous**

## O 90: Post-Deadline Session

Time: Thursday 20:00–21:00 Location: TRE Phy

**Contributed Post-Deadline Talks**

## O 91: Invited Talk (Andrey Turchanin)

Time: Friday 9:30–10:15 Location: TRE Phy

**Invited Talk** O 91.1 Fri 9:30 TRE Phy

**From organic monolayers to free-standing 2D carbon materials: Carbon nanomembranes, graphene and their heterostructures** — •Andrey Turchanin — Faculty of Physics, University of Bielefeld

In this talk it will be demonstrated how monolayers of aromatic molecules can be employed to engineer novel free-standing 2D carbon materials. By electron or photon irradiation, aromatic monolayers are converted into dielectric carbon nanomembranes (CNMs) with a thickness of one molecule, which can be tuned from about 0.5 to 3 nm. CNMs possess high mechanical stability and similar to graphene or other atomically thin 2D materials (e.g., hBN, MoS2) can be separated from their original substrates and transferred onto various other substrates, fabricated as suspended sheets or stacked into multilayer films with precise control over their thickness. By annealing CNMs are converted into graphene. This approach enables both scalable productions of graphene and direct writing of CNM or graphene micro and nanostructures employing e-beam or extreme UV lithography. Layer-by-layer assembly of vertical CNM/graphene heterostructures opens many doors to the engineering of novel materials with tunable electronic, optical and chemical properties. Their characterization by complementary spectroscopy, microscopy, electric and magnetoelectric transport measurements as well as implementation in novel field-effect devices will be presented.

# O 92: Symposium One-dimentional Metals: Reality or Fiction (DS jointly with HL, O, TT)

Time: Friday 9:30–12:30 Location: HSZ 02

**Invited Talk** O 92.1 Fri 9:30 HSZ 02

**Atomic-scale dopant wires for quantum computer architectures** — •Michelle Y Simmons — Centre of Excellence for Quantum Computation and Communication Technology, University of New South Wales, Sydney, NSW 2052, Australia

Down-scaling has been the leading paradigm of the semiconductor industry since the invention of the first transistor in 1947. As silicon electronics approaches the atomic scale, interconnects and circuitry become comparable in size to the active device components. Maintaining low electrical resistivity at this scale is challenging because of the presence of confining surfaces and interfaces. We report on the fabrication of wires in silicon-only one atom tall and four atoms wide-with exceptionally low resistivity ˜ 0.3 milliohm-centimeters. By embedding phosphorus atoms within a silicon crystal with an average spacing of less than 1 nanometer we achieved a diameter-independent resistivity [1]. Atomistic tight-binding calculations confirm the low resistivity of these atomic-scale wires [2], which pave the way for single-atom device architectures for both classical and quantum information processing. I will demonstrate how we have incorporated these wires into single atom transistors [3] and performed single-shot spin read-out of precisely-positioned P donor electron spins as potential qubits in Si [4].

[1] B. Weber et al., Science 335, 6064 (2012). [2] H. Ryu et al., Nanoscale 5, 8666 (2013). [3] M. Fuechsle et al., Nature Nanotechnology 7, 242 (2012). [4] H. Buch et al., Nature Communications 4, 2017 (2011).

**Invited Talk** O 92.2 Fri 10:10 HSZ 02

**$1+\delta$: Tuning the Dimensionality of Organic Conductors** — •Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart

Organic charge-transfer salts are prime candidates for tuning the dimension by applying pressure. Strictly one-dimensional systems, such as the Fabre salts $(\mathrm{TMTTF})_2X$, are Mott insulators that undergo a deconfinement transition towards a Luttinger liquid and eventually a two-dimensional Fermi liquid if the interchain interaction increases with pressure. The deconfinement transition can be identified when the transverse hopping integral $2t_\perp = \Delta_\rho$, the Mott gap. Ab-initio density functional theory allows us to study the influence of temperature and pressure on the electronic band structure.

Quasi-one-dimensional organic conductors, like the Bechgaard salts $(\mathrm{TMTSF})_2X$, exhibit a cross-over from a Luttinger liquid to a Fermi liquid behavior upon cooling and application of external pressure. Frequency and temperature dependent transport measurement yield a change in power-laws and Luttinger exponent.

Often the metallic phase is not stable in reduced dimensions: at low temperatures the electronic charges and spins tend to arrange themselves in an orderly fashion due to relatively strong correlations. There are a growing number of molecular materials where electronic degrees of freedom and electronic interactions are directly responsible for electric polarization and ferroelectric transition, termed electronic ferroelectricity. Recently, it was discovered that charge order not only produces ferroelectricity but also breaks the symmetry of the magnetic degree of freedom in organic quantum spin chains.

**Coffee break (20 min)**

**Invited Talk** O 92.3 Fri 11:10 HSZ 02

**Spectral and transport properties of one-dimensional correlated electrons** — •Volker Meden — Institut für Theorie der Statistischen Physik, RWTH Aachen University

Two-particle interactions strongly alter the low-energy physics of electrons confined to one spatial dimension. Excitations cannot be described by fermionic quasi-particles. Metallic systems of this type fall into the Luttinger liquid universality class and are characterized by power-law decay of correlation functions. I will give an overview over the one-particle spectral and transport properties of such systems including a discussion of the model dependent low-energy scale beyond which Luttinger liquid power laws are observable. Leaving the framework of equilibrium physics I will report on recent progress in understanding the non-equilibrium steady state as well as relaxation dynamics of isolated and contacted quantum wires.

**Invited Talk** O 92.4 Fri 11:50 HSZ 02

**Atomic nanowires on surfaces: Spectroscopic reality versus theoretical fiction** — •Ralph Claessen — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Solids with electrons confined to only one spatial dimension are predicted to behave quite different from conventional metals. Many-body theory finds that electronic interactions may lead to Peierls-type instabilities or even a breakdown of Landau's quasiparticle picture, which works so well in higher dimensions. Atomic nanowires formed by self-organized growth of metal atoms on suitable semiconductor surfaces can be viewed as closest approach to perfect 1D electron confinement, and therefore serve well as model systems for experimental tests of the expected 1D physics. In my presentation I will discuss current experiments on atomic nanowires, using photoelectron spectroscopy and scanning tunneling microscopy as experimental probes, and compare the results to corresponding theoretical predictions. Examples include the observation of Tomonaga-Luttinger behavior as well as the possible detection of (quasi-)1D antiferromagnetic order.

# O 93: Topological Insulators (MA jointly with DS, HL, O, TT)

Time: Friday 9:30–12:00 Location: HSZ 04

O 93.1 Fri 9:30 HSZ 04

**Experimental characterization and simulation of quasi-particle-interference in the Bi-bilayer topological insulator** — •Matteo Michiardi[1], Andreas Eich[2], Gustav Bihlmayer[3], Alex A. Khajetoorians[2], Jens Wiebe[2], Jianli Mi[4], Bo B. Iversen[4], Philip Hofmann[1], and Roland Wiesendanger[2] — [1]Department of physics and astronomy, Aarhus University, Denmark — [2]Institute of Applied Physics, University of Hamburg, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [4]Center for Materials Crystallography, Aarhus University, Denmark

Topological insulators (TI) are a new class of materials that host gapless surface states with spin helicity. While several 3D TIs have been discovered, the interest in 2D TI systems that can host topological edge state is rising. A single bilayer of bismuth is predicted to be such a 2D TI. Here we present an experimental and theoretical study of a Bi-bilayer grown on 3D TI $\mathrm{Bi_2Se_3}$. The use of $\mathrm{Bi_2Se_3}$ as substrate allows the epitaxial growth of the bilayer in the rhombohedral structure, as shown by Scanning Tunnelling Microscopy. We calculate the band structure of the Bi-bilayer/$\mathrm{Bi_2Se_3}$ system by Density Function Theory (DFT) and experimentally study the quasi particle interference (QPI) on the bilayer. In order to clarify the scattering channels responsible for the QPI, we perform simulations based on the Joint Density of States method starting from our DFT calculations. The comparison with the experimental results reveals a good match for a wide range of binding energies for both occupied and unoccupied states.

O 93.2 Fri 9:45 HSZ 04

**Quasiparticle self-consistent *GW* study of bismuth under strain** — •Irene Aguilera, Christoph Friedrich, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

It has been recently claimed on the basis of ARPES measurements that bulk bismuth is a topological semimetal. The discrepancies between this result and previous *ab-initio* calculations were attributed to the failure of density functional theory (DFT) in the prediction of band gaps, because the topological or trivial character of Bi depends only on the "sign" of the very small direct band gap at the L point. We show that bulk Bi is indeed predicted by DFT in the local-density approximation (LDA) to be a trivial semimetal, with a surprisingly overestimated gap at L. We have performed quasiparticle self-consistent *GW* (QS*GW*) calculations for bulk bismuth that support its trivial character. The QS*GW* gap at L as well as the energy overlap between the electron and hole pockets are in much better agreement with experiments than the LDA ones. Thus, the QS*GW* approach appears as the right tool to study the trivial-to-topological transition that Bi experiences under stress, as a result of a change of sign of the gap at L. We have analyzed the effect of strain on the topological properties of bulk Bi. Whereas LDA predicts that an impractical stress is needed for such a transition, QS*GW* shows that bulk Bi becomes a topological semimetal already under very small stress. This work is supported by the Helmholtz Virtual Institute for Topological Insulators (VITI).

O 93.3 Fri 10:00 HSZ 04

**Combined STM/STS- and ARPES-investigation of the quaternary Topological Insulator $\mathbf{Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}}$** — •Thomas Bathon[1], Felix Reis[1], Christoph Seibel[2], Hendrik Bentmann[2], Paolo Sessi[1], Friedrich Reinert[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We present a combined scanning tunneling microscopy/spectroscopy (STM/STS) and angular-resolved photoemission spectroscopy (ARPES) characterization of the electronic properties of the quaternary compound $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$. ARPES-data evidence that this compound is still a Topological Insulator (TI) with a single Dirac cone, which is characteristic for the $Bi_2X_3$-class. The topological properties of the surface state, i.e. forbidden backscattering, have been confirmed by Fourier-transformed differential conductance ($dI/dU$) maps. Measurements performed both above and below the Fermi level allow us to determine the energy dispersion relation, the carrier velocity, and—by extrapolation to zero momentum—the position of the Dirac point. The observed scattering vectors are not as well-defined as those observed in binary compounds, probably due to substitutional disorder which results in a spatial fluctuation of the chemical potential. Our investigations illustrate how the properties of the well-known TI $Bi_2Te_3$ can be changed by chemical substitution.

O 93.4 Fri 10:15 HSZ 04

**Surface and bulk contributions to the electronic structure of the topological insulator $\mathbf{Sb_2Te_3(0001)}$** — •Christoph Seibel[1,2], Hendrik Bentmann[1,2], Henriette Maass[1,2], Jürgen Braun[3], Jan Minár[3], Kenya Shimada[4], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe — [3]Department Chemie, Physikalische Chemie, Universität München, Butenandtstraße 5-13, D-81377 München — [4]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

Photon energy dependent angle-resolved photoemission measurements were performed to disentangle surface and bulk contributions to the electronic structure of the 3D topological insulator (TI) $Sb_2Te_3$. We discover a penetration of the topological surface state (TSS) into the bulk valence band regime where it coexists with bulk states without considerable hybridization. Our results indicate an emerging $k_\perp$-dispersion of the TSS at higher binding energies, which we attribute to an increasing bulk character. These observations deviate from previous findings for the isostructural TIs $Bi_2Se_3$ and $Bi_2Te_3$. Our results are supported by fully relativistic one-step photoemission calculations. [1] Seibel *et al.* PRB 86, 161105(R) (2012)

**15 min. break**

O 93.5 Fri 10:45 HSZ 04

**Spin-dependent unoccupied electronic structure of the topological insulator $\mathbf{Sb_2Te_3}$** — •Anna Zumbülte[1], Anke B. Schmidt[1], Markus Donath[1], Peter Krüger[2], Gregor Mussler[3], and Detlev Grützmacher[3] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

Studies on three-dimensional topological insulators focus mainly on the well-known systems of $Bi_2Se_3$ and $Bi_2Te_3$ and the related ternary compounds. Theoretical predictions of chalcogenides as topological insulators with a single Dirac cone [1] include an additional compound, $Sb_2Te_3$. There, due to p-type doping of the available samples, the Dirac point lies above the Fermi level, making it inaccessible to photoemission experiments unless the surface is modified with an adsorbate [2]. Consequently, the electronic structure of this system has been left almost unstudied.

We present spin- and angle-resolved inverse-photoemission measurements of the unoccupied electronic states of $Sb_2Te_3$. In addition to the Dirac state, further spin-dependent features have been obtained which show a distinct Rashba splitting. The experimental data will be discussed along with bandstructure calculations.

[1] H. Zhang *et al.*, Nat. Phys. **5**, 438 (2009)

[2] C. Seibel *et al.*, Phys. Rev. B **86**, 161105 (2012)

O 93.6 Fri 11:00 HSZ 04

**Comparitive study of the ternary topological insulators $\mathbf{Bi_2Se_2Te}$ and $\mathbf{Bi_2Te_2Se}$** — •Felix Reis[1], Thomas Bathon[1], Christoph Seibel[2], Hendrik Bentmann[2], Paolo Sessi[1], Friedrich Reinert[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The 3D topological insulators $Bi_2Se_2Te$ and $Bi_2Te_2Se$ have been investigated by combining the complementary experimental techniques scanning tunneling microscopy (STM/STS) and angular-resolved photoemission spectroscopy (ARPES). With low temperature STM/STS technique we investigate the structural and electronic properties of both systems. Fourier-transformed quasi-particle interference (QPI) maps give access to the scattering events within the topological surface state. Taking QPI maps for several energies allows us to obtain information on the position of the Dirac point and the carrier velocity by fitting the linear energy dispersion relation of the Dirac fermions. These results will be compared with the band structure as obtained by ARPES measurements.

O 93.7 Fri 11:15 HSZ 04

**A large-energy-gap oxide topological insulator based on the superconductor BaBiO3** — •Binghai Yan[1,2,3], Martin Jansen[1], and Claudia Felser[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden — [3]Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg University of Mainz, 55099 Mainz

Topological insulators are a new class of quantum materials that are characterized by robust topological surface states (TSSs) inside the bulk-insulating gap, which hold great potential for applications in quantum information and spintronics as well as thermoelectrics. One major obstacle is the relatively small size of the bulk bandgap, which is typically around 0.3eV for the known topological insulator materials. Here we demonstrate through ab initio calculations that a known superconductor BaBiO3 (BBO) with a Tc of nearly 30 K emerges as a topological insulator in the electron-doped region. BBO exhibits a large topological energy gap of 0.7 eV, inside which a Dirac type of TSSs exists. As the first oxide topological insulator, BBO is naturally stable against surface oxidization and degradation, distinct from chalcogenide topological insulators. An extra advantage of BBO lies in its ability to serve as an interface between TSSs and superconductors to realize Majorana fermions for future applications in quantum computation.

Reference: B. Yan, M. Jansen, C. Feler, Nature Physics 9, 709*711 (2013) (arXiv:1308.2303).

O 93.8 Fri 11:30 HSZ 04

**Topological surface states of HgTe and Heulser compounds** — •Shu-Chun Wu[1], Binghai Yan[1,2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany. — [2]Max Planck Institute for Physics of Complex Systems, Dresden, Germany.

We studied the topological electronic structures of HgTe and half Heusler compounds (e.g.: $XYZ$, $X$ = rare earth elements, $Y$ = trasition metal and $Z$ = main group elements) by both *ab initio* calculations. The topological surface structures were investigated by the Wannier function based tight-binding method. The effects of external strains induced from the substrate and surface terminations are taken into account by the atomic positions. Our results agree well with recent photoemission experiments.

O 93.9 Fri 11:45 HSZ 04

**Sputter Deposition of Half-Heusler Topological Insulators** — •Benedikt Ernst, Daniel Ebke, Stanislav Chadov, Gerhard Fecher, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

Heusler compounds have exhibited manifold physical properties in the recent years and attracted a lot of interest in the field of spintronic applications due to their half-metallic properties. Recently, a topological insulating state has been predicted by theory for some of these compounds.

In this work, we have prepared Heusler materials such as LaPdBi and LaPtBi for which a topological insulating behavior was predicted. Co-deposition by DC- and RF magnetron sputtering was used to prepare corresponding thin films. To realize an epitaxial film growth in the crystallographic C1$_b$ structure on MgO-substrates, a buffer layer was applied and optimized. Initial transport properties will be discussed with regard to the film composition and the crystallographic properties.

## O 94: Graphene: Bi- and Multi-Layers (HL jointly with MA, O, TT)

Time: Friday 9:30–11:00 Location: POT 081

O 94.1 Fri 9:30 POT 081

**Atomistic simulations of dislocations in bilayer graphene** — •Konstantin Weber[1], Christian Dolle[2], Florian Niekiel[2], Benjamin Butz[2], Erdmann Spieker[2], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Center for Nanoanalysis and Electron Microscopy, FAU Erlangen-Nürnberg

The atomic structure and the properties of basal-plane dislocations in bilayer graphene, the thinnest imaginable crystal that can host such 1D defects, has been investigated by atomistic simulations based on the registry-dependent potential of Kolmogorov and Crespi [1] and the classical AIREBO potential.

Our calculations show that the dislocations lead to a pronounced buckling of the graphene bilayers in order to release strain energy, leading to a complete delocalization of the residual compressive/tensile strain in the two graphene sheets [2]. Furthermore, the absence of a stacking-fault energy, a unique peculiarity of bilayer graphene, gives rise to a splitting of the dislocations into equidistant partials with alternating Burgers vectors [2]. Thus, dislocations in bilayer graphene show a distinctly different behavior than corresponding dislocations in graphite or other 3D crystals.

[1] A. Kolmogorov, V. Crespi, *Phys. Rev. B* **71**, 235415 (2005).

[2] B.Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H.B. Weber, B. Meyer, E. Spieker, *Nature*, (2013) (accepted for publication).

O 94.2 Fri 9:45 POT 081

**Study of the magnetoresistance of biased graphene bilayers** — •Dmitri Smirnov[1], Galina Y. Vasileva[1,2], Yurij B. Vasilyev[2], Pavel S. Alekseev[2], Yurij L. Ivanov[2], Hennrik Schmidt[1], Alexander W. Heine[1], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Ioffe Physical Technical Institute, Russian Academy of Sciences, St. Petersburg

We demonstrate magnetotransport behaviour of bilayer graphene. In contrast to monolayer graphene, bilayer has a parabolic band structure with a zero band gap, which can be opened by applying an electrical field perpendicular to the samples [1]. One of the consequences of such a band structure is the coexistence of two different types of charge carriers with the Fermi energy placed near the charge neutrality point.

Several bilayer graphene samples with different electrical properties (charge neutrality point, mobility) have been investigated. A positive and negative magnetoresistance is observed for electrons and holes. We can show that that the positive magnetotransport can be described well with a two carrier Drude model which allows us a new approach to probe parameters of electrons and holes separately.

[1] McCann, E., and V. Fal'ko Phys. Rev. Lett. 96, 086805 (2006)

O 94.3 Fri 10:00 POT 081

**Transport in Dual Gated Encapsulated Bilayer Graphene** — •Jonas Hesselmann[1], Stephan Engels[1,2], Bernat Terrés[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

Bilayer graphene (BLG) is a promising material which combines superior electronic properties like high charge carrier mobilities with the possibility of opening a band gap. The band gap can be induced by applying a perpendicular electric field resulting in a gap in the order of a few 10 meV. This makes BLG a possible candidate for future nanoelectronic applications. Here, we present the fabrication and low temperature (T=2K) transport measurements of dual gated BLG which is encapsulated in hexagonal boron nitride serving as an atomically flat gate dielectric. We show that the investigated devices exhibit mobilities of up to 80.000 cm$^2$/Vs. Quantum Hall effect measurements show a distinct sequence of Hall plateaus together with a full symmetry breaking of the eightfold degenerate zero Landau level. By temperature dependent measurements we investigate the energy gap opening as function of a perpendicular electric field. We find that the transport via localized states at low temperatures exhibits a strong asymmetric behavior with respect to the sign of the applied electric field while the temperature activated transport is fully symmetric.

O 94.4 Fri 10:15 POT 081

**An emergent momentum scale and low energy theory for the graphene twist bilayer.** — •Sam Shallcross, Nicolas Ray, Dominik Weckbecker, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

We identify an angle dependent *momentum scale* as the fundamental property of a bilayer composed of mutually rotated graphene layers [1]. This leads to (i) a numerical method that increases, for the twist bilayer, the efficiency of the standard tight-binding method by a factor of $\approx 10^3$, at no loss of accuracy, and (ii) a low energy theory that can be deployed, without distinction, for both the low angle regime and the large angle regime. In the low angle regime this leads to a theory that is close to that of Bistritzer *et al.* [2], but differs in the choice of momentum scale. In the large angle this approach yields electronic versions of the Hamiltonians first derived on symmetry grounds by Mele [3]. We use these low energy approaches to give an overview of the $T = 0$ electronic properties of the twist bilayer system, with a particular focus on the localization of electrons, mixing of single layer graphene states by the interaction, and low energy density of states features.

[1] S. Shallcross, S. Sharma, and O. Pankratov, *Phys. Rev. B* **87**, 245403, 2012.

[2] R. Bistritzer and A. H. MacDonald. *Proc. Natl Acad. Sci.*, **108:12233**, 2010.

[3] E. J. Mele. *Journal of Physics D Applied Physics*, **45:154004**, 2012.

O 94.5 Fri 10:30 POT 081

**RKKY interaction in the AB stacked graphene bilayer: interstitial impurities and a diverging propagator.** — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

The interaction between spin polarised impurities in graphene displays a number of novel features that arise both from the valley degree of freedom that graphene possesses, as well as the linearly vanishing density of states at the Dirac point [1,2]. Multilayer graphene systems offer both the possibility of realistic interstitial (i.e., interlayer) impurities, as well as novel electronic features. In particular, the Bernal stacked (AB) bilayer exhibits low energy (chiral) bands as well as high energy bonding and anti-bonding bands. We demonstrate that at the bonding to anti-bonding *gap edge* there is an logarithmic divergence $\log(E - E_g)$ in the propagator on one sublattice, with $E$ the energy and $E_g$ the energy of the bonding to anti-bonding gap (0.38 eV). This leads to a number of dramatic consequences for the RKKY interac-

tion, most notably: (i) a $R^{-5/2}$ impurity interaction at the gap edge, and, (ii) for interstitial impurities a discontinuous change in the Fermi surface spanning vector that drives the RKKY at the gap edge. We further derive the finite temperature behaviour of this system on the basis of finite temperature perturbation theory.
[1] M.Sherafati, and S.Satpathy, Phys. Rev. B 84, 125416, 2011.
[2] F.Parhizgar, and M.Sherafati, and R.Asgari, and S.Satpathy, Phys. Rev. B 87, 165429, 2013.

O 94.6 Fri 10:45 POT 081

**Conductivity of two-dimensional charge carriers with non-parabolic dispersion** — Bretislav Sopik[1], Janik Kailasvuori[2,3], and •Maxim Trushin[4] — [1]Central European Institute of Technology, Masaryk University, Kamenice 735, 62500 Brno, Czech Republic — [2]International Institute of Physics, Universidade Federal do Rio Grande do Norte, 59078-400 Natal-RN, Brazil — [3]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [4]University of Konstanz, Fachbereich Physik, M703 D-78457 Konstanz

We investigate the conductivity of two-dimensional charge carriers with the non-parabolic dispersion $k^N$ with $N$ being an arbitrary natural number assuming the delta-shaped scattering potential as a major source of disorder. We employ the exact solution of the Lippmann-Schwinger equation to derive an analytical Boltzmann conductivity formula valid for an arbitrary scattering potential strength. We proceed further with a numerical study based on the finite size Kubo formula which assesses the applicability range of our analytical model. We find that for any $N > 1$, the conductivity demonstrates a linear dependence on the carrier concentration in the limit of a strong scattering potential strength. This finding agrees with the conductivity measurements performed recently on chirally stacked multilayer graphene [1] where the lowest two bands are non-parabolic and the adsorbed hydrocarbons might act as strong short-range scatterers.

[1] L. Zhang, Y. Zhang, J. Camacho, M. Khodas I. Zaliznyak, Nature Physics **7**, 953-957 (2011).

## O 95: Micro- and Nanopatterning (DS jointly with O)

Time: Friday 9:30–11:15 Location: CHE 89

O 95.1 Fri 9:30 CHE 89

**Effect of periodic pre-patterned structures on ripple wavelength and propagation velocity on ion-irradiated surfaces** — •Detlef Kramczynski[1], Bernhard Reuscher[2], and Hubert Gnaser[1,2] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institute for Surface and Thin-Film Analysis (IFOS), 67663 Kaiserslautern, Germany

Glass surfaces were patterned by milling periodic trench structures with wavelengths from 150 to 750 nm in a focused ion beam (FIB) system. Upon exposure to 30 keV Ga$^+$ ion irradiation under an incidence angle of 52° with respect to the surface normal, these patterns were found to transform into "ripple"-like nanostructures. Their evolution was monitored in situ for ion fluences up to $2.5 \times 10^{18}$ Ga$^+$ ions/cm$^2$ using the scanning electron microscope incorporated in the FIB. With increasing fluence, the wavelengths of the ripples were found to stay constant (and equal to their original feature size) while they propagate across the surface, in a direction which coincides with the projection of the ion beam's incident direction onto the surface. The propagation velocity was determined to scale inversely proportional to the wavelength, being in the range (60-100) nm/($10^{17}$ ions/cm$^2$). On pristine surface areas (which had not been pre-patterned) ripples were also formed by ion bombardment. However, their wavelength was found to increase with ion fluence from initially ~250 nm to ~420 nm.

O 95.2 Fri 9:45 CHE 89

**structural evolution upon thermal annealing for Fe ion irradiated Si(100)** — •behnam khanbabaee[1], jörg grenzer[2], stefan facsko facsko[2], and ullrich pietsch[1] — [1]Universität Siegen, Festkörperphysik,Siegen, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

Off-normal irradiation of Si(100) by Fe ions leads to the surface patterning. In order to understand the mechanism of pattern formation, chemical reactions between Fe and Si atoms have to be considered to influence the surface instability required for pattern formation. Since the as-irradiated surface area is amorphous, we examined the recrystallization process of the Fe-Si layer formed by off-normal 20 keV irradiation using a Si(100) substrate comparing the effect of low (1*10ˆ16 ions/cmˆ2) and high (5*10ˆ17 ions/cmˆ2) fluencies, where only the higher fluence leads to patterned surface. The samples were annealed up to a temperature of 800°C and characterized by in-situ grazing incidence X-ray diffraction (GI-XRD). Depth profiling by GI-XRD confirmed that $\epsilon$-FeSi was formed close to the surface changing to a $\beta$-FeSi2 phase with lower Fe content at larger depths. While the polycrystalline $\beta$-FeSi2 phase dominates for higher ion fluencies, a nearly equal ratio between $\epsilon$-FeSi and $\beta$-FeSi2 is found for lower ones. Our results suggest that phase distribution is related to the Fe concentration profile and can be considered as the relevant factor in the process of pattern formation.

O 95.3 Fri 10:00 CHE 89

**Nano-structured surfaces produced by low energy ion beam sputtering of amorphous Fe$_x$Si$_{1-x}$ films** — •Kun Zhang, Christoph Brüsewitz, and Hans Hofsäss — II. Physikalisches Institut, Universität Göttingen, Göttingen, Germany

It is well known that metallic surfactants induce pronounced dot and ripple patterns on Si substrate surfaces during normal ion incidence sputter erosion. These surfactant atoms are co-deposited on the substrate surface either from intentional co-deposition or inadvertently contaminations from sputtering of the vacuum chamber walls. In the present contribution we investigate the pattern formation on amorphous Fe$_x$Si$_{1-x}$ thin films with different Fe atomic fraction x, irradiated with Xe ions of 5 keV and 10 keV energies and normal incidence. In this situation the Fe atoms work as surfactants, but are supplied from the bulk of the substrate. The resulting surface morphologies were examined ex-situ by AFM, while the Fe concentration and its depth profile were determined with RBS and high resolution RBS. Nanopattern forms on the substrates with x = 0.02 - 0.08. In this case Fe atoms accumulate in the surface near region ( 13 nm in depth) after ion irradiation, revealing a phase separation towards a FeSi2 phase. For the samples with x >0.09, the average Fe concentration near the surface exceeds x=0.33 and the surface remains flat. For x <0.02 no pattern formation occurs. The results give further evidence of phase separation as a major drive force for surfactant induced the pattern formation.

O 95.4 Fri 10:15 CHE 89

**Redeposition during ion-beam erosion can stabilize well-ordered nanostructures** — •Christian Diddens and Stefan J. Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster

We investigate the redeposition effect, i.e. the reattachment of eroded particles on the surface, in the context of self-organized pattern formation on semiconductor targets during ion-beam erosion. Within the framework of a continuum model for this non-local, inherently complicated process, we present (i) the distribution of redepositing particles on the surface, (ii) an approximation of the redeposition effect in terms of the surface height and (iii) the spatio-temporal evolution of one- [1] two-dimensional [2,3] surface morphologies subject to combined erosion and redeposition. We are able to conclude that an interplay of erosion, diffusion and redeposition can reproduce the hexagonally arranged nanodots found in experiments in extended regions of the parameter space.

[1] C. Diddens and S. J. Linz, Eur. Phys. J. B, 86 (2013) 397
[2] C. Diddens and S. J. Linz, EPL, 104 (2013) 17010
[3] C. Diddens and S. J. Linz, (in preparation)

O 95.5 Fri 10:30 CHE 89

**Nanoscale low energy electron induced graphitization in tetrahedral amorphous carbon thin films** — •Frederik Klein and Thomas Mühl — Leibniz Institute for Solid State and Materials Research Dresden, PF 270116, D-01171 Dresden, Germany

Under ambient or vacuum conditions diamond and related materials like tetrahedral amorphous carbon (ta-C) are in a metastable state. By application of energy the material is able to undergo a phase change to a graphitic or $sp^2$-hybridised state. We induce local phase changes in ta-C thin films by eV and low keV electron beams in ultrahigh vacuum provided by a scanning tunneling microscope (STM) and a scanning electron microscope (SEM), respectively. These are accompanied by huge changes in many physical properties such as electrical conductivity.

The graphitization is analyzed by STM-based current-distance spectroscopy and conductive atomic force microscopy (c-AFM). The total tip-sample circuit contains the tunneling gap resistance in series with the resistance of the carbon thin film $R_{\mathrm{carbon}}$. An analysis of the STM spectra provides the tunneling barrier height $\Phi$ and $R_{\mathrm{carbon}}$.

We observe a decrease of $R_{\mathrm{carbon}}$ as well as an increase of $\Phi$ in the graphitized areas. However, an expected surface elevation due to a reduction of the material's mass density cannot be seen.

O 95.6 Fri 10:45 CHE 89

**Surface nanostructuring of fused silica assisted by laser-induced self-assembling of thin metal layers: Theory and experiment** — •Pierre Lorenz[1], Michael Klöppel[2,3], Tomi Smausz[4], Tamas Csizmadia[4], Frank Frost[1], Martin Ehrhardt[1], Klaus Zimmer[1], Bela Hopp[1], and Pu Li[2] — [1]Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany — [2]Simulation and Optimal Processes Group, Institute of Automation & Systems Engineering, Ilmenau University of Technology, POB 10 05 65, 98684 Ilmenau, Germany — [3]Institute of Scientific Computation, Department of Mathematics, TU Dresden, 01062 Dresden — [4]Department of Optics and Quantum Electronics, University of Szeged, H-6720 Szeged, Dóm tér 9, Hungary

The introduced laser method demonstrates a novel concept of complex nanostructuring of dielectric surfaces assisted by a laser-induced molten metal layer deformation process. This method allows the fast, large-scale, and cost-effective production of randomly distributed surface nanostructures with a lateral dimension down to 10 nm. However, for an optimizing of this process a profound physical understanding is necessary. For this, the process was simulated under the assumption of the heat equation and the Navier-Stokes equations. Furthermore, the resultant structures were investigated dependent on the metal layer thickness and the laser parameter by AFM and SEM. Additionally, the dynamics of the deformation process were analysed by time-dependent reflection and transmission as well as time-dependent optical microscopic measurement.

O 95.7 Fri 11:00 CHE 89

**Interference Lithography Combined with Hard Anodization Leading to Highly Ordered Nanoporous Alumina** — Josep M. Montero Moreno[1], •Robert Zierold[1], Martin Waleczek[1], Stephan Martens[1], Victor Vega Martinez[2], Victor M. Prida[2], and Kornelius Nielsch[1] — [1]Institut für Angewandte Physik, Universität Hamburg — [2]Department of Physics, University of Oviedo

A perfect order of the pores in nanoporous alumina is desired for application in the fields magneto-optical and opto-electronic devices, photonic crystals, solar cells, fuel cells, and chemical and biochemical sensing systems, to name a few.

We present the fabrication of thick nanoporous $Al_2O_3$ membranes with mono-oriented, perfect hexagonal packing of pores, and precise control of all structural parameters over large areas by matching the conditions of three-beam laser interference lithography and subsequent hard anodization. The periodic concavities after the patterning step in the aluminum surface guide the pore nucleation during the anodization, and the self-ordering phenomenon guarantees the maintenance of the predefined arrangement throughout the entire layer.

The cylindrical pores—diameters adjustable between 20 and 450 nm with advanced post-processing techniques such as atomic layer deposition or selective-chemical etching—are uniform in shape and widely tunable in their dimensions with aspect ratios as high as 500. With that technique, the interpore distance can be easily and accurately tuned in the range of 200 to 500 nm without time-consuming prefabrication of hard-masking stamps.

## O 96: Atomic Layer Deposition (DS jpointly with O)

Time: Friday 9:30–12:30 Location: CHE 91

**Invited Talk** O 96.1 Fri 9:30 CHE 91

**Synthesis, Characterization, and Application of Tunable Resistance Coatings** — •Jeffrey W. Elam — Argonne National Laboratory, Argonne, IL, USA

We used atomic layer deposition (ALD) to synthesize nanocomposite coatings comprised of M:Al2O3 where M= W or Mo using alternating exposures to trimethyl aluminum (TMA) and H2O for the Al2O3 ALD and alternating MF6/Si2H6 exposures for the metal ALD. By varying the ratio of metal and the Al2O3 ALD cycles, we can tune precisely the resistance of these coatings over a very broad range from 1012-105 Ohm-cm. These films exhibit Ohmic behavior and resist breakdown even at high electric fields of 107 V/m. Moreover, the self-limiting nature of ALD allows us to grow these films inside of porous substrates and on complex, 3D surfaces. To investigate the growth mechanism we employed in situ QCM and FTIR absorption spectroscopy studies. For the Mo:Al2O3 films, QCM showed that the Mo ALD inhibits the Al2O3 ALD and vice versa. Surprisingly, FTIR revealed that the reducing agent for the Mo is not the Si2H6, but rather the TMA exposure from the subsequent Al2O3 ALD cycle. Cross sectional TEM revealed the film structure to be metallic nanoparticles (˜1 nm) embedded in an amorphous matrix. We utilized these coatings to fabricate large-area microchannel plates for large-area photodetectors, and as charge drain coatings in MEMS devices for a prototype electron beam lithography tool.

O 96.2 Fri 10:00 CHE 91

**ALD on Multi-Stacked Polystyrene Opals for Thermal Barrier Coatings** — •Robert Zierold[1], Martin Waleczek[1], Josep M. Montero Moreno[1], Roman Kubrin[2], Hooi Sing Lee[3], Alexander Petrov[3], Manfred Eich[3], Gerold A. Schneider[2], and Kornelius Nielsch[1] — [1]Institut für Angewandte Physik, Universität Hamburg — [2]Institut für Keramische Hochleistungswerkstoffe, Technische Universität Hamburg-Harburg — [3]Institut für Optische und Elektronische Materialien, Technische Universität Hamburg-Harburg

Thermal Barrier Coatings (TBC) are used to protect thermally highly loaded metallic components, such as turbine blades in gas engines, from excessive heat and thus prolong the life time of the component.

Herein, we present a novel synthesis route for multi- stacked, photonic crystals made of titania and zirconia revealing a multi-bandgap structure in the infrared, a prerequisite for a TBC. Sequential self-assembly of monodisperse polystyrene particles with different diameters between 315 and 756 nm results in multi-stacked direct opals. The polymer template is then conformally molded by low temperature ALD—with its capabilty to coat complex nanostructures without shadowing effects due to its self-limited nature—processes with $TiO_2$ and $ZrO_2$ from the precursors titanium isopropoxide (TTIP) or tetrakis(ethylmethylamino) zirconium (TEMAZ), respectively, and $H_2O$. Subsequently, calcination of the polystyrene leads to high quality photonic crystals. Optical characterization of the tailor-made samples reveals reflectance peaks in the near infrared corresponding to the different stop-gaps of the individual layers with different periodicities.

O 96.3 Fri 10:15 CHE 91

**New opportunities with Plasma enhanced atomic layer deposition (PE-ALD) of oxides** — •Massimo Tallarida[1], Karsten Henkel[1], Hassan Gargouri[2], Jörg Häberle[1], Bernd Gruska[2], Matthias Arens[2], and Dieter Schmeisser[1] — [1]Brandenburg University of Technology, Konrad Wachsmann Allee, 17, 03046, Cottbus Germany — [2]Sentech Instruments GmbH, Schwarzschildstrasse 2, 12489 Berlin, Germany

Thermal Atomic layer deposition (T-ALD) of oxides is obtained by the pulsed alternation of a metal precursor and an oxygen source, typically $H_2O$ or $O_3$, and the reactions leading to ALD are thermally activated. With plasma enhanced ALD (PE-ALD), instead, the oxygen source is represented by an oxygen-containing plasma. The higher reactivity of the plasma-generated species extend the capabilities of ALD: improved film quality and increased flexibility in process conditions, such as growth at low temperature, are typical advantages of PE-ALD over T-ALD. We report on results on the preparation of thin (<100 nm) aluminum oxide ($Al_2O_3$) films on silicon substrates using T-ALD and PE-ALD in the SENTECH SI ALD LL system. Films were deposited in the temperature range between room temperature (RT) and 200°C. We characterized the films with spectroscopic ellipsometry (thickness, refractive index, growth rate) over 4” wafers and with X-ray photoelectron spectroscopy. All films resulted in a high degree of homogeneity, independent of the deposition temperature. Investigations with capacitance-voltage and conductance-voltage measurements showed a very low interface states density for the PE-ALD films.

O 96.4 Fri 10:30 CHE 91

**X-ray linear dichroism in atomic layer deposited Titanium dioxide layers** — •Chittaranjan Das, Massimo Tallarida, and Dieter Schmeisser — Applied physics and sensors,BTU Cottbus, Germany

Among the various metal oxides TiO2 has been investigated because of its wide range of applications in various fields such as self-cleaning, photocatalysis, solar cell, water splitting, bio-implants. In order to increase its efficiency in water splitting and solar cell energy conversion, it is necessary to understand the crystal structure and electronic properties of thin films. Generally the process of synthesis may modify the electronic properties of TiO2. In the present work we show X-ray linear dichroism (XLD) measurements of TiO2 thin films of different polymorphs. Titania thin films were produced by atomic layer deposition (ALD) and were characterized in-situ with X-ray photoelectron and absorption spectroscopy at synchrotron radiation center BESSY-II. We found that that all titania phases show XLD at Ti-L and O-K edges, but the intensity of XLD is different for different phases. We discuss our data in terms of the partial density of states.

O 96.5 Fri 10:45 CHE 91

**Control of thickness of SiO2 interfacial layer for photocatalytic water splitting on Si photocathodes** — •Chittaranjan Das, Massimo Tallarida, and Dieter Schmeisser — Applied physics and sensors,BTU Cottbus, Germany

Silicon with a band gap of 1.1eV is an excellent candidate for visible photocatalytic water splitting. But p-type Si has a low quantum yield and are less efficient for water splitting [1]. It has been shown that preventing oxidation of Si surface can shift the onset potential for water reduction by about 300mV towards more positive [2]. We investigated in detail the influence of the SiO2 layer thickness on the onset potential for water splitting on Si photocathodes: we used p-type Si substrates covered with SiO2 layers of varying thickness. Then, we deposited a thin TiO2 film on using atomic layer deposition (ALD) to inhibit Si oxidation during the electrochemical experiment. In this way we could shift the onset potential up to 200mV, depending on the SiO2 thickness.

[1]E. L. Warren, S. W. Boettcher, M. G. Walter, H. A. Atwater, and N. S. Lewis: J. Phys. Chem. C 115 (2011) 594. [2]B. Seger, Anders B. Laursen, P. C. K. Vesborg, T. Pedersen, O. Hansen, S. Dahl, I. Chorkendorff, Angew. Chem. Int. Ed. 2012, 51, 9128 *9131

## Coffee break (15 min)

O 96.6 Fri 11:15 CHE 91

**Atomic layer deposition of $Sr_xTi_{1-x}O_y$: Stoichiometry variation and layer characterization** — •Solveig Rentrop[1], Barbara Abendroth[1], Hartmut Stöcker[1], Ralph Strohmeyer[1], Jura Rensberg[2], Juliane Walter[1], and Dirk C. Meyer[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg — [2]Institut für Festkörperphysik, Universität Jena

Resistance switching of metal-insulator-metal (MIM) capacitor structures is one of the possible routes for future non-volatile random access memories. A promising ternary dielectric for MIM devices is $Sr_xTi_{1-x}O_y$. In this material, the layer composition is found to determine dielectric and optical properties as well as the band gap.

Here, we present studies on the atomic layer deposition of amorphous $SrTiO_3$ from $Sr(iPr_3Cp)_2$, $Ti[N(CH_3)_2]_4$ and $H_2O$ at substrate temperatures of 300 °C and 320 °C, resp. By changing the Sr/Ti pulse ratio, we are able to tailor the stoichiometry from stoichiometric to Sr or Ti excess. The layer composition is obtained from X-ray fluorescence spectroscopy and Rutherford backscattering. The tuned band gap value is determined by using a Tauc plot of the ellipsometric absorption coefficient. Moreover, we investigated the dependencies of optical constants, layer density and surface morphology on the layer composition.

Carbon incorporated during deposition increases the leakage current. By X-ray photoelectron spectroscopy the carbon content was measured after Ar ion cluster sputtering. The results show that we are able to deposit carbon free $Sr_xTi_{1-x}O_y$ layers for different Sr/Ti ratios.

O 96.7 Fri 11:30 CHE 91

**$Ta_2O_5$ by thermal-activated ALD** — •Marcel Junige[1], Ralf Tanner[1], Christian Wenger[2], Grzegorz Lupina[2], Matthias Albert[1], and Johann W. Bartha[1] — [1]Technische Universität Dresden — [2]IHP GmbH, Frankfurt (Oder), Germany

$Ta_2O_5$ is a dielectric material with a comparably high permittivity as well as refractive index and thus gains interest for several electronic or optical applications. Atomic Layer Deposition (ALD) is a vacuum technique, which enables the coating of complex-shaped surfaces by alternatively applying self-terminating physicochemical reactions.

We investigated the thermal-activated ALD using the halogen-free metal-organic precursor TBTEMT and ozone gas ($O_3$) as co-reactant at an actual deposition temperature of 215 °C. We pre-heated a Silicon sample for 30 min at the respective process conditions and pre-cleaned the initial surface for 180 s in $O_3$ in order to remove ambient carbon contaminations prior to the ALD.

In-situ real-time Spectroscopic Ellipsometry with a highest possible sampling rate of ca. 1 data point/s confirmed a timewise saturation of the TBTEMT adsorption and of the subsequent ligand removal. An ellipsometric multi-time analysis of a deposition run with 100 ALD cycles determined the homogeneous growth per cycle around 0.64 Å/cycle, the refractive index at 500 nm wavelength around 2.1 and the Tauc optical band gap around 4.3 eV, indicating an amorphous phase. In-vacuo X-ray Photoelectron Spectroscopy revealed a $Ta_2O_5$ film of high purity with a tantalum-to-oxygen ratio of (29:71) at.% as well as carbon and nitrogen contaminants below the detection limit.

O 96.8 Fri 11:45 CHE 91

**Simulation of the deposition and growth of nano-crystalline MgF2 films via the low-temperature atom beam deposition method** — Sridhar Neelamraju, •Johann Christian Schön, and Martin Jansen — MPI for Solid State Research, D-70569 Stuttgart

We model the deposition of magnesium difluoride (MgF2) clusters on a sapphire substrate and the subsequent growth of ordered MgF2-phases via the low-temperature atom beam deposition method. For the modeling procedure we use empirical potentials to describe the interactions within the substrate and the MgF2 deposit, and between the deposited atoms and the substrate. First, we established that primarily MgF2- and Mg2F4-clusters form in the gas phase, and thus the deposition could be described by the adsorption of such molecules on the substrate at low temperatures [1]. Next, the deposited MgF2-layers are annealed, and the structure of the resulting amorphous and nano-crystalline compounds is analyzed and compared with the results (pair distribution functions) of the experimental deposition [2]. We show that the appearance of an (at standard conditions) kinetically unstable CaCl2-type phase in the experiment [3] is due to the concurrent existence of a nano-crystalline CdI2-type modification of MgF2 predicted in earlier theoretical studies [4].

[1] S. Neelamraju et al., J. Chem. Phys. 137:194319 (2012); S. Neelamraju et al., Phys. Chem. Chem. Phys. 14:1223 (2012) [2] X. Mu et al., J. Appl. Cryst. 46:1105 (2013) [3] A. Bach et al., Inorg. Chem. 50:1563 (2011) [4] M.A.C. Wevers et al., J. Solid State Chem. 136:223 (1998)

O 96.9 Fri 12:00 CHE 91

**Structural changes in $HfO_2$ thin films: thickness and doping dependence** — •Simone Brizzi[1], Massimo Tallarida[1], Christoph Adelmann[2], Lars-Ake Ragnasson[2], Sven Van Elshocht[2], and Dieter Schmeisser[1] — [1]Brandenburg University of Technology, Konrad-Wachsmann Allee 17, 03046 Cottbus, Germany — [2]Imec, Kapeldreef 75, B-3001 Leuven, Belgium

In this work we show results regarding MOCVD and ALD $HfO_2$ as well as Al-doped $HfO_2$. We use Synchrotron Radiation Photoemission Spectroscopy (SRPES) to determine Hf/O atomic ratios and X-ray Absorption Spectroscopy (XAS) to investigate the electronic properties related to their crystallization. MOCVD films are synthesized at temperatures ranging from ambient to 400°C and show structures from completely amorphous to monoclinic. ALD films are amorphous as deposited, and can crystallize after post-deposition anneal depending on the percentage of Al-doping. We discuss PES results in order to determine how close to stoichiometry the Hf/O atomic ratios of the films are, as well as the doping level. From XAS data, instead, we can point out how orbital hybridizations are related to structural and physical properties.

O 96.10 Fri 12:15 CHE 91

**Charging effect in HfO2 films deposited on SiO2/Si by atomic layer deposition** — •Silma Alberton Correa, Simone Brizzi, Massimo Tallarida, and Dieter Schmeisser — Department of Applied Physics and Sensors, Brandenburg University of Technology, 03046 Cottbus, Germany

Thin films of hafnium oxide (HfO2) deposited by atomic layer deposition (ALD) have been studied extensively as a high-k replacement for the SiO2 gate in field effect transistors. The use of ALD process allows one to grow homogeneous thin films at low temperatures with a precise control of thickness [1]. Some important electrical considerations for the application of a high-k dielectric include the presence of fixed charge (Qf) and charge trapping in the dielectric. For instance, in the case of Al2O3 thin films deposited on Si, the thickness of the interfacial SiO2 layer was identified as a key fundamental parameter determining Qf [2]. A similar trend can be also expected in HfO2/Si structures. Therefore, in this work, we proposed an in situ evaluation of photon induced charge trapping in HfO2 films deposited on SiO2/Si structures. For that, tetrakis-di-methyl-amino-hafnium (TDMAHf) and H2O were employed as precursors to deposit HfO2 films on SiO2/Si samples with variable thickness of the SiO2 interlayer. Measurements were performed by Synchrotron Radiation Photoemission Spectroscopy (SR-PES). Results indicated that the charging process is dependent on the thickness of the SiO2 interlayer and on the quality of the HfO2 film. [1] M. Leskelä and M. Ritala, Thin Solid Films 409, 138 (2002). [2] G. Dingemans et al., J. Appl. Phys. 110, 093715 (2011).

## O 97: Organic/bio Molecules on Metal Surfaces IV

Time: Friday 10:30–13:00 Location: TRE Phy

O 97.1 Fri 10:30 TRE Phy

**Dispersion Corrected DFT Calculations for the Adsorption of Phthalocyanines on Au(111)** — •Johann Lüder, Olle Eriksson, Biplab Sanyal, and Barbara Brena — Uppsala University, Box-516, 75120 Uppsala, Sweden

An accurate description of physisorbed systems including dispersion, e.g. van der Waals, forces is still a challenge in density functional theory (DFT). We have investigated the adsorption of the technological relevant metal-free Phthalocyanine ($H_2Pc$) and Copper-Phthalocyanine (CuPc) on Au(111). We compared several available methods including pair-potentials and sparse-matter functionals for a monolayer of $H_2Pc$ on Au(111). The calculations of $H_2Pc$ on Au(111) showed that accurate results were obtained with optB86b-DF1 and the Tkatchenko-Scheffler (TS) method. The adsorption of CuPc on the same surface was studied with the TS method, and the accuracy of the obtained results was confirmed by recent experimental X-ray standing wave measurements.

O 97.2 Fri 10:45 TRE Phy

**From terpyridine species to metal organic coordination networks** — •Thomas Dienel[1], Roland Widmer[1], Ralph Koitz[2], Marcella Iannuzzi[2], A. Dieter Schlüter[3], Jürg Hutter[2], and Oliver Gröning[1] — [1]nanotech@surfaces Lab, Empa, Überlandstrasse 129, CH-8600 Dübendorf, Schweiz — [2]Department of Chemistry, University of Zurich, CH-8057 Zürich, Schweiz — [3]Department of Materials, Institute of Polymers, ETH Zürich, CH-8093 Zürich, Schweiz

Substrate-supported metal organic coordination networks offer the possibility to adjust electronic and magnetic properties on the nanometer scale and represent a step towards the realization of two-dimensional polymers [1]. Here, we report on the adsorption behavior of trifunctional terpyridine monomers on coinage metals by means of low-temperature scanning tunneling microscopy. On copper (Cu(111)), the orientation of the terpyridine molecules exhibits a pronounced anisotropy, while a similar behavior was not observed for silver and gold. This is analyzed by density functional theory, revealing specific registries between the monomers and the corresponding substrates. We discuss the impact of this registry on the formation of self-assembled metal organic coordination networks by copper or iron adatoms.

[1] T. Bauer, Z. Zheng, A. Renn, R. Enning, A. Stemmer, J. Sakamoto, A.D. Schlüter, Angewandte Chemie International Edition, 50, 7879-7884 (2011).

O 97.3 Fri 11:00 TRE Phy

**Surface-assisted synthesis of large hydrocarbon macrocycles: Honeycombenes and their organometallic intermediates** — Qitang Fan[1], Cici Wang[1], Yong Han[1], Junfa Zhu[1], Min Chen[2], Hans-Jörg Drescher[2], Malte Zugermeier[2], Han Zhou[2], Julian Kuttner[2], Gerhard Hilt[2], Wolfgang Hieringer[3], and •J. Michael Gottfried[2] — [1]National Synchrotron Radiation Laboratory, University of Science and Technology of China — [2]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [3]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

Honeycombenes constitute a novel class of hexagonal hydrocarbon macrocycles, which are made by surface-assisted synthesis. The basic representative is [18]-honeycombene or hyperbenzene, a hexagon consisting of 18 phenyl rings.[1] The macrocycle was synthesized by surface-assisted Ullmann coupling of six 4,4”-dibromo-m-terphenyl (DBTP) precursor molecules on Cu(111). Hyperbenzene assembles to form close-packed islands with hexagonal symmetry. As intermediates of the surface Ullmann reaction, stable cyclic and linear organometallic species with C-Cu-C bonds have been observed. Their large diameters (2 nm for [18]-honeycombene) make the honeycombenes promising candidates for nanotroughs that could host metal and semiconductor particles or large organic molecules. [1] Q. Fan, C. Wang, Y. Han, J. Zhu, W. Hieringer, J. Kuttner, G. Hilt, J. M. Gottfried, Angew. Chem. Int. Ed. 52 (2013) 4668.

O 97.4 Fri 11:15 TRE Phy

**Hydrogen-bonded networks of triarylamine molecules on noble metal surfaces** — •Christian Steiner[1], David Gessner[1], Ute Meinhardt[2], Bettina Gliemann[2], Milan Kivala[2], and Sabine Maier[1] — [1]Department of Physics, University of Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Germany

Hydrogen bonding is a highly directional interaction that has successfully been applied towards the construction of complex supramolecular architectures both in bulk and on surfaces. Here, we present a low temperature scanning tunneling microscopy study of hydrogen-bonded networks on noble metal surfaces using triarylamine derivatives functionalized with diaminotriazine and carboxylic moieties as molecular building blocks. While on Au(111) extended hexagonal hydrogen-bonded networks with different pore-sizes are formed, the strong surface-molecule interaction leads to different hydrogen-bonded assemblies on Cu(111). In addition, we performed comparative STM measurements of the same triarylamine networks formed from solution on HOPG in ambient conditions and discuss their structure and stability. Such self-assembled organic nanostructures formed at room temperature and atmospheric pressure are highly appealing with respect to applications.

O 97.5 Fri 11:30 TRE Phy

**Steering on-surface polymerization of dibromopyrene on metal substrates** — •Fei Song[1], Tuan Anh Pham[1], Jonas Bjork[2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, the Netherlands — [2]Department of Physics Chemistry and Biology, Linkoping University, Sweden

Self-assembly of functional molecular building blocks into supramolecular structures has attracted a wealth of attention in the past due to its potential usage in molecular devices [1]. However, a drawback of such regular nanostructures is, due to their comparably weak intermolecular interactions, poor thermal and chemical stability. Consequently, robust structures with covalently bonded architectures have attracted much attention as a new alternative route towards the design of nanostructures [2]. Herein, we discuss the formation of stable molecular networks on different metal substrates through on-surface polymerization of the molecular precursor dibromopyrene. The investigations were carried out by using a combination of scanning tunneling microscopy, x-ray photoemission spectroscopy, and density functional theory. We demonstrate that the surface-confined polymerization can be steered by the chosen substrate. [1] Schenning, A. P. H. J.; Meijer, E. W. Chem. Commun. 2005, 26, 3245. [2] Grill, L.; Dyer, M.; Lafferentz, L.; Persson, M.; Peters, M. V.; Hecht, S. Nature Nanotech. 2007, 2, 687.

O 97.6 Fri 11:45 TRE Phy

**Predicting the mechanochemical behavior of multivalent thiol ligands on gold surfaces from free energy relationships** — •Martin Zoloff Michoff, Jordi Ribas-Arino, and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780, Bochum, Germany

Free energy relationships have been widely used in physical organic chemistry in the past 50 years to predict the reactivity of molecules in solution. Recently, it has been shown that this kind of analysis can also be applied to molecular systems adsorbed on transition metal surfaces [1]. In the last 10 years, we have been interested in our group in the mechanochemical properties of thiols adsorbed on metallic surfaces such us Au or Cu [2]. We will present a significant amount of data that shows that the binding strength and the mechanical behavior of the thiol – gold bond can be predicted in terms of the electronic properties of the molecular systems and making use of free energy relationships. On one side, we have focused on monothiols, because they provide a straightforward way of tuning their electronic structure properties by means of changing a substituent in the molecule. On the other, we have also investigated multivalent thiolated molecules, which are more interesting from the point of view of their potential applications, such as providing the anchoring for biocompatible polymers used to coat gold nanoparticles in medical applications [3].

[1]R. A. van Santen *et al. Chem. Rev.* **2010**, *110*, 2005–2048. [2] J. Ribas-Arino, D. Marx *Chem. Rev.* **2012**, *112*, 5412–5487. [3] J. V. Jokerst *et al. Nanomedicine* **2011**, *6*, 715–728.

O 97.7 Fri 12:00 TRE Phy

**Subphthalocyanine based nanocrystals** — •Marta Trelka[1,2], Anaïs Medina[3], David Écija[2], Christian Urban[2], Oliver Gröning[4], Roman Fasel[4], José Gallego[5], Christian Claessens[3], Roberto Otero[2,6], Tomás Torres[3,6], and Rodolfo Miranda[2,6] — [1]University of Bielefeld, 33615 Bielefeld, Germany — [2]Universidad Autónoma de Madrid, 28049 Madrid, Spain — [3]Universidad Autónoma de Madrid, 28049 Madrid, Spain — [4]Empa Swiss Federal Laboratories for Materials Testing and Research, 3602 Thun, 8600 Dübendorf, Switzerland — [5]Instituto de Ciencia de Materiales de Madrid, 28049 Madrid, Spain — [6]Instituto Madrileño de Estudios Avanzados en Nanociencia, 28049 Madrid, Spain

We will present Scanning Tunneling Microscopy studies on Subphthalocyanie (SubPc) molecules that lead to the formation of 3D nanocrystals on a Cu(111) surface. Subphthalocyanine molecules are significantly large macrocycle aromatic structures with a boron atom in the center. Strong molecule-molecule interactions can be expected due to the high dipole moment along the boron-ligand axis. For molecules with a chlorine atom linked to the boron axis, the formation of the organic nanocrystals is found to increase the coverage of sublimated molecules on the surface. The nanocrystals grow up to third layer creating trimers imaged as a bright protrusion. In the studies, the importance of the dipole moment for the growth process is presented. Taking into account the obtained data it is concluded that organic molecules can lead to growth at a metal surface into nanocrystals.[1]

[1] SubPc based nanocrystals Chem. Comm. (2011) 47,9986-9988

O 97.8 Fri 12:15 TRE Phy

**Fabrication of ssDNA/oligo(ethylene glycol) monolayers and complex nanostructures and brushes by promoted exchange reaction** — M. Nuruzzaman Khan and •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

Using a representative test system, we present here a versatile approach to prepare mixed monolayers of thiolate-bound single stranded DNA (ssDNA) and oligo(ethylene glycol) substituted alkanethiols (OEG-AT) in a broad range of compositions as well as ssDNA/OEG-AT patterns of desired shape imbedded into biorepulsive background. The procedure involves two steps. First, primary, well-defined OEG-AT monolayer on a solid support is exposed to electrons or UV light in either homogeneous or lithographic fashion. Second, the promoted (by the irradiation in the first step) exchange reaction between the damaged OEG-AT species in the film and ssDNA substituents in solution occurs, resulting in formation of ssDNA/OEG-AT monolayer or pattern. The composition of the mixed films or ssDNA/OEG-AT spots (lithography) can be precisely adjusted by electron or UV dose in almost entire composition range. The above procedure relies on commercially available compounds and is applicable to both thiolate substituted and disulfide type ssDNA, both symmetric and asymmetric. The fabricated OEG-AT/ssDNA templates and patterns can be, if necessary, extended into the z-dimension by surface-initiated enzymatic polymerization, which may result in formation of highly ordered ssDNA brushes and in sculpturing complex ssDNA brush patterns.

O 97.9 Fri 12:30 TRE Phy

**Conformation Selection by Charge State Dependent Deposition of Unfolded Proteins** — •Gordon Rinke[1], Stephan Rauschenbach[1], Ludger Harnau[2,3], Alyazan Albarghash[1], Mathias Pauly[1], and Klaus Kern[1,4] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, Stuttgart — [2]Max- Planck-Institute for Intelligent Systems, Heisenbergstr. 3, Stuttgart — [3]IV. Institute for Theoretical Physics, University Stuttgart, Pfaffenwaldring 57, Stuttgart — [4]Institut de Physique de la Matiere Condensee, Ecole Polytechnique Federale de Lausanne, Switzerland

The conformation of polymers or proteins often define the electronic and mechanical properties of the single molecule just as well as the meso- and macro scale material properties. It is determined by the chemical interaction with itself and the environment in thermal equilibrium, which means that typically it cannot be addressed actively. Here we show that the conformation of unfolded Cytochrome proteins on a surface can be steered actively between fully extended and completely compact by electrospray ion beam deposition. The charge state and the deposition energy are free parameters in this approach, which can be used independently to control the molecules mechanical stiffness and the intensity of the collision. A quantitative analysis of the obtained conformations with scanning tunneling microscopy and molecular dynamics simulations show that, in addition to the initial gas phase conformation, the mechanical deformation during the ion surface-collision contributes significantly to the final conformation. Thus our methodology adds a new dimension to vacuum processing of molecules.

O 97.10 Fri 12:45 TRE Phy

**Planarized Cyano-Functionalized Triarylamines on Coinage Metal Surfaces: Intermolecular vs. Molecule/Substrate Interactions** — •Kathrin Müller[1], Stefano Gottardi[1], Juan Carlos Moreno Lopez[1], Handan Yildirim[2], Ute Meinhardt[3], Abdelkader Kara[2], Milan Kivala[3], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Department of Physics, University of Central Florida, Orlando, USA — [3]Department of Chemistry and Pharmacy, University Erlangen-Nürnberg, Germany

The formation of well-ordered molecular networks on surfaces has gained increasing attention over the last decades due to their application in devices for molecular electronics. However, the intermolecular as well as the molecule/substrate interactions, which govern the self-assembly process, are often not well understood. We conducted a detailed study of a cyano-functionalized triarylamine molecule on different coinage metal surfaces. By using scanning tunneling microscopy and density functional theory studies we found that the substrates play a crucial role in the self-assembly process. While on Au(111) two different well-ordered phases with micrometer sized domains were found, on Cu(111) only small patches of close packed molecules were observed next to a disordered phase. In contrast only one close-packed phase with micrometer sized islands was found on Ag(111). This study shows that although coinage metal surfaces are considered to be passive they can strongly influence the molecular self-assembly, due to their different electronic and structural corrugation.

# O 98: Plasmonics and Nanooptics V

Time: Friday 10:30–13:00 Location: TRE Ma

O 98.1 Fri 10:30 TRE Ma

**Evidence for graphene plasmons in the visible spectral range probed by molecules** — •Philipp Lange, Günter Kewes, Nikolai Severin, Oliver Benson, and Jürgen P. Rabe — Humboldt-Universität zu Berlin, Department of Physics, 12489 Berlin, Germany

Graphene is considered to be plasmon active only up to the infrared based on combined tight binding model and random phase approximation calculations. Here we show that the optical properties of graphene as measured by ellipsometry and simulated by density functional theory imply the existence of strongly localized graphene plasmons in the visible with a line width of 0.1 eV. Using small emitters that provide the high wave vectors necessary to excite graphene plasmons at optical frequencies we demonstrate graphene plasmon induced excitation enhancement by nearly 3 orders of magnitude.

O 98.2 Fri 10:45 TRE Ma

**Electroluminescence of single oligothiophene wire suspended in a STM junction.** — •Gaël Reecht[1], Fabrice Scheurer[1], Virginie Speiser[1], Fabrice Mathevet[2], Yannick Dappe[3], and Guillaume Schull[1] — [1]IPCMS , Strasbourg, France — [2]Laboratoire de Chimie des Polymères, Paris, France — [3]IRAMIS CEA, Saclay, France

In a pioneering experiment [1], it has been demonstrated that the fluorescence of a single molecule could be excited using a scanning tunnelling microscope (STM). In this case the molecule was separated from the electrodes by thin insulating layers. For direct molecule-electrode contacts experiments [2], luminescence mechanisms intrinsic to the molecule are quenched because of the strong hybridization with the electrode states. Combining direct molecule-electrode coupling and fluorescence in a same junction is therefore a challenging key issue towards molecular optoelectronic devices.

Here we used the tip of a low temperature STM to lift a unique $\pi$-conjugated polymer chain from a Au(111) surface. For positive sample voltage, passing current through the suspended molecular wire induced an emission of light whose spectral and voltage dependencies are consistent with the fluorescence of the wire junction mediated by localized plasmons. For the opposite polarity the emission is strongly attenuated. Our molecular contact junction can therefore be viewed as a single molecular wire light emitting diode.

[1]. X. H. Qiu, and al. Science 299, 542 (2003).

[2]. N. L. Schneider, and al. Phys. Rev. Lett.109, 186601 (2012).

O 98.3 Fri 11:00 TRE Ma

**Bloch Oscillations in Plasmonic Waveguide Arrays** — •Alexander Block[1], Christopf Etrich[2], Felix Bleckmann[1], Thorsten Limböck[1], Carsten Rockstuhl[2], and Stefan Linden[1] — [1]Physikalisches Institut, Bonn, Germany — [2]Institut für Festkörpertheorie und -optik, Jena, Germany

We present the experimental observation of spatial Bloch oscillations in arrays of dielectric-loaded surface plasmon polariton waveguides. By fabricating strips of PMMA on a gold film via gray-scale electron beam lithography, it is possible to guide surface plasmon polaritons. We study the evanescent coupling of light propagating through arrays of such plasmonic waveguides which is described by coupled mode theory. The equation of motion for the evolution of the light field along the waveguides takes the same form as the crystal electron wavefunction's time evolution in the tight binding model of solid state physics. Therefore, we can visualize quantum mechanical condensed matter phenomena in a coherent, yet classical wave environment by mapping the probability distribution to the surface plasmon intensity distribution in real space which is directly imaged via leakage radiation microscopy. We observed plasmonic Bloch oscillations by fabricating waveguide arrays with linearly increasing effective refractive indices. This gradient mimics the linear potential gradient of a DC electric field as required for Bloch oscillations of crystal electrons. The results clearly show the expected spatial Bloch oscillation of a shape retaining Gaussian beam wave package. These results excellently agree with finite-difference time-domain simulations, which are also presented.

O 98.4 Fri 11:15 TRE Ma

**Fabrication of hybrid nanostructures composed of quantum dots and plasmonic nanoparticles** — •Manuel Peter, Cody Friesen, and Stefan Linden — Physikalisches Institut, Universität Bonn, Nußallee 12, 53115 Bonn, Germany

In this contribution, we present a two-step electron lithography process for the reliable positioning of colloidal quantum dots in the vicinity of plasmonic nanoparticles with sub-50-nm spatial accuracy. In the first lithography step, gold nanoparticles are fabricated with spectral features at the emission wavelength of the used quantum dots ($\lambda$=780 nm). Following this, a second layer of PMMA is deposited on the sample. Then a mask is written with the electron beam to define the positions for the colloidal quantum dots. After development, the surface of the substrate as well as that of the quantum dots are chemically modified such that a linker molecule can bind the quantum dots to the predefined spots. After removing the PMMA mask, we obtain hybrid nanostructures composed of gold nanoparticles and quantum dots. With our fabrication method, we will be able to precisely control all geometrical parameters of the hybrid nanostructures. This opens interesting opportunities to study the interaction of quantum dot with particle plasmon resonances via fluorescence microscopy and life-time measurements.

O 98.5 Fri 11:30 TRE Ma

**Linear colloidal assemblies with adjustable dimensions and plasmonics** — •Christoph Hanske, Moritz Tebbe, Vera Bieber, Mareen Müller, Munish Chanana, Nicolas Pazos-Perez, and Andreas Fery — Physical Chemistry II, University of Bayreuth, 95440 Bayreuth, Germany

Topographical templating is a powerful technique to assemble simple colloids into complex structures with advanced optical functionality. We present the fabrication of linear colloidal arrangements by convective assembly of spherical particles on wrinkled substrates. The method does not rely on conventional lithographic processes and yields highly regular structures over macroscopic areas.[1] In a subsequent transfer step additional features with micron- or even submicron-sized dimensions can be introduced through the use of patterned target substrates.[2] We discuss the role of the underlying surface chemistry and demonstrate how this assembly strategy can be employed to manipulate the plasmonic properties of metallic nanoparticles. In UV-Vis/NIR investigations linear arrangements of close-packing spherical gold particles display a pronounced polarization dependent spectral response. The observed anisotropy is caused by strong plasmonic coupling between adjacent particles and can be described in analogy to the transversal and longitudinal modes common for gold nanorods.

O 98.6 Fri 11:45 TRE Ma

**Fano resonances in T-like configured nanospheroids** — •Manuel Gonçalves[1], Taron Makaryan[2], Hayk Minassian[3], Armen Melikyan[4], and Othmar Marti[1] — [1]Ulm University - Inst. of Experimental Physics, Ulm, Germany — [2]Yerevan State University - Radiophysics Department, Yerevan Armenia — [3]Yerevan Physics Institute, Yerevan, Armenia — [4]Russian-Armenian (Slavonic) University, Yerevan, Armenia

Nowadays the growing interest towards systems of metallic nanoparticles is often conditioned by the possibility of revealing Fano resonancies in surface plasmon (SP) oscillations. In this communication we consider plasmonic coupling effects in metallic spheroidal nanoparticles when they form T-like configuration. While identical spheroids do not present Fano resonances, proper choice of aspect ratios of non identical spheroids makes possible strong dipole-quadrupole coupling. When the length of the horizontal spheroid is approximately twice of the length of vertical one Fano resonance takes place if the incident light is polarized along the vertical spheroid and leads of pronounced atenuation in the scattering. Calculations were carried out using COMSOL Multiphysics software for Au spheroids of several aspect ratios and interparticle separations. At the Fano resonance, calculations of near field distribution show that the energy of surface plasmon (SP) oscillations is mainly concentrated in the horizontal spheroid. It is important to note that due to the symmetry of the system the dipole moment of horizontal spheroid vanishes, and the radiation losses are conditioned only by the SP oscillations in the vertical one.

O 98.7 Fri 12:00 TRE Ma

**Electrochemical route to large-area mono-crystalline gold platelets for plasmonic applications** — •Bettina Frank[1], Adrian Ruff[2], Sabine Ludwigs[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Institute of Polymer Chemistry, University of Stuttgart, Germany

We fabricate high-quality gold platelets for plasmonic applications using an electrochemical approach. This process consists of dissolution of a sacrificial gold electrode by cyclic voltammetry in HCl-water-based electrolytes with a 3-electrode setup. Within a specific negative voltage range the Au ions are reduced back to gold atoms and can rearrange in micrometer-sized monocrystalline hexagons, triangles and truncated triangles. Placed underneath the sacrificial electrode, any kind of substrate collects the high-quality microstructures. The particles can be tailored in size, thickness, and number per area, depending on the electrochemical parameters. Sizes of several tens of micrometers can be reached, and thicknesses are in the 10-100 nm range. To demonstrate single-crystallinity, we perform AFM surface analysis which demonstrates that our structures are extremely flat, down to monoatomic flatness. TEM studies confirm the single-crystallinity via electron diffraction by showing the exact hexagonal arrangement of the gold atoms. Our single-crystalline gold platelets will serve as bulk material for high quality plasmonic structures and long-range propagation.

O 98.8 Fri 12:15 TRE Ma

**CMOS-compatible switchable plasmonic perfect absorber** — •Andreas Tittl[1], Behrad Gholipour[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCOPE, University of Stuttgart, Germany — [2]Centre for Disruptive Photonic Technologies, Nanyang Technological University, Singapore

We demonstrate experimentally, for the first time, a CMOS-compatible switchable plasmonic perfect absorber based on the phase-change material germanium antimony telluride (GST). Our design incorporates an array of square aluminum nanopatches stacked above a GST spacer layer and an aluminum mirror. We target the atmospheric window in the 3 to 5 $\mu$m spectral range, which is of great importance for infrared detection and metrology. Furthermore, the Al/GST material system ensures full compatibility with industrial CMOS fabrication techniques. Our structures exhibit tunable absorbance >90% starting at a wavelength of 2.5 $\mu$m, which can be switched off by thermal heating of the sample above the transition temperature of 160°C. This pronounced switching behavior enables a multitude of applications ranging from infrared imaging to localized reaction control.

O 98.9 Fri 12:30 TRE Ma

**Matrix induced growth: a versatile tool for preparing crystalline Au nanoparticles for photonic applications** — •Christian Katzer[1], Philipp Naujok[1], Hendrik Bernhardt[1], Gabriele Schmidl[2], Robert Müller[2], Wolfgang Fritzsche[2], and Frank Schmidl[2] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholzweg 5, D-07743 Jena — [2]Institute of Photonic Technology (IPHT), Albert-Einstein-Str. 9, D-07745 Jena

In the past years different methods such as wet chemical synthesis were used to fabricate metal nanoparticles for photonic applications. In order to overcome typical solution based problems like aggregation of particles, new in-situ methods of preparing them directly on the substrate surface are highly favoured. The authors present a novel in-situ method of fabricating crystalline gold nanoparticles by a thin film controlled self-organization technique using two different thin film matrices ($YBa_2Cu_3O_{7-\delta}$ and $SrTiO_3$). We will show that it is possible to individually control the size and the distribution of the nanoparticles as well as their shape. Thus, it is also possible to fabricate highly anisotropic particles which are of great interest due to the local field enhancement. All can be achieved by adjusting process parameters that are easily accessible. As one might have to extract the nanoparticles from the surrounding matrix material to realise photonic applications we will present our findings concerning the matrix dissolution.

[1] C. Katzer et al., J. Nanopart. Res. 14, 1285 (2012)

[2] C. Katzer et al., Proc. SPIE 8807, Nanophotonic Materials X, doi:10.1117/12.2024058

O 98.10 Fri 12:45 TRE Ma

**Manipulating and probing the growth of plasmonic nanoparticle arrays using light** — Oral Ualibek[1], Ruggero Verre[2], Brendan Bulfin[1], •Karsten Fleischer[1], John F. McGilp[1], and Igor V. Shvets[1] — [1]School of Physics, Trinity College Dublin, Ireland — [2]Department of Applied Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden

Highly ordered self-assembled silver nanoparticle (NP) arrays have been produced by glancing angle deposition on faceted c-plane $Al_2O_3$ templates. The NP shape can be tuned by changing the substrate temperature during deposition. Reflectance anisotropy spectroscopy has been used to monitor the plasmonic evolution of the sample during the growth. The structures showed a strong dichroic response related to NP anisotropy and dipolar coupling. Furthermore, multipolar resonances due to sharp edge effects between NP and substrate were observed. Analytical and numerical methods have been used to explain the results and extract semi-quantitative information on the morphology of the NPs. The results provide insights on the growth mechanisms by the glancing angle deposition. Finally, it has been shown that the NP morphology can be manipulated by a simple illumination of the surface with an intense light source, inducing changes in the optical response. This opens up new possibilities for engineering plasmonic structure over large active areas.

## O 99: Scanning Probe Methods III

Time: Friday 10:30–13:00 Location: GER 38

O 99.1 Fri 10:30 GER 38

**Sensing the spin environment at atomic dimensions** — •Shichao Yan[1], Deung-Jang Choi[1], Jacob Burgess[1], Steffen Rolf-Pissarczyk[1], and Sebastian Loth[1,2] — [1]Max Plank Institute for the Structure and Dynamics of Matter, Hamburg — [2]Max Planck Institute for Solid State Research, Stuttgart

Electronic pump-probe spectroscopy is a versatile tool to study dynamic processes in tunnel junctions with nanosecond time resolution. We apply this technique to low temperature scanning tunneling microscopy and study spin dynamics of Fe nanostructures. Regular patterns of Fe atoms can be assembled with the tip of the STM on a copper nitride surface on Cu(100) and studied individually. The spin relaxation time of Fe trimers is found to be extremely sensitive to variations in their spin environment. We use this sensitivity to sense the presence of another spin. By attaching one transition metal atom to the STM tip and approaching it to the Fe trimer on the surface we deduce the coupling strength between the magnetic atoms. In addition, by monitoring minute changes of the Fe trimer's spin relaxation time, the magnetic state of long-lived spin chains can be sensed even at several nanometers distance.

O 99.2 Fri 10:45 GER 38

**Magnetic force microscopy sensors with multi-component stray field sensitivity** — •Christopher Friedrich Reiche[1], Silvia Vock[1], Bernd Büchner[1,2], and Thomas Mühl[1] — [1]Leibniz-Institut für Festköper- und Werkstoffforschung IFW Dresden — [2]Institut für Festkörperphysik, Technische Universität Dresden

Magnetic force microscopy (MFM) is a powerful tool for mapping the spatial distribution of one component of a magnetic stray field gradient. We employ iron filled carbon nanotubes as monopole-like magnetic tips [1] for quantitative MFM. Our advanced sensor design enables us to consecutively perform quantitative measurements of one in-plane and the out-of-plane stray field component with the same sensor [2]. By developing novel sensor concepts we not only improve the in-plane sensitivity of our sensors but also expand their scope of application. Furthermore, we investigate the applicability of our sensors to general scanning force microscopy methods.

[1] F. Wolny, T. Mühl, U. Weissker, K. Lipert, J. Schumann, A. Leonhardt, and B. Büchner, Nanotechnology 21, 435501 (2010)

[2] T. Mühl, J. Körner, S. Philippi, C. F. Reiche, A. Leonhardt, and B. Büchner, Appl. Phys. Lett. 101, 112401 (2012)

O 99.3 Fri 11:00 GER 38

**Electron-phonon coupling of hot and low-energy electrons studied with SP-STM** — •Anika Schlenhoff, Stefan Krause, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg

Heat dissipation in electronic devices influences their performance and reliability. As dimensions approach the nanoscale, understanding thermal phenomena on a local scale becomes crucial. In spin-polarized scanning tunneling microscopy (SP-STM) the atom-size probe tip allows for a very local current injection. By changing the tip-sample distance, the current can be varied by orders of magnitude.

In our experiments, we inject low-energy tunneling electrons at $U = 200\,\mathrm{mV}$ and hot field-emitted electrons at $U = 5\,\mathrm{V}$ into a superparamagnet, consisting of about 50 iron atoms on a W(110) substrate [1]. In both cases, increasing the current significantly rises its thermal switching frequency, indicating considerable Joule heating. Astonishingly, for the same power a lower effective temperature increase of the nanomagnet is observed for the hot field-emitted electrons. Our experiments reveal that the Joule heating depends not only on the power but also on the electron energy. The results will be discussed in terms of different relaxation mechanisms for the respective electron energies. Within a simple model taking the heat flow from the nanomagnet to the substrate into account [2], we quantify the electron-phonon coupling for the hot and the low-energy electrons.

[1] A. Schlenhoff *et al.*, Phys. Rev. Lett. **109**, 097602 (2012).

[2] W. A. Little, Can. J. Phys. **37**, 334 (1959).

O 99.4 Fri 11:15 GER 38

**Determination of the electron-phonon coupling in ultra-thin Pb films with STM** — Michael Schackert[1], Tobias Märkl[1], •Jasmin Jandke[1], Martin Hölzer[2], Sergey Ostanin[2], Eberhard K.U. Gross[2], Arthur Ernst[2,3], and Wulf Wulfhekel[1] — [1]Karlsruhe Institute of Technology, Physikalisches Instiut, Wolfgang-Gaede Straße 1, 76131 Karlsruhe, Germany — [2]Max Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [3]Wilhelm-Ostwald Institut für Physikalische und Theoretische Chemie, Linnéstraße 2, Universität Leipzig, 04103 Leipzig, Germany

In conventional superconductors, Cooper pairs form due to electron-electron interaction via virtual phonon exchange. A central quantity in this process is the effective phonon spectrum, also known as Éliashberg function which determines the superconducting properties of the material. Using scanning tunneling microscopy (STM) below 800 mK in UHV we found a new method to locally determine the Éliashberg function directly by performing the inelastic tunneling spectroscopy in the normal state. As a first model system we investigated thin Pb islands on Cu(111), wich are in the normal-state due to the proximity effect and therefore the STM-ITS signal is not superposed by the signature of the SC gap. We find a pronounced dependence of the electron-phonon coupling on the island thickness which is in good agreement with ab initio calculations.

O 99.5 Fri 11:30 GER 38

**Scanning force and Kelvin probe force microscopy studies of vicinal Si(111) with atomic resolution** — •Carmen Pérez León, Holger Drees, Michael Marz, and Regina Hoffmann-Vogel — Karlsruher Institut für Technologie (KIT), Physikalisches Institut and DFG-Center for Functional Nanostructures (CFN), D-76131 Karlsruhe

Stepped well-ordered surfaces can be used as nanotemplates for the fabrication of one-dimensional nanostructures. Vicinal Si(111) surfaces inclined towards the $[\bar{1}\bar{1}2]$ direction contain steps with the height of one and three interplanar distances at temperatures below 870°C [1]. With increasing miscut angle the amount of triple steps also increases [1,2]. For an angle of 10 °, only triple steps appear between regularly spaced (111) terraces with a width equal to that of a cell of the Si(111)-$7 \times 7$ surface structure [2]. We have investigated the atomic structure of the 10 °-miscut vicinal Si(111) surface with with frequency-modulation scanning force microscopy (FM-SFM) and Kelvin probe force microscopy (KPFM) at room temperature. Although measurements of step edges are challenging for SFM and KPFM, we have obtained atomic resolution of the structure and the surface potential distribution on the triple step between the Si(111)-$7 \times 7$ terraces.

[1] S. A. Teys, K. N. Romanyuk, R. Zhachuk and B. Z. Olshanetsky, Surf. Sci. **600**, 4878 (2006).

[2] A. Kirakosian, R. Bennewitz, J. N. Crain, Th. Fauster, J.-L. Lin, D. Y. Petrovykh and F. J. Himpsel, Appl. Phys. Lett. **79**, 1608 (2001).

O 99.6 Fri 11:45 GER 38

**Kelvin Probe Force Microscopy Studies of Lead Islands on Si(111)** — •Thomas Späth[1], Carmen Pérez León[1], Michael Marz[1], Hilbert v. Löhneysen[1,2], and Regina Hoffmann-Vogel[1] — [1]Karlsruher Institut für Technologie (KIT), Physikalisches Institut and DFG-Center for Functional Nanostructures (CFN), D-76131 Karlsruhe — [2]Karlsruher Institut für Technologie (KIT), Institut für Festkörperphysik, D-76021 Karlsruhe

Quantum size sffects (QSE) become pronounced when the thickness of a metal film approaches the de Broglie wavelength of the confined electrons. QSE lead to an oscillatory behavior of many physical properties as a function on the thickness of the metallic film. We have studied the influence of the QSE on the work function of Pb islands on Si(111). Pb was evaporated in ultra-high vacuum at room temperature on the Si(111)-$7 \times 7$ surface. The height and local work function of the islands were simultaneously characterized by non-contact atomic force microscopy and Kelvin probe force microscopy. To prevent dewetting, the measurements were performed at approx. 110 K. The observed height of the islands ranges between four and nine monolayers. The local work-function difference shows an even-odd oscillatory dependence on the island's height, in good agreement with calculations [1] and previous results [2]. The amplitude of the oscillation decreases with increasing film thickness.

[1] C. M. Wei and M. Y. Chou, Phys. Rev. B **66**, 233408 (2002).

[2] J. Kim, S. Y. Qin, W. Yao, Q. Niu, M. Y. Chou, and C. K. Shih, Proc. Natl. Acad. Sci. USA **107**, 12761 (2010).

O 99.7 Fri 12:00 GER 38

**Modifying the atomic structure of a single Pb layer by STM** — •Michael Caminale[1], Augusto A. Leon Vanegas[1], Agnieszka Stepniak[1], Hirofumi Oka[1], Dirk Sander[1], and Jürgen Kirschner[1,2] — [1]MPI-Halle — [2]MLU Halle-Wittenberg

The highly complex atomic structure of one single layer of Pb on Si(111) has been extensively investigated in the past by scanning tunneling microscopy (STM) [1-2]. It has been shown that in a narrow coverage interval of 0.1 ML the system exhibits a quasi-infinite number of structural phases constructed hierarchically with an increasing atomic density. This is ascribed to the existence of two competing unit cells for the Pb atoms, respectively identified as $\sqrt{3} \times \sqrt{3}$ (10.44 atoms/nm$^2$) and $\sqrt{7} \times \sqrt{3}$ (9.4 atoms/nm$^2$). The combination of these leads to a rich set of phases [2]. We report the manipulation of a structural phase of Pb/Si(111) by STM-induced structural manipulation at 380 mK. A reversible modification of the atomic arrangement on a scale from $15{\times}15$ nm$^2$ to $80{\times}80$ nm$^2$ is achieved by exploiting the tip-surface interaction by two different strategies: (i) by the application of a milliseconds-long voltage pulse for a constant tunneling current; (ii) by a milliseconds-long ramping of the tip-surface distance for a constant bias value. Combined atomically resolved STM and tunneling spectroscopy measurements give a structural and electronic characterization of the phase change. The results are discussed in view of tip-surface interactions, mass transfer and surface atomic diffusion.

[1] D. R. Heslinga et al. Phys. Rev. Lett. 64, 1589 (1990). [2] M. Hupalo et al. Phys. Rev. Lett. 90, 216106 (2003).

O 99.8 Fri 12:15 GER 38

**The role of Si trimers in the Si/Pt(111) surface alloy** — •M. Švec[1], M. Ondráček[1], P. Hapala[1], P. Merino[2], P. Mutombo[1], M. Vondracek[1], S. Polyak[1], V. Chab[1], M. Blanco-Rey[3], P. de Andres[3], J. A. M. Gago[3], and P. Jelinek[1] — [1]FZÚ AVČR, Praha CZ — [2]CAB-INTA, Madrid ES — [3]ICMM-CSIC, Madrid ES

Silicon is deposited onto crystalline Pt and the resulting structure is investigated in a great detail. An ensemble of surface-science techniques (STM-AFM, ARUPS, SRPES, LEED-IV) is employed to characterize the system and to deduce an atomistic model for the complex geometry of the Si-(r19xr19)R23.4°/Pt(111) structure. Theoretical simulations achieve a very good agreement with the experimental techniques and corroborate beyond any doubt that it is a surface alloy. Generality of the model is briefly discussed, based on similarities found in analogous systems. These findings render unlikely any formation of silicene or germanene on Pt(111) and other noble metal surfaces.

O 99.9 Fri 12:30 GER 38

**Current driven forces in molecular junctions** — Zsolt Majzik, Prokop Hapala, Ondrej Krejci, Martin Setvin, and •Pavel Jelinek — Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

We performed simultaneous nc-AFM/STM measurements over acetophenon molecule deposited on Si(100) p-doped surface in an upright position. Simultaneously tunnelling current and frequency shift as function of tip-sample distance and bias voltage allows us to identify presence of new current driven force acting in molecular junction. In far distance regime, we observe well-known parabolic dependence of frequency shift on applied voltage due to long-range electrostatic force. In close distance regime, the new attractive force emerges at positive bias voltage. What more the force changes sign with further tip approach. We will discuss the origin of the force and the sign change with distance.

O 99.10 Fri 12:45 GER 38

**Investigations of the surface structure of Pt and Fe/Pt by PAES, XPS and STM** — •Samantha Zimnik[1,2], Christian Piochacz[1,2], Sebastian Vohburger[2], and Christoph Hugenschmidt[1,2] — [1]Technische Universität München, Physik Department,Lehrstuhl E21, James-Franck-Straße, D-85748 Garching, Germany — [2]Technische Universität München, Forschungs-Neutronenquelle Heinz Maier-Leibnitz, Lichtenbergstraße 1, D-85748 Garching, Germany

The characterization of the elemental composition of surfaces is of high importance for the understanding of many surface processes such as surface segregation or oxidation. These processes may significantly affect the macroscopic properties of thin films or nano particles such as the magnetization in the system Fe/Pt. Positron annihilation induced Auger Electron Spectroscopy (PAES) is a powerful technique to gather information about the elemental composition of only the topmost atomic layer of a sample. The positron beam facility NEPOMUC at the research reactor Heinz Maier-Leibnitz delivers a high-intensity positron beam with an intensity of $10^9$ $e^+/s$. Thus, time-dependent PAES becomes possible and enables an in-situ observation of the surface segregation process.

The upgraded surface spectrometer at NEPOMUC uses the complementary techniques PAES, XPS and STM for a comprehensive surface analysis and enables the characterization of the elemental composition and the surface topology. Recent studies on the surface of Pt and Fe/Pt with PAES, XPS and STM will be presented.

## O 100: Surface Dynamics II

Time: Friday 10:30–13:00 Location: PHY C 213

O 100.1 Fri 10:30 PHY C 213

**A short-pulse facility for time and angle-resolved photoemission experiments at the synchrotron light source DELTA** — •Sven Döring[1,2], Stefan Cramm[1,2], Mathias Gehlmann[1,2], Lukasz Plucinski[1], Markus Höner[2], Holger Huck[2], Maryam Huck[2], Robert Molo[2], Peter Ungelenk[2], Shaukat Khan[2], and Claus M. Schneider[1] — [1]PGI-6, Forschungszentrum Jülich — [2]Zentrum für Synchrotronstrahlung, DELTA, TU Dortmund

At the synchrotron light source DELTA (TU Dortmund), a short-pulse facility is under commissioning. The U250 undulator of the storage ring is used to generate coherent sub-ps pulses at higher harmonics of a seeding laser. The VUV beamline BL5 operated by a group from PGI-6 (FZ Jülich) guides those pulses into an end-station that is optimized for angle and spin-resolved photoemission spectroscopy experiments. A part of the seeding laser pulse is brought into the end-station via a separate beamline and can be used as a pump beam for pump-probe experiments. With those time and angle-resolved photoemission experiments that are now feasible with this unique setup we will, in the near future, study magnetization dynamics of thin ferromagnetic films on metal surfaces.

The modifications of the photoemission setup that were necessary to conduct time-resolved experiments and the current status of the short-pulse facility will be described.

O 100.2 Fri 10:45 PHY C 213

**Time-resolved two-photon photoemission of NiO(100) ultrathin films** — •Konrad Gillmeister[1], Mario Kiel[1], and Wolf Widdra[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Although NiO is one of the most important models for a correlated electron system, not much is known about the electron dynamics across its charge-transfer band gap. Here we focus on the dynamics of unoccupied states for well-ordered NiO ultrathin films. The films with thicknesses up to nine monolayers (ML) have been grown via molecular beam epitaxy on Ag(001).

Based on two-photon photoemission spectroscopy, we find for all films unoccupied Ni 3*d* states in the range of 1.5 to 2.8 eV above $E_F$. The lifetimes of these states are well below 20 fs. This ultrafast dynamics in the presence of the large NiO bandgap points towards the importance of electron correlation for the decay mechanism. At higher energies a series of image potential states is present starting from one NiO monolayer up to nine ML. The states are identified from their parabolic dispersion. With increasing film thickness, the lifetime of the n=1 image state decreases non-monotonically from 30 to 9 fs.

O 100.3 Fri 11:00 PHY C 213

**Electronic structure and exciton formation dynamics at the ZnO($10\bar{1}0$) surface** — •Jan-Christoph Deinert, Daniel Wegkamp, Michael Meyer, Clemens Richter, Julia Stähler, and Martin Wolf — Fritz-Haber-Institut der MPG, Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

Zinc oxide (ZnO) is a promising electrode material for optoelectronic applications. It is transparent to visible light (band gap of 3.4 eV), natively n-type doped and abundant. Notably, the electronic properties of its interfaces with - possibly functional - organic molecules are not well understood, e. g. only recently the effect of ZnO metallization by hydrogen adsorption and formation of a surface charge accumulation layer (SCA) has been elucidated in detail. We employ a pump-probe technique to gain insight into the dynamics of excited carriers at hydrogen-terminated ZnO surfaces: time-resolved two-photon photoelectron spectroscopy (2PPE). Above band gap excitation at the ($10\bar{1}0$) surface leads to the population of states in the conduction band (CB). These states decay on a few ten fs timescale via LO phonon scattering, where scattering rates show no distinct temperature dependence. At energies below the bulk CB, however, the excited electron dynamics deviate strongly from that ultrafast behaviour. We observe exciton formation within two ps after excitation, 50 meV *below* the Fermi energy. These surface excitons exhibit lifetimes exceeding several hundred ps. Remarkably, the signature of the surface excitons is quenched by increasing the charge density in the SCA. This is due to enhanced screening as the charge density approaches the Mott limit.

O 100.4 Fri 11:15 PHY C 213

**Ultrafast Water Dynamics at the Water-Surfactant-Air Interface** — •Ruth A. Livingstone, Mischa Bonn, and Ellen H. G. Backus — Department of Molecular Spectroscopy, Max Planck Institute for Polymer Research, 55128 Mainz, Germany

Time resolved spectroscopy has revealed exciting new insights into how energy is transferred in interfacial water. The surfactant SDS (sodium dodecyl sulfate) is an important constituent of cleaning products, and has been widely used as a model in surface and colloidal chemistry. At the water-air interface the SDS solution forms a self assembled surfactant monolayer. Our recent study looks at the interaction of water with SDS at this interface on a molecular level. By using time-resolved two-dimensional sum-frequency generation spectroscopy (2DSFG) we found that there are two distinct types of water present at the air-SDS-water interface. In one type, the water molecules are strongly interacting with the SDS layer; while in the other, the water molecules behave more like bulk water. Interestingly, we observed extremely fast energy transfer between these two different types of water.

O 100.5 Fri 11:30 PHY C 213

**2D-Polymer superstructure dynamics on graphene mapped by ultrafast low-energy electron diffraction** — •Max Gulde, Simon Schweda, Sascha Schäfer, and Claus Ropers — IV. Physical Institute, University of Göttingen, Germany

Time-resolved diffraction methods currently serve as powerful tools to elucidate the ultrafast structural dynamics of bulk media. Corresponding experimental developments for the investigation of transient processes on surfaces and other 2D systems have proven to be challenging. Here, we present the implementation of ultrafast low-energy electron diffraction (ULEED) in a laser pump / electron probe setup allowing for a temporal resolution of few picoseconds.

The surface sensitivity of ULEED is utilized to investigate the dynamical behavior of an ultrathin bilayer system, composed of a polymethyl methacrylate (PMMA) superstructure on a freestanding, single layer graphene substrate. In particular, ultrafast partial melting of two-dimensional folded chain crystals is observed, paralleled by the appearance of an expanded amorphous phase. The structural evolution of the crystallites and the amorphous phase are mapped, showing characteristic time constants between 50 ps and 300 ps.

O 100.6 Fri 11:45 PHY C 213

**Rotation and translation in surface diffusion of pentacene on pentacene: Extracting different processes from Helium-3 spin echo measurements.** — •Paul Rotter[1], Antonia Morherr[1], Barbara Lechner[2], David Chisnall[2], Andrew Jardine[2], John Ellis[2], William Allison[2], Bruno Eckhardt[1], and Gregor Witte[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Cavendish Laboratory, Cambridge, CB3 0HE, UK

We advance surface diffusion investigation to comparatively large organic adsorbates on organic surfaces. In this study a coplanar monolayer of pentacene chemisorped on Cu(110) was used as a well characterized organic surface on which isolated pentacene molecules diffuse. Helium-3 spin echo measurements provide a complete statistical description of the adsorbate motion at adequate length scales (nm) and time scales (ps). The potential energy landscape is explored via molecular mechanics and is used for molecular dynamics simulations to compare to experimental results for different azimutal surface directions. An analytical model is derived, which links our observations to known diffusion characteristics and explains key features of the measurements. It turns out that a diffusing molecule lies flatly on the surface but rotates its long axis between two preferred orientations. Thereby the anisotropy of a pentacene molecule considerably impacts its movement across the surface.

O 100.7 Fri 12:00 PHY C 213

**Dynamics of $O_2$ on Pd(100) – Unfreezing the surface** — •Vanessa Jane Bukas[1], Angela den Dunnen[2], Jörg Meyer[1], Ludo Juurlink[2], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Universiteit Leiden, The Netherlands

Despite its progress, state-of-the-art quantitative modeling in the field of gas-surface dynamics still faces considerable challenges when it comes to faithfully reproducing experimental data. We find such a discrepancy upon comparing measured sticking curves for $O_2$ on Pd(100) with our first-principles results. Within the latter approach, we perform molecular dynamics simulations on a neural network interpolated potential derived from density-functional theory and accounting for all six molecular degrees of freedom [1]. Suspecting as source for the discrepancy the prevalent frozen surface approximation (FSA) underlying this approach, we extend our model to additionally include surface mobility in the form of a surface oscillator (SO), and a generalized langevin oscillator (GLO). While following the same dissociation mechanism, even a simple SO model significantly enhances the system's reactivity and already yields remarkable agreement to experiment. Allowing for energy dissipation to the bulk within the GLO approach further reproduces molecular chemisorption at low surface temperatures as also suggested by electron energy loss spectroscopy [2]. Overall, our results thus underscore the importance of overcoming the FSA for adsorbates heavier than the prototypical $H_2$.

[1] V. J. Bukas *et al.*, Z. Phys. Chem., **227**, 1523 (2013).
[2] C. Nyberg *et al.*, Solid State Commun. **44**, 251 (1982).

O 100.8 Fri 12:15 PHY C 213

**Vibrational properties of $O_2$ on Ag(100): multiple adsorption sites vs. Fermi resonances?** — Daniel Strobusch, Jörg Meyer, and •Christoph Scheurer — TU München, Garching, Germany

Adsorption of molecular oxygen on the Ag(100) surface is commonly believed to occur competitively on *both* hollow and bridge sites. A double peak for the oxygen stretch mode observed in high-resolution energy electron loss spectroscopy (HREELS) in combination with semiempirical cluster calculations [1,2] have been invoked as evidence. However, recent density functional theory (DFT) calculations question this picture [3]. In this work, we propose that side-on adsorption of the oxygen molecule on the fourfold hollow site *alone* can reconcile the DFT results with the experimentally measured vibrational properties. We calculate the latter with a full quantum dynamical treatment at the vibration configuration interaction (VCI) level of theory [4] based on a six-dimensional DFT potential energy. This yields excellent agreement with the observed overtone and combination bands [2]. Guided and supported by electronic structure calculations, we propose a model based on the occurrence of a Fermi resonance to explain the HREELS double peak and its coverage dependence. We will discuss implications for other surfaces and larger adsorbates.

[1] L. Vattuone *et al.*, Surf. Sci. **377**, 671 (1997).
[2] F. Buatier de Mongeot *et al.*, J. Chem. Phys. **106**, 9297 (1997).
[3] V. J. Bukas *et al.*, Z. Phys. Chem., **227**, 1523 (2013).
[4] D. Strobusch, M. Nest and C. Scheurer, J. Comp. Chem. **34**, 1210 (2013).

O 100.9 Fri 12:30 PHY C 213

**Vibrational properties of alkali nitrate solutions: from clusters to the water/vapor interface** — •Gang Huang[1], Marie-Pierre Gaigeot[2], and Marialore Sulpizi[1] — [1]Institute for physics, Johannes Gutenberg University, Staudingerweg 7,55099, Mainz, Germany — [2]LAMBE UMR8587, University of Evry Val d'Essonne, Blvd F. Mitterrand, Bat Maupertuis, 91025 EVRY, France

The structure of ions at the vapor/aqueous interface, as well as their influence on the water's hydrogen bond network is of special interest to the atmospheric chemistry community. We use Density Functional Theory-based molecular dynamics to investigate the structure and dynamics of solvated alkali nitrate in water clusters and at the vapor-aqueous interface.

Vibrational density of states (VDOS) are calculated to extract the vibrational signatures for the ions and the surrounding water molecules. We find that in the clusters alkali-nitrate induces a redshift of hydrogen-bonded O-H stretch peaks while in the full water/vapor interface there is an overall blueshift of the hydrogen bonded OH-stretching band. Results are rationalized in term of contact vs water separated ion pairs and confronted with recent surface specific vibrational spectroscopy experiments [1].

[1]A. M. Jubb, W. Hua, and H. Allen, Ann. Rev. Phys. Chem. 63, 107 (2012)

O 100.10 Fri 12:45 PHY C 213

**Rotational Excitation Spectroscopy with the Scanning Tunneling Microscope** — •Fabian Donat Natterer, François Patthey, and Harald Brune — Institute of Condensed Matter Physics, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

The great potential of inelastic electron tunneling spectroscopy with the scanning tunneling microscope (STM) is based on its unmatched spatial resolution that allows for a study of the magnetic, electronic and vibrational properties of individual atoms and molecules. Complementary information about surface processes could be harvested from rotational excitations of molecules, but hitherto remained elusive. Here we show rotational excitation spectroscopy (RES) with the STM for hydrogen, its isotopes, and mixtures thereof, physisorbed on graphene and on hexagonal boron nitride. In consequence of strict symmetry requirements for molecules with identical nuclei (Pauli principle), a certain alignment of nuclear spins demands a specific set of rotational levels $J$. For this reason, the molecular nuclear spin states can be derived from the measured rotational levels. We observed excitation energies at 44 and 21 meV, corresponding to rotational transitions $J = 0 \rightarrow 2$ for hydrogen and deuterium. Notably, these values identify the nuclear spin isomers para-$H_2$ and ortho-$D_2$. For $H_2$:HD:$D_2$ mixtures, we observe RES transitions of all three isotopes, irrespective of where the spectra were recorded; a sign of a collective excitation. Our results mark the potential of STM-RES in the study of nuclear spin states of homonuclear molecules with unprecedented spatial resolution.

# O 101: Molecular Films: Electronics, Photovoltaics and Structure

Time: Friday 10:30–12:30 Location: WIL A317

O 101.1 Fri 10:30 WIL A317

**Towards computational solar cell design: Calculating *ab initio* charge-transfer coupling elements for large systems** — •Christoph Schober, Harald Oberhofer, and Karsten Reuter — Technische Universität München, Germany

Organic solar cells promise outstanding application possibilities, but current systems lack the efficiency to be economically viable. Improvements are often the result of experimental intuition or empirical knowledge, rather than strategic design. Towards a computer-aided design we need to understand, amongst others, the complex mechanism of charge propagation in (possibly amorphous) materials. To this end, Hamiltonian charge-transfer coupling elements are a key ingredient linking microscopic structure and the charge mobilities that determine the device efficiency. To make the calculation of these coupling elements numerically tractable for complex systems we implement a fragment molecular orbital scheme in FHIaims, a highly parallelized all-electron *ab initio* code that due to its atom-centered basis sets is ideally suited to tackle the non-periodicity of organic solar cell materials. We use the self-consistent density of the fragments to construct the system Hamiltonian with correct number of electrons, and additionally implement an embedding scheme that allows to consider the generally neglected second fragment and therewith take polarization effects into account. We present charge-transfer coupling elements for a number of systems previously used for benchmarking and for larger molecules used as hole transport material for organic solar cells.

O 101.2 Fri 10:45 WIL A317

**Nanometer Scale Optical and Photocurrent Microscopy of Organic Optoelectronic Materials** — Marius van den Berg, Kai Braun, Alfred J. Meixner, and •Dai Zhang — Institute of Phyiscal and Theoretical Chemistry, University of Tübingen, Tübignen

Optoelectronic material is the basic component in photovoltaic, photodetector, or transistor system. In organic photovoltaic, the photon-electron conversion efficiency is strongly influenced by the local donor/acceptor morphology, such as crystallinity, or domain size [1, 2]. To get insight into this topic, we monitor the absorption and photocurrent from organic semiconductor blends using a home-built white light transmission setup. To image the distributions and local morphology of donor or acceptor materials, we use Raman and photoluminescence spectroscopy combined with a parabolic mirror assisted confocal optical microscope. Such optical signals can be correlated with topography information through an integrated shear-force scanning probe microscope. The intensity ratios between the donor photoluminescence and the local photocurrent under different bias voltages will be discussed, with respect to the charge transfer processes. Furthermore, photodegradation of the optoelectronic materials will be systematically compared, regarding the changing of photoluminescence, and Raman signals as well as the photocurrent decays.

References: [1] Zhang, D., Heinemeyer, U., Stanciu, C., et al, Phys. Rev. Lett., 2010, 104, 056601. [2] Wang, X., Azimi, H., Zhang, D., et al, Small, 2011, 7, 2793.

O 101.3 Fri 11:00 WIL A317

**Pulsed laser deposited ZnO nanostructures with a sol-gel ZnO coating for hybrid solar cells** — •Sven Käbisch[1,2], Thomas J. K. Brenner[3], Norbert H. Nickel[1], and Norbert Koch[1,2] — [1]Helmholtz-Zentrum Berlin GmbH — [2]Humboldt-Universität zu Berlin, Institut für Physik — [3]Universität Potsdam, Hybrid Photovoltaics & Optoelectronics Group

Hybrid solar cells aim to combine high cross sections for light absorption common for organic semiconductors with high mobility of charge carriers in inorganic semiconductors. Besides the generation and collection of charge carriers in a hybrid solar cell, the charge separation process at the inorganic/organic interface determines the power conversion efficiency (PCE) of the device. Zinc oxide (ZnO) nanostructures and planar layers were deposited by a pulsed laser deposition process on O-terminated Al-doped ZnO planar layers. Subsequently, poly[(bis-(2-ethylhexyl)-cyclopentadithiophene)-alt-benzothiadiazole] (PCPDTBT) was spin-coated on the ZnO nanostructures. The fabrication of the hybrid solar cell was finished by thermal evaporation of molybdenum trioxide and gold as the top electrode. Prior to the formation of the hybrid ZnO/PCPDTBT junction, some of the planar and nanostructured ZnO electrodes were subjected to a surface modification by drop-casting of sol-gel ZnO. Owing to the presence of the structurally imperfect sol-gel layer, the performance of the solar cells could be increased by a factor of 7 for planar and 15 for nanostructured hybrid junctions. This increase of the PCE is explained in terms of an improved charge separation at the ZnO/PCPDTBT interface.

O 101.4 Fri 11:15 WIL A317

**Electric Potential Distributions in Space Charge Regions of Molecular Organic Adsorbates: The Distributed States Model** — •Eric Mankel[1,2], Corinna Hein[3], Maybritt Kühn[1,2], Thomas Mayer[1,2], and Wolfram Jaegermann[1,2] — [1]TU Darmstadt, Surface Science Div., Darmstadt — [2]InnovationLab GmbH, Heidelberg — [3]TU Darmstadt, Electronic Materials Div., Darmstadt

We study the evolution of the electric surface potential for organic semiconductor adsorbates on different high work function substrates using photoelectron spectroscopy. Usually, the surface potential of these materials shows a typical progression in dependence of the adsorbate layer thickness indicating the formation of a space charge region around the contact. We found that these curve shapes cannot be fully explained by the Schottky model which is usually the standard to describe potential distributions in contact space charge regions. Therefore, the Schottky model has been extended assuming a continuous density of states distribution (DOS) in energy. The differences between the Schottky model and the distributed states model (DSM) will be discussed. Finally, both models are applied to measured values of the surface potential evolution of some exemplary organic molecules on varying substrates. We find that the surface potential evolution of the DSM describes the measured potential much more accurately than the surface potential evolution of the Schottky model. Although if this does not prove unequivocally the presence of a DOS in organic semiconductors their amount is estimated in the framework of the new model being between $10^{18}$ cm$^{-3}$eV$^{-1}$ and $10^{19}$ cm$^{-3}$eV$^{-1}$.

O 101.5 Fri 11:30 WIL A317

**Analysis of constructive quantum interference effects in single molecule circuits with parallel backbones** — •Hector Vazquez[1], Rachid Skouta[2], Severin Schneebeli[2], Maria Kamenetska[3], Ronald Breslow[2], Latha Venkataraman[3], and Mark S. Hybertsen[4] — [1]Institute of Physics, AS CR, Prague, Czech Republic — [2]Dept. of Chemistry, Columbia University, USA — [3]Dept. of Appl. Phys. and Appl. Mathem., Columbia University, USA — [4]Center for Functional Nanomaterials, Brookhaven National Laboratory, USA

Quantum interference effects play an important role in single molecule transport. Several examples of destructive quantum interference in molecular transport have been measured [1,2]. Recently, we studied the conductance superposition law in molecular circuits and demonstrated constructive quantum interference effects [3]. We showed that molecules with two branches bound in parallel to the electrodes can exhibit more than twice the conductance of the single backbone counterparts.

Here we extend our analysis to quantify the effect of junction geometry on the conductance of single and double backbone molecules. In this talk I will present results from DFT-NEGF based methods, and discuss the role of junction structure (eg. molecular rotations) in observing clear signatures of interference effects.

[1] J. Am. Chem. Soc. 133, 9556 (2011). [2] Nat. Nanotechnol. 7, 305 (2012). [3] Nat. Nanotechnol. 7, 663 (2012).

O 101.6 Fri 11:45 WIL A317

**Structurally and kinetically controlled on-surface polymerization** — •Johanna Eichhorn[1], Wolfgang M. Heckl[1,2], and Markus Lackinger[1,2] — [1]Physik-Department & TUM School of Education, Technische Universität München, 80799 München, Germany — [2]Deutsches Museum, 80538 München, Germany

On-surface polymerization of functionalized building blocks is an established route to synthesize defined, periodic, covalently linked nanostructures. The arrangement of reactive side groups defines the network topology. The usage of different functional groups with different binding energies facilitates a controlled sequential coupling. Here, we present a hierarchical polymerization based on Ullmann-coupling by sequential dehalogention using bromine and iodine as leaving groups.

Room temperature deposition of 1-(4'-iodophenyl)-3,5-bis(4'-bromophenyl)benzene on Au(111) exclusively activates the iodine-phenyl bond dissociation, whereas the bromine-phenyl bonds remain stable. Subsequent dimerization yields new dumbbell shaped building block which self-assemble into large, periodic islands. Thermal annealing up to 375°C was used to also activate homolysis of the bromine substituents and initiate subsequent polymerization into covalent reticular networks. To compare the polymerization of building blocks with different bond topology, we also studied the direct polymerization of the monomer by deposition onto a preheated substrate. For both protocols the influence on the network quality of different kinetic reaction parameters was studied.

O 101.7 Fri 12:00 WIL A317

**On-surface Synthesis of Extended Graphdiyne Wires by Stepped Surface Templating of Terminal Alkyne Homo-Coupling** — Borja Cirera[1], Yi-Qi Zhang[1], Jonas Björk[2], Svetlana Klyatskaya[3], Zhi Chen[3], Mario Ruben[3], Johannes V. Barth[1], and •Florian Klappenberger[1] — [1]Physik Department E20, TU München, Germany — [2]Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden — [3]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany

The success of carbon allotropes strongly refreshed the attraction towards low-dimensional hydrocarbon materials like carbyne, graphyne, or graphdiyne originally targeted by acetylenic solution chemistry. Recently, we introduced homo-coupling of terminal alkynes on a noble metal surface to the field of covalent on-surface synthesis. Here, we overcome the missing chemoselectivity of this method by templating the coupling reaction of linear diethynyl-terphenyl monomers with step edge alignment on the vicinal Ag(877) surface. This approach allowed us to suppress side-reactions resulting in irregularly-branched polymers on the planar surface and rendering possible the fabrication of 300 Å-long strands of a novel 1D hydrocarbon material. The extended-graphdiyne molecular wire is classified by density functional theory electronic structure calculations as a direct band gap semiconductor material. Our method puts a great variety of carbon-rich materials within reach and should also be applicable to other classes of tectons.

O 101.8 Fri 12:15 WIL A317

**Coupling of Brominated Tetrathienoanthracene on Crystalline Copper and Silver** — •Rico Gutzler[1,2,3], Luis Cardenas[1,2], Josh Lipton-Duffin[1], Dmitrii F. Perepichka[2], and Federico Rosei[1] — [1]Institut National de la Recherche Scientifique, Université du Québec, 1650 boulevard Lionel-Boulet, Varennes, QC J3X 1S2, Canada — [2]Department of Chemistry, McGill University, 801 Sherbrooke Str. West, Montreal, QC H3A 0B8, Canada — [3]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

We report the synthesis of extended 2D organic networks on copper and silver from thiophene-based molecules. A combination of STM and XPS yields insight into the reaction pathways from single molecules towards the formation of two-dimensional organometallic and polymeric structures via Ullmann reaction dehalogenation and C-C coupling. The thermal stability of the molecular networks is probed by annealing to temperatures of up to 500 °C. On Cu(111) only organometallic structures are formed, while on Ag(111) both organometallic and covalent polymeric networks were found to coexist. The ratio between organometallic and covalent bonds could be controlled by means of the annealing temperature. The thiophene moieties start degrading at 200 °C on the copper surface, whereas on silver the degradation process becomes significant only at 400 °C. Our work reveals how the interplay of a specific surface type and temperature steers the formation of organometallic and polymeric networks and describes how these factors influence the structural integrity of two-dimensional organic networks.

## O 102: Graphene: Interaction with the Substrate (HL jointly with DY, MA, O, TT)

Time: Friday 11:15–13:00 Location: POT 081

O 102.1 Fri 11:15 POT 081

**Phonons of graphene on metallic and semiconductor surfaces, an ab-inito approach** — •Alejandro Molina-Sanchez and Ludger Wirtz — Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg

The interaction of graphene with substrates can alter its electronic and vibrational properties and is relevant for the practical use of graphene. In this work, we describe the graphene-substrate interaction through the theoretical study of the vibrational properties. We focus on three paradigmatic cases where the interaction strength changes gradually: graphene@BN, graphene@Ir(111), and graphene@SiC (i.e., the buffer layer). We use ab-initio methods to obtain the phonon modes, the density of states, and the strength of the electron-phonon coupling. When we deal with large supercells, we use an unfolding scheme to visualize the phonon bands in the primitive unit cell. Thus, we can distinguish clearly the changes in the phonon dispersion of perturbed-graphene with respect to the one of pristine graphene. Graphene on boron nitride exhibits a weak interaction but a non-negligible shift of the 2D Raman band. We explain this observation as due to a weakening of the electron-phonon interaction via screening of electron-electron correlation by the dielectric substrate. Graphene on iridium, also displays weak interaction but the underlying material is a metal. This leads to an even more pronounced screening of the electron-electron interaction in graphene. In the last case, we study the buffer layer of graphene on silicon carbide. The hybridization of graphene with silicon carbide changes the electronic structure of graphene and the phonon bands.

O 102.2 Fri 11:30 POT 081

**The (3×3)-SiC($\bar{1}\bar{1}\bar{1}$) reconstruction: Surface phase equilibria near the graphene formation regime on 3C-SiC($\bar{1}\bar{1}\bar{1}$)** — •Lydia Nemec[1], Florian Lazarevic[2], Patrick Rinke[1], Volker Blum[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]AQcomputare GmbH, Chemnitz — [3]MEMS Department, Duke University, Durham, NC, USA

To refine the growth quality of epitaxial graphene on the C-side of SiC and improve the resulting electronic character of these films, it is important to understand the atomic- and electronic-structure of the interface. A phase mixture of different surface phases is observed just when surface graphitization first sets in. However, the atomic structure of some of the competing surface phases, as well as of the SiC-graphene interface, is unknown.

We performed a density functional theory study on the C-side of the polar SiC($\bar{1}\bar{1}\bar{1}$) surface using the all-electron, numeric, atom-centered basis function code FHI-aims. The formation energy of different reconstructions and model systems for the interface is presented within the thermodynamically allowed range.

The surface energies of the known (2×2) phase is compared with several structural models of the (3×3) phase proposed in the literature. In comparison all the previously suggested (3×3) models are higher in energy than the known (2×2) phase. We present a new model for the (3×3) reconstruction. Its formation energy crosses that of the (2×2) phase just at the carbon rich limit of the chemical potential, which could explain the observed phase mixture.

O 102.3 Fri 11:45 POT 081

**Reststrahl band assisted photocurrents in epitaxial graphene layers** — •P. Olbrich[1], C. Drexler[1], L.E. Golub[2], S.N. Danilov[1], V.A. Shalygin[3], V.A. Shalygin[3], R. Yakimova[4], S. Lara-Avila[5], S. Kubatkin[5], B. Redlich[6], R. Huber[1], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]State Polytechnic University, St. Petersburg, Russia — [4]Linköping University, Linköping, Sweden — [5]Chalmers University of Technology, Göteborg, Sweden — [6]FOM Institute for Plasma Physics, Nieuwegein, The Netherlands

We report on the observation of reststrahl band assisted photocurrents in epitaxial graphene on SiC. The samples were excited by the infrared radiation from the tunable free electron laser "FELIX" and a $CO_2$ gas laser [1]. We show that the photoresponse due to linearly (circularly) polarized mid-infrared light is strongly enhanced (suppressed) in the vicinity of the reststrahl band of SiC. Our data, in particular a complex spectral behavior, are well described by the developed theory taking into account photon drag and photogalvanic effects affected by an enhanced light-matter interaction in the range of substrate's negative dielectric function in its reststrahl band. Moreover, our work demonstrates that substrate phonons strongly influence the transport properties of the carriers in graphene.

[1] P. Olbrich *et al.*, arXiv:1308.0123

O 102.4 Fri 12:00 POT 081

**Towards superlattices: Lateral bipolar multibarriers in graphene** — •Martin Drienovsky[1], Franz-Xaver Schrettenbrunner[1], Andreas Sandner[1], Ming-Hao Liu[2], Fedor Tkatschenko[2], Klaus Richter[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik Universität Regensburg — [2]Institut für Theoretische Physik Universität Regensburg

We report on transport properties of monolayer-graphene (MLG) with a laterally modulated charge carrier density profile. For that we employed a planar back gate and striped top gate electrodes of 25 nm width and a spacing of 100 nm up to 200 nm, separated from the MLG by an $Al_2O_3$ dielectric. Tuning of top and back gate voltages gives rise to multiple potential barriers and wells, enabling the investigation of resistance either in the unipolar or the bipolar transport regime. In the latter pronounced single- and multibarrier Fabry-Pérot (FP) resonances are observed. The experimental data of different devices with alternating numbers of top gate stripes and pitch, taken at different temperatures, is consistent with a ballistic transport calculation, employing a realistic potential profile, extracted from classical electrostatic simulation combined with the quantum capacitance model. The origin of resistance oscillations in our multibarrier graphene system can be explained in the FP-picture, without resorting to an artificial band structure.

O 102.5 Fri 12:15 POT 081

**Scanning Tunnelling Spectroscopy of Moiré Patterns on Graphene/Rh(111)** — •Anne Holtsch, Tobias Euwens, Hussein Schanak, and Uwe Hartmann — Institut für Experimentalphysik, Universität des Saarlandes, Saarbrücken

The lattices of graphene and Rh(111) provide a difference of approximately 9% between the two lattice constants. This mismatch results in the formation of a Moiré pattern with a lattice constant of 2.9 nm. Each unit cell of the pattern exhibits four regions where the graphene lattice is aligned differently with respect to the Rh(111) atoms. Scanning tunnelling microscopy and spectroscopy are used to investigate changes in the electronic properties at the four regions of the Moiré unit cell. Density functional theory (DFT) calculations show that a decreasing C-Rh distance at different symmetry points coincides with an increasing interaction strength between graphene and Rh(111) [1]. The locations of the minima in the dI/dV curves are identical for the different symmetry regions. Beyond the minimum, the symmetry points show differences in the dI/dV curves according to the C-Rh interaction strength.

[1] M. Iannuzzi and J. Hutter, Surf. Sci. 605, 1360 (2011).

O 102.6 Fri 12:30 POT 081

**Varied Moiré patterns of graphene/Rh(111) measured by scanning tunnelling microscopy** — •Tobias Euwens, Anne Holtsch, Hussein Schanak, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken

Scanning tunnelling microscopy measurements on graphene deposited on a Rh(111) surface are conducted to investigate the superstructures that originate from the different lattice parameters of the graphene and the substrate. Different kinds of superstructures, also called Moiré patterns, can be seen in the resulting images. Their origin lies in either the surface inhomogenities of the Rh(111) substrate or in the form of folds and steps in the graphene itself. Knowing the properties of the growth of graphene on the rhodium surface is important for the construction of more complex graphene-based electronics. Understanding the specific structure of the Moiré patterns can help in that regard as it relays information about the angle between the carbon and the rhodium lattice and potential reasons for the twisting between the two lattices.

O 102.7 Fri 12:45 POT 081

**Impact of the substrate on the electronic properties of graphene** — •Hussein Shanak, Anne Holtsch, Tobias Euwens, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken

Electronic properties of graphene grown on different substrates such as Rh, Cu and SiO2 were investigated using scanning tunnelling microscopy and spectroscopy. The different kinds of substrates result in different types of superstructures due to the mismatch between graphene and substrate. Comparison of the electronic properties obtained for graphene on the different substrates leads to a better understanding of the graphene doping behaviour. Additionally, the existence of different superstructures leads to different growing properties of the materials on top of graphene itself.

## O 103: Graphene (DS jointly with TT, MA, HL, DY, O)

Time: Friday 11:30–13:15 Location: CHE 89

O 103.1 Fri 11:30 CHE 89

**Plasma-enhanced chemical vapor deposition of graphene on copper substrates** — •Nicolas Wöhrl, Oliver Ochedowski, Steven Gottlieb, and Volker Buck — Universität Duisburg-Essen und CENIDE, 47057 Duisburg, Germany

In this work we present the synthesis of graphene on copper by microwave Plasma-enhanced Chemical Vapor Deposition (PE-CVD) process. The special construction of the plasma source allows the deposition at a wide range of different process parameters giving a fast and inexpensive method to synthesize graphene. Additional advantages of the plasma deposition of graphene are lower substrate temperatures compared with thermal CVD processes. The PE-CVD process uses hydrogen and methane as reaction gases exactly like thermal CVD process does. The gaseous precursors are decomposed in the plasma and the catalytic influence of copper and the minor solubility of carbon in copper lead to the growth of one monolayer of graphene. Plasma parameters are varied to investigate the influence on the graphene properties. Raman spectroscopy and AFM measurements are used as nondestructive tools for the characterization of the synthesized graphene films. Especially Raman spectroscopy is used as an efficient tool to determine the number of graphene layers, the disorder and the defect density. We present a possible way to produce large area of monolayer graphene on a copper based substrate. This technology can help to make graphene available for industrial applications.

O 103.2 Fri 11:45 CHE 89

**Continuous wafer-scale graphene on cubic-SiC(001)** — •Victor Aristov[1,2], Olga Molodtsova[2], Alexei Zakharov[3], Dmitry Marchenko[4], Jaime Sánchez-Barriga[4], Andrei Varykhalov[4], Marc Portail[5], Marcin Zielinski[6], Igor Shvets[7], and Alexander Chaika[1,7] — [1]ISSP RAS, Chernogolovka, Moscow dist. 142432, Russia — [2]HASYLAB at DESY, D-22607 Hamburg, Germany — [3]MAX-lab, Lund University, Box 118, 22100 Lund, Sweden — [4]HZB für Materialien und Energie, D-12489 Berlin, Germany — [5]CNRS-CRHEA, 06560 Valbonne, France — [6]NOVASiC, BP267-F73375 Le Bourget du Lac Cedex, France — [7]CRANN, School of Physics, Trinity College, Dublin 2, Ireland

The atomic and electronic structure of graphene synthesized on commercially available cubic SiC(001)/Si(001) wafers have been studied. LEED, LEEM, PEEM, STM and ARPES data prove the wafer-scale continuity and uniform thickness of the graphene overlayer and reveal that the graphene overlayer consists of only a few monolayers with physical properties of quasi-freestanding graphene: atomic-scale rippling, asymmetric distributions of carbon-carbon bond lengths etc. In addition, graphene overlayer consists of rotated nanometer-sized ribbons with four different lattice orientations connected through the grain boundaries. Thus, this graphene could be adapted for graphene-based electronic technologies and directly patterned using Si-electronic lithographic process. Supported by RFBR grant 14-02-00949, by Marie Curie IIF grant (7th ECFP) and by SPP 1459 of DPG.

O 103.3 Fri 12:00 CHE 89

### Characterization of single and few layer of molybdenum disulfide with spectroscopic imaging ellipsometry

— •P. H. Thiesen[1], B. Miller[2], C. Röling[1], E. Parzinger[2], A. W. Holleitner[2], and U. Wurstbauer[2] — [1]Accurion GmbH, Göttingen, Germany — [2]Technische Universität München, Walter Schottky Institut, 85748 Garching, Germany

Molybdenum disulfide is a layered transition metal dichalcogenide. From the point of current research, 2D-materials based on MoS2 are very promising because of the special semiconducting properties. The bulk material has an indirect 1.2 eV electronic bandgap, but single layer MoS2 has a direct 1.8 eV bandgap. The monolayer can be used in prospective electronic devices like transistors or photo detectors. Like in the initial period of graphene research, the issue is to identify and characterize MoS2 crystallites of microscopic scale. Imaging ellipsometry is a nondestructive optical method in thin film metrology with a lateral resolution down to 1 micro meter. Imaging ellipsometry has been applied to characterize graphene flakes of few micrometer size [1],[2] and also to identify single layer steps in multilayer graphene/graphite stacks [3]. Delta and Psi Spectra of MoS2 monolayers as well as maps of the ellipsometric angles will be presented. The practical aspect of single layer identification will be addressed and the capability of ellipsometric contrast micrographs as a fast tool for single layer identification will be demonstrated. [1] Wurstbauer et al., Appl. Phys. Lett. 97, 231901 (2010) [2] Matkovic et al. J. Appl. Phys. 112, 123523 (2012) [3] Albrektsen et al. J. Appl. Phys. 111, 064305 (2012)

O 103.4 Fri 12:15 CHE 89

### Charge and Spin Transport in Turbostratic Graphene and Graphene Nanoribbons

— •Nils Richter[1], Sebastian Schweizer[2], Ajit Kumar Patra[2], Yenny Hernandez[3], Akimitsu Narita[3], Xinliang Feng[3], Petr Ostrizek[1], Klaus Müllen[3], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]FB Physik, Universität Konstanz, 78457 Konstanz, Germany — [3]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

We present two specially selected allotropes of graphene: Turbostratic graphene (TG) and graphene nanoribbons (GNRs).

TG discs are graphitic microstructures where the twisting of adjacent layers leads to an electronic decoupling. Electrical transport measurements reveal quantum effects such as weak localization and huge charge carrier mobilities (100,000 cm$^2$/Vs) in protected bulk layers [1]. In non-local spin valves we find efficient spin injection over micrometer distances showing large spin diffusion lengths.

Using electromigrated nanojunctions we are able to investigate electrical and spin transport in chemically synthesized GNRs. As they are dispersed in a solvent [2] they can be drop cast on such junctions. With GNRs of different widths and edge geometries we will probe the exciting unconventional properties that have been predicted for these nanostructures [3].

[1] Y. Hernandez et al., arXiv:1301.6087 (under review 2013). [2] A. Narita et al., Nature Chem., in press, DOI: 10.1038/NCHEM.1819. [3] O. Yazyev, Rep. Prog. Phys. 73, 056501 (2010).

O 103.5 Fri 12:30 CHE 89

### Graphene functionalisation with N and O: reversible or permanent modification of the electronic properties?

— •Peter Brommer[1,2], Alex Marsden[1], Neil Wilson[1], Gavin Bell[1], and David Quigley[1,2] — [1]Department of Physics, University of Warwick, Coventry, UK — [2]Centre for Scientific Computing, University of Warwick, Coventry, UK

For many applications it is essential to modify the electronic properties of graphene in a controlled fashion. This can be achieved via oxygen and nitrogen functionalisation in ultra-high vacuum, leading to a system in which electronic and structural properties can be systematically studied. Low dose oxygen functionalisation ($<$ 5 atomic percent) can be reversed completely by annealing at 200 °C, while nitrogen permanently integrates itself into the material. Here we present insights from DFT calculations on this system, such as the low-energy configurations and simulated transmission electron microscopy (TEM) images, binding energies and effective band structures of the N and O decorated graphene sheets. We directly compare our results with experiments on CVD grown graphene. Angle-resolved photoemission spectroscopy (ARPES) resolves the band structure changes on functionalization, whilst X-ray photoelectron spectroscopy (XPS) provides information about the chemical environment of the defect atoms. Combined, the computational and experimental data can offer insights into the structural changes induced by the functionalisation process and their consequences on the electronic properties of the material.

O 103.6 Fri 12:45 CHE 89

### Revealing the ultrafast process behind the photoreduction of graphene oxide

— •Daniel S. Badali[1], Regis Y.N. Gengler[1], Dongfang Zhang[1], Kostantinos Dimos[2], Kostantinos Spyrou[2], Dimitrios Gournis[2], and R.J. Dwayne Miller[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg Center for Ultrafast Imaging, University of Hamburg, Hamburg, Germany — [2]Department of Material Science and Engineering, University of Ioannina, Ioannina, Greece

Because of its unique electronic and structural properties, graphene has brought two-dimensional materials to the foreground of material science and nanoelectronic research. As such, reliable methods for producing graphene are in demand and have significant impact on the field of thin films. In recent years it has been found that irradiating dispersions of graphene oxide in water with ultraviolet light has led to the production of graphene. Although this has been observed in a variety of experimental conditionals, the exact mechanism of the reduction has remained elusive until now. To this end, we have performed careful optical pump-probe measurements which have revealed the chemistry of this process: rather than direct photoreduction, the reduction is mediated by solvated electrons which have been liberated from water molecules by the ultraviolet light. We show that this occurs on an ultrafast timescale in the tens of picoseconds range. Characterization of the final product confirms the removal of oxygen containing groups and the restoration of the honeycomb carbon network of graphene.

O 103.7 Fri 13:00 CHE 89

### Tuning of structural, electronic and optical properties in twisted bilayer MoS$_2$

— •Jens Kunstmann[1], Arend M. van der Zande[1], Alexey Chernikov[1], Daniel A. Chenet[1], YuMeng You[1], XiaoXiao Zhang[1], Timothy C. Berkelbach[1], Pinshane Y. Huang[2], Lei Wang[1], Fan Zhang[1], Mark Hybertsen[1,3], David A. Muller[2], David R. Reichman[1], Tony F. Heinz[1], and James C. Hone[1] — [1]Columbia University, New York, New York, 10027, USA — [2]Cornell University, Ithaca, New York, 14853, USA — [3]Brookhaven National Laboratory, Upton, New York 11973, USA

With the rise of graphene, atomically thin 2D materials have become the focus of many researchers worldwide. Among them, group 6 transition metal dichalcogenides, such as MoS$_2$ are new 2D direct gap semiconductors, have been used as field effect transistors and are promising for applications in valleytronics. However, little is understood about the interlayer interactions between 2D materials. We measured dozens of MoS$_2$ bilayers with well-defined twist angle by stacking single crystal monolayers using ultraclean transfer techniques. We observe that continuous changes in the interlayer twist angle lead to strong, continuous tuning in the indirect optical transitions, the Raman modes, the second harmonic generation, and the reflection spectra. We use electronic structure calculations to show that the tuning in the indirect band transitions arise from an increase of the bilayer separation caused by the van der Waals repulsion of sulfur atoms. These results indicate the possibility of producing new 2D materials with desired properties by tailoring the interlayer alignment in 2D heterostructures.

# O 104: Invited Talk (Alec Wodtke)

Time: Friday 13:15–14:00 Location: TRE Phy

**Invited Talk** O 104.1 Fri 13:15 TRE Phy

**Toward a Dynamical Understanding of Surface Chemistry** — •Alec Wodtke — Department of Dynamics at Surfaces, Max Planck Institute for biophysical Chemistry, Göttingen, Germany — Institute for Physical Chemistry, Georg-August University, Göttingen, Germany

Great strides in our understanding of surface chemistry have been made over the last two decades due to constantly improving computational methods that rely on the Born-Oppenheimer (electronically adiabatic) approximation and exploit the power of modern electronic structure theory, especially density functional theory. Despite this progress, describing and understanding the atomic-scale motion involved in surface reactions remains a daunting challenge. The central difficulty concerns the question: how is energy exchanged between an adsorbate and elementary excitations of the solid? To observe and understand the atomic-scale motion involved in energy conversion processes occurring in collisions between molecules and solid surfaces is a central goal of our group. Using modern molecular beams methods in state-to-state scattering experiments, we obtain a wealth of observational data. Emphasizing quantitative comparison to first principles theories, we find that energy conversion can occur by unexpected mechanisms, where the electronically adiabatic approximation separating the time scales of electronic and nuclear motion is found to be invalid. One important outcome of this work is the realization that Born-Oppenheimer breakdown can be induced by simple electron transfer events that are common in surface chemistry.