Surface Science Division
Fachverband Oberflächenphysik (O)

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Overview of Invited Talks and Sessions

(Lecture rooms HSZ 01, HSZ 101, GER 38, TRE Phy, TRE Ma,
WIL A317, WIL B321, WIL C107, WIL C307, and REC/PHY C213;
Poster P1A, P1C, P2-EG, P2-OG1, P2-OG2, P2-OG3, and P2-OG4)

Invited Talks

O 1.1	Mon	9:30–10:15	TRE Phy	**Electron Spin Resonance of single atoms on surfaces** — •Andreas Heinrich
O 10.1	Mon	15:00–15:45	TRE Phy	**Overview of the development of ultrafast scanning tunneling microscopy** — Dominik Peller, Tyler L. Cocker, Ping Yu, Rupert Huber, •Jascha Repp
O 13.1	Mon	15:00–15:30	GER 38	**Towards efficient orbital-dependent density functionals for weak and strong correlation** — •Igor Ying Zhang, Patrick Rinke, John P. Perdew, Matthias Scheffler
O 25.1	Tue	9:30–10:15	TRE Phy	**Electrochemistry: A new frontier for a theoretical surface scientist** — •Axel Gross
O 27.1	Tue	10:30–11:00	TRE Phy	**The role of nonadiabatic friction in chemical dynamics at metal surfaces** — •Reinhard Maurer
O 30.1	Tue	10:30–11:00	GER 38	**Including spin effects in the strong-coupling limit of DFT** — •Paola Gori-Giorgi, Juri Grossi, Derk Pieter Kooi, Klaas Giesbertz, Michael Seidl, Aron Cohen, Paula Mori-Sanchez
O 32.1	Tue	10:30–11:00	WIL C307	**Electrical detection of spin-polarized transport on topological insulator via four-probe spectroscopy** — •An-Ping Li, Saban Hus, Corentin Durand, Xiaoguang Zhang, Giang Nguyen, Yong Chen
O 32.5	Tue	11:45–12:15	WIL C307	**Probing electron transport with atomic scale precision** — •Christian A. Bobisch
O 34.1	Tue	10:30–11:00	HSZ 101	**Self-Assembly at the Liquid/Solid Interface: Playing on the Nanoscale and Taming Molecules** — •Manfred Buck
O 36.1	Tue	14:00–14:30	TRE Phy	**Attosecond control of excited electrons and nuclei in gas- and condensed-phase systems** — •Thomas Pfeifer
O 36.2	Tue	14:30–15:00	TRE Phy	**Probing ultrafast electron and spin dynamics in momentum, space, and time - chances and opportunities of a surface science end station at ELI-ALPS** — •Stefan Mathias
O 36.3	Tue	15:00–15:30	TRE Phy	**Attosecond electron dynamics on surfaces and layered systems** — •Reinhard Kienberger
O 36.4	Tue	15:30–16:00	TRE Phy	**Coinicdence ARPES on molecules** — •Reinhard Doerner
O 38.1	Tue	14:00–14:30	WIL A317	**Tuning excitonic excitations in molecular layers** — •Martin Weinelt, Cornelius Gahl
O 40.1	Tue	14:00–14:30	WIL C307	**Performances of the new low temperature ultrahigh vacuum 4 scanning tunneling microscopes** — •christian Joachim, Delphine Sordes, Corentin Durand, We-Hyo Soe, Marek Kolmer
O 43.1	Tue	15:30–16:00	WIL C307	**STM-induced light emission: from molecular LED to subnanometric optical microscopy.** — •Guillaume Schull

O 66.1	Wed	9:30–10:15	TRE Phy	**Probing catalytic surface reactions in real time** — •Anders Nilsson
O 68.1	Wed	10:30–11:00	TRE Phy	**Electronic orders in light-driven materials** — •Philipp Werner, Yuta Murakami, Hugo Strand, Shintaro Hoshino, Martin Eckstein
O 68.2	Wed	11:00–11:30	TRE Phy	**Pump/probe photoemission spectroscopy in charge density wave insulators** — •James Freericks
O 68.3	Wed	11:30–12:00	TRE Phy	**Controlling magnetism and pairing in a periodically driven Hubbard model** — •Stephen Clark, Jonathan Coulthard, Juan Jose Mendoza-Arenas, Martin Eckstein, Dieter Jaksch, Andrea Cavalleri
O 68.4	Wed	12:00–12:30	TRE Phy	**Ultrafast Terahertz and XUV ARPES Probes of Quantum Materials Dynamics** — •Robert A. Kaindl
O 68.5	Wed	12:30–13:00	TRE Phy	**Ultrafast spin interactions revealed with terahertz radiation** — •Tobias Kampfrath
O 71.1	Wed	10:30–11:00	GER 38	**Electronic excitations in 2D materials and heterostructures** — •Kristian Sommer Thygesen
O 77.1	Wed	15:00–15:30	WIL A317	**Carbon Nanomembranes (CNM) : 2D Materials Beyond Graphene** — •Armin Gölzhäuser
O 79.1	Wed	15:00–15:30	WIL C307	**Sensing the Quantum Limit in Scanning Tunneling Spectroscopy: From the Josephson Effect to Quantum Tunneling** — •Christian R. Ast
O 83.1	Thu	9:30–10:15	TRE Phy	**Molecular adsorption on oxide surfaces: Insights from first-principles calculations** — •Bernd Meyer
O 87.1	Thu	10:30–11:00	WIL C307	**Structure and redox dynamics of ultrathin ceria films and nanostructures** — •Jan Ingo Flege
O 93.1	Thu	15:00–15:30	TRE Phy	**Oxygen and Oxide Cluster Functionalized Graphene for Model Catalytic Studies** — •Zdenek Dohnalek
O 93.2	Thu	15:30–16:00	TRE Phy	**Oxide model interfaces from ultrahigh vacuum conditions to liquid environments** — •Jörg Libuda
O 95.1	Thu	15:00–15:30	WIL A317	**Visualizing surface X-ray diffraction: the active phase of CO oxidation model catalysts** — •Johan Gustafson
O 97.1	Thu	15:00–15:30	REC/PHY C213	**The challenge of atomic resolution in liquid and ambient conditions with AFM** — •Alfred J. Weymouth
O 97.2	Thu	15:30–16:00	REC/PHY C213	**Single-molecule magnets: The influence of the surface** — •Katharina Diller
O 98.1	Thu	15:00–15:30	WIL C307	**Spin-charge transport phenomena on the atomic scale** — •Christoph Tegenkamp
O 98.2	Thu	15:30–16:00	WIL C307	**Electronic properties of functional organic materials at surfaces** — •Petra Tegeder
O 99.1	Thu	16:00–16:30	GER 38	**Spectacular success of DFT in predicting novel topological phases** — •Arun Bansil
O 101.1	Thu	17:00–17:30	TRE Phy	**Density Functional Theory in Surface Science and Catalysis - Successes and Limitations** — •Felix Studt
O 105.1	Fri	9:30–10:15	TRE Phy	**The Surface Chemistry of Anatase (001) and Rutile (110) in Solution: Atomically Flat Surfaces and Near-Ideal Organic Monolayers** — •Melissa Hines
O 109.1	Fri	10:30–11:00	WIL A317	**Discovery of 1D spin-polarized states at step edges of topological crystalline insulators** — •Paolo Sessi
O 110.1	Fri	10:30–11:00	GER 38	**Ceramics for Metal-Organic Frameworks (MOFs) based devices** — •Paolo Falcaro
O 112.1	Fri	13:15–14:00	HSZ 01	**Helical Molecules and Surfaces: Self-Assembly, Spin Filtering and Unidirectional Motors** — •Karl-Heinz Ernst

Invited talks of the joint symposium SYLI

See SYLI for the full program of the symposium.

SYLI 1.1	Mon	9:30–10:00	HSZ 02	**Interfacial challenges in solid- state Li ion: some perspectives from theory** — •Alan Luntz, Saskia Stegmaier, Johannes Voss, Karsten Reuter

SYLI 1.2	Mon	10:00–10:30	HSZ 02	**Will solid electrolytes enable lithium metal anodes in solid state batteries?** — •Jürgen Janek, Dominik Weber, Wolfgang Zeier
SYLI 1.3	Mon	10:30–11:00	HSZ 02	**Hybrid Electrolytes for Solid-State Batteries** — •Hans-Dieter Wiemhöfer
SYLI 1.4	Mon	11:15–11:45	HSZ 02	**Neutron diffraction on solid-state battery materials** — •Helmut Ehrenberg, Anatoliy Senyshyn, Mykhailo Monchak, Sylvio Indris, Joachim Binder
SYLI 1.5	Mon	11:45–12:15	HSZ 02	**Sulfate-based Solid-State Batteries** — •Yuki Katoh

Invited talks of the joint symposium SYQO

See SYQO for the full program of the symposium.

SYQO 1.1	Thu	9:30–10:00	HSZ 02	**Quantum dot based quantum technologies** — •Pascale Senellart
SYQO 1.2	Thu	10:00–10:30	HSZ 02	**Controlled strong coupling of a single quantum dot to a plasmonic nanoresonator at room temperature** — Heiko Gross, Joachim M. Hamm, Tommaso Tufarelli, Ortwin Hess, •Bert Hecht
SYQO 1.3	Thu	10:30–11:00	HSZ 02	**High efficiency and directional emission from a nanoscale light source in a planar optical antenna** — •Mario Agio
SYQO 1.4	Thu	11:30–12:00	HSZ 02	**Tailoring quantum states by measurement** — •Jörg Wrachtrup
SYQO 1.5	Thu	12:00–12:30	HSZ 02	**Quantum optics and quantum control at the nanoscale with surface plasmon polaritons** — •Stéphane Guérin

Invited talks of the joint symposium SYLM

See SYLM for the full program of the symposium.

SYLM 1.1	Thu	15:00–15:30	HSZ 02	**Light matter interaction in TMDs and their heterostructures** — •Ursula Wurstbauer
SYLM 1.2	Thu	15:30–16:00	HSZ 02	**Quantum optics with deterministically positioned quantum emitters in a two-dimensional semiconductor** — •Brian Gerardot
SYLM 1.3	Thu	16:00–16:30	HSZ 02	**Light-matter coupling with atomic monolayers in microcavities** — •Christian Schneider
SYLM 1.4	Thu	17:00–17:30	HSZ 02	**Properties of Synthetic 2D Materials and Heterostructures** — •Joshua Robinson
SYLM 1.5	Thu	17:30–18:00	HSZ 02	**Exciton spectroscopy in transition metal dichalcogenide monolayers and van der Waals heterostructures** — •Bernhard Urbaszek
SYLM 1.6	Thu	18:00–18:30	HSZ 02	**Strain-induced single-photon emitters in layered semiconductors** — •Rudolf Bratschitsch

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Fri	10:30–11:00	HSZ 02	**Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations** — •Weitao Yang
SYES 1.2	Fri	11:00–11:30	HSZ 02	**Multi-reference density functional theory** — •Andreas Savin
SYES 1.3	Fri	11:30–12:00	HSZ 02	**Density functionals from machine learning** — •Kieron Burke
SYES 1.4	Fri	12:00–12:30	HSZ 02	**Taming Memory-Dependence in Time-Dependent Density Functional Theory** — •Neepa Maitra
SYES 1.5	Fri	12:30–13:00	HSZ 02	**Quantum Embedding Theories** — •Fred Manby

Sessions

O 1.1–1.1	Mon	9:30–10:15	TRE Phy	**Overview Talk: Andreas Heinrich**
O 2.1–2.5	Mon	9:30–12:15	HSZ 02	**Symposium Interfacial Challenges in Solid-State Li Ion Batteries**
O 3.1–3.10	Mon	10:30–13:00	TRE Phy	**Scanning Probe Techniques: Method Development I**
O 4.1–4.10	Mon	10:30–13:00	TRE Ma	**Plasmonics and Nanooptics I: Light-Matter Interactions**

O 5.1–5.10	Mon	10:30–13:00	WIL A317	**Organic-Inorganic Hybrid Systems and Organic Films I**
O 6.1–6.10	Mon	10:30–13:00	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - I**
O 7.1–7.9	Mon	10:30–12:45	WIL C107	**Electronic Structure of Surfaces: Magnetism and Spin Phenomena**
O 8.1–8.10	Mon	10:30–13:00	REC/PHY C213	**2D Materials Beyond Graphene I**
O 9.1–9.10	Mon	10:30–13:00	WIL C307	**Solid-Liquid Interfaces: Structure, Spectroscopy I**
O 10.1–10.1	Mon	15:00–15:45	TRE Phy	**Overview Talk: Jascha Repp**
O 11.1–11.7	Mon	15:00–16:45	TRE Ma	**Plasmonics and Nanooptics II: Light-Matter Interaction**
O 12.1–12.7	Mon	15:00–16:45	WIL A317	**Organic-Inorganic Hybrid Systems and Organic Films II**
O 13.1–13.12	Mon	15:00–18:15	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - II**
O 14.1–14.10	Mon	15:00–17:30	WIL C107	**Electronic Structure of Surfaces: Magnetism and Spin Phenomena II**
O 15.1–15.5	Mon	15:00–16:15	WIL B321	**Solid-Liquid Interfaces: Structure, Spectroscopy II**
O 16.1–16.4	Mon	15:45–16:45	IFW A	**SYLI: Interfacial Challenges in Solid-State Li Ion Batteries - Interface-dominated behaviour**
O 17.1–17.9	Mon	15:45–18:00	TRE Phy	**Scanning Probe Techniques: Method Development II**
O 18.1–18.6	Mon	16:00–17:30	WIL C307	**Semiconductor Substrates: Structure, Epitaxy and Growth**
O 19.1–19.10	Mon	16:00–18:30	REC/PHY C213	**2D Materials Beyond Graphene II**
O 20.1–20.7	Mon	16:30–18:15	WIL B321	**Solid-Liquid Interfaces: Reactions and Electrochemistry - Experiment I**
O 21.1–21.6	Mon	17:00–18:30	TRE Ma	**Plasmonics and Nanooptics III: Light-Matter Interaction**
O 22.1–22.6	Mon	17:00–18:30	WIL A317	**Organic-Inorganic Hybrid Systems and Organic Films III**
O 23.1–23.3	Mon	17:15–18:00	IFW A	**SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - sulphate- and phosphate-based electrolytes**
O 24.1–24.4	Mon	17:30–18:30	WIL C307	**Semiconductor Substrates: Adsorption**
O 25.1–25.1	Tue	9:30–10:15	TRE Phy	**Overview Talk: Axel Groß**
O 26.1–26.5	Tue	10:15–11:30	IFW A	**SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - NMR studies**
O 27.1–27.7	Tue	10:30–12:30	TRE Phy	**Surface Dynamics: Theory**
O 28.1–28.10	Tue	10:30–13:00	TRE Ma	**Plasmonics and Nanooptics IV: Light-Matter Interaction**
O 29.1–29.10	Tue	10:30–13:00	WIL A317	**Organic-Inorganic Hybrid Systems and Organic Films IV**
O 30.1–30.9	Tue	10:30–13:00	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - III**
O 31.1–31.10	Tue	10:30–13:00	WIL C107	**Oxide and Insulator Surfaces: Structure, Epitaxy and Growth I**
O 32.1–32.8	Tue	10:30–13:00	WIL C307	**Focus Session: Charge Transport at Surfaces and Nanostructures with Multi-probe Techniques I**
O 33.1–33.10	Tue	10:30–13:00	REC/PHY C213	**Nanostructures at Surfaces: Metals, Oxides and Semiconductors I**
O 34.1–34.6	Tue	10:30–12:15	HSZ 101	**Solid-Liquid Interfaces: Reactions and Electrochemistry - Experiment II**
O 35.1–35.4	Tue	12:15–13:15	HSZ 101	**Solid-Liquid Interfaces: Reactions and Electrochemistry - Theory I**
O 36.1–36.4	Tue	14:00–16:00	TRE Phy	**ELI-ALPS: A New European Light Source for Ultrafast Surface Science**
O 37.1–37.8	Tue	14:00–16:00	TRE Ma	**Plasmonics and Nanooptics V: Light-Matter Interaction**

O 38.1–38.7	Tue	14:00–16:00	WIL A317	**Organic-Inorganic Hybrid Systems and Organic Films V**
O 39.1–39.8	Tue	14:00–16:00	WIL C107	**Oxide and Insulator Surfaces: Structure, Epitaxy and Growth II**
O 40.1–40.4	Tue	14:00–15:15	WIL C307	**Focus Session: Charge Transport at Surfaces and Nanostructures with Multi-probe Techniques II**
O 41.1–41.8	Tue	14:00–16:00	REC/PHY C213	**Nanostructures at Surfaces: Metals, Oxides and Semiconductors II**
O 42.1–42.8	Tue	14:00–16:00	WIL B321	**Solid-Liquid Interfaces: Reactions and Electrochemistry - Theory II**
O 43.1–43.1	Tue	15:30–16:00	WIL C307	**Gaede Prize Talk**
O 44.1–44.8	Tue	18:30–20:30	P1A	**Metal Substrates: Structure, Epitaxy and Growth**
O 45.1–45.26	Tue	18:30–20:30	P1A	**Organic-Inorganic Hybrid Systems and Organic Films**
O 46.1–46.24	Tue	18:30–20:30	P1A	**Electronic Structure of Surfaces: Spectroscopy, Surface States**
O 47.1–47.8	Tue	18:30–20:30	P1A	**Electronic Structure of Surfaces: Magnetism and Spin Phenomena**
O 48.1–48.6	Tue	18:30–20:30	P1A	**Oxide and Insulator Surfaces: Structure, Epitaxy and Growth**
O 49.1–49.6	Tue	18:30–20:30	P1A	**Oxide and Insulator Surfaces: Adsorption**
O 50.1–50.7	Tue	18:30–20:30	P1A	**Semiconductor Substrates: Structure, Epitaxy, Growth and Adsorption**
O 51.1–51.24	Tue	18:30–20:30	P1C	**Nanostructures at Surfaces: 1D and 2D Structures and Networks**
O 52.1–52.13	Tue	18:30–20:30	P1C	**Nanostructures at Surfaces: Dots, Particles, Clusters**
O 53.1–53.12	Tue	18:30–20:30	P1C	**Nanostructures at Surfaces: Other Aspects**
O 54.1–54.5	Tue	18:30–20:30	P1C	**Metallic Nanowires on Semiconductor Surfaces**
O 55.1–55.14	Tue	18:30–20:30	P2-EG	**Graphene**
O 56.1–56.20	Tue	18:30–20:30	P2-EG	**2D Materials beyond Graphene**
O 57.1–57.7	Tue	18:30–20:30	P2-EG	**Ultrafast Electron and Spin Dynamics**
O 58.1–58.4	Tue	18:30–20:30	P2-EG	**Surface Science: Misc.**
O 59.1–59.32	Tue	18:30–20:30	P2-OG1	**Plasmonics and Nanooptics**
O 60.1–60.11	Tue	18:30–20:30	P2-OG2	**Solid-Liquid Interfaces: Structure, Spectroscopy, Reactions and Electrochemistry**
O 61.1–61.8	Tue	18:30–20:30	P2-OG2	**Heterogeneous Catalysis**
O 62.1–62.4	Tue	18:30–20:30	P2-OG2	**Surface Dynamics**
O 63.1–63.17	Tue	18:30–20:30	P2-OG3	**Focus Session: Charge Transport at Surfaces and Nanostructures with Multi-probe Techniques**
O 64.1–64.13	Tue	18:30–20:30	P2-OG3	**Scanning Probe Techniques: Method development**
O 65.1–65.12	Tue	18:30–20:30	P2-OG4	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond**
O 66.1–66.1	Wed	9:30–10:15	TRE Phy	**Overview Talk: Anders Nilsson**
O 67.1–67.5	Wed	10:15–11:30	IFW A	**SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - defects, structure and thermodynamics**
O 68.1–68.5	Wed	10:30–13:00	TRE Phy	**Focus Session: Non-equilibrium Dynamics in Light-driven Materials: Theory Meets Experiment**
O 69.1–69.8	Wed	10:30–12:30	TRE Ma	**Plasmonics and Nanooptics VI: Light-Matter Interactions and Characterisation**
O 70.1–70.10	Wed	10:30–13:00	WIL A317	**2D Materials Beyond Graphene III**
O 71.1–71.9	Wed	10:30–13:00	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - IV**
O 72.1–72.9	Wed	10:30–12:45	WIL C107	**Oxide and Insulator Surfaces: Adsorption I**
O 73.1–73.10	Wed	10:30–13:00	REC/PHY C213	**Nanostructures at Surfaces: Metals, Oxides and Semiconductors III**
O 74.1–74.4	Wed	11:45–12:45	IFW A	**SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - hybrid and structured electrolytes**
O 75.1–75.15	Wed	15:00–18:45	TRE Phy	**Ultrafast Electron and Spin Dynamics**
O 76.1–76.12	Wed	15:00–18:00	TRE Ma	**Plasmonics and Nanooptics VII: Applications and Other Aspects**

O 77.1–77.10	Wed	15:00–17:45	WIL A317	**2D Materials Beyond Graphene IV**
O 78.1–78.13	Wed	15:00–18:15	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - V**
O 79.1–79.12	Wed	15:00–18:15	WIL C307	**Electronic Structure of Surfaces: Spectroscopy, Surface States I**
O 80.1–80.4	Wed	15:45–16:45	IFW D	**SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - Structure - property relationships II**
O 81.1–81.10	Wed	16:00–18:30	WIL C107	**Oxide and Insulator Surfaces: Adsorption II**
O 82.1–82.10	Wed	16:00–18:30	REC/PHY C213	**Nanostructures at Surfaces: Graphene and Other Aspects**
O 83.1–83.1	Thu	9:30–10:15	TRE Phy	**Overview Talk: Bernd Meyer**
O 84.1–84.7	Thu	9:30–12:30	POT 51	**Focus Session: Semiconductor Materials and Nanostructure for Photocatalysis**
O 85.1–85.10	Thu	10:15–13:00	ZEU 114	**Thin Films, Nanostructures and Nanoparticles I**
O 86.1–86.10	Thu	10:30–13:00	WIL A317	**Graphene: Electronic Properties, Structure and Substrate Interaction I**
O 87.1–87.9	Thu	10:30–13:00	WIL C307	**Metal Substrates: Structure, Epitaxy and Growth**
O 88.1–88.13	Thu	10:30–13:45	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VI**
O 89.1–89.9	Thu	10:30–12:45	TRE Phy	**Oxide and Insulator Surfaces: Adsorption III**
O 90.1–90.9	Thu	10:30–12:45	WIL C107	**Surface Dynamics: Experiments**
O 91.1–91.10	Thu	10:30–13:00	REC/PHY C213	**Nanostructures at Surfaces: Molecular Systems I**
O 92.1–92.5	Thu	10:30–13:00	TRE Ma	**Gerhard Ertl Young Investigator Award**
O 93.1–93.6	Thu	15:00–17:00	TRE Phy	**Heterogeneous Catalysis: Experiment**
O 94.1–94.13	Thu	15:00–18:15	TRE Ma	**Graphene: Electronic Properties, Structure and Substrate Interaction II**
O 95.1–95.12	Thu	15:00–18:15	WIL A317	**Metal Substrates: Adsorption of Atoms and Inorganic Molecules**
O 96.1–96.11	Thu	15:00–17:45	WIL C107	**Metallic Nanowires on Semiconductor Surfaces**
O 97.1–97.12	Thu	15:00–18:30	REC/PHY C213	**Nanostructures at Surfaces: Molecular Systems II**
O 98.1–98.2	Thu	15:00–16:00	WIL C307	**Nanostructures at Surfaces: 1D Systems**
O 99.1–99.9	Thu	16:00–18:30	GER 38	**Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VII**
O 100.1–100.10	Thu	16:00–18:30	WIL C307	**Electronic Structure of Surfaces: Spectroscopy, Surface States II**
O 101.1–101.5	Thu	17:00–18:30	TRE Phy	**Heterogeneous Catalysis: Theory I**
O 102.1–102.3	Thu	17:45–18:30	WIL C107	**New Methods: Theory**
O 103	Thu	19:00–19:30	HSZ 01	**Annual Meeting of the Surface Science Division**
O 104	Thu	19:30–20:30	HSZ 01	**Post-Deadline Session**
O 105.1–105.1	Fri	9:30–10:15	TRE Phy	**Overview Talk: Melissa Hines**
O 106.1–106.10	Fri	10:30–13:00	WIL C107	**Electronic Structure of Surfaces: Spectroscopy, Surface States III**
O 107.1–107.10	Fri	10:30–13:00	TRE Phy	**Heterogeneous Catalysis: Theory II**
O 108.1–108.10	Fri	10:30–13:00	TRE Ma	**Graphene: Adsorption, Intercalation and Other Aspects**
O 109.1–109.9	Fri	10:30–13:00	WIL A317	**Tribology and Structure of Surfaces: Misc.**
O 110.1–110.9	Fri	10:30–13:00	GER 38	**Molecular Films: Morphology, Electronics, Photovoltaics**
O 111.1–111.10	Fri	10:30–13:00	REC/PHY C213	**Nanostructures at Surfaces: Molecular Systems III**
O 112.1–112.1	Fri	13:15–14:00	HSZ 01	**Overview Talk STM and Molecular Machines: Karl-Heinz Ernst**
O 113.1–113.10	Fri	10:15–13:00	ZEU 114	**Thin Films, Nanostructures and Nanoparticles II**

Annual General Meeting of the Surface Science Division

Thursday 19:00–19:30 HSZ 01

- Report of the Chairman

- Presentation of the Gerhard Ertl Young Investigator Award
- Miscellaneous

O 1: Overview Talk: Andreas Heinrich

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

Invited Talk O 1.1 Mon 9:30 TRE Phy

Electron Spin Resonance of single atoms on surfaces — •Andreas Heinrich — Ewha Womans University, Seoul, South Korea — Center for Quantum Nanoscience, IBS Research, South Korea

The scanning tunneling microscope is an amazing experimental tool because of its atomic-scale spatial resolution. This can be combined with the use of low temperatures, culminating in precise atom manipulation and spectroscopy with microvolt energy resolution. In this talk I will apply these techniques to the investigation of the quantum spin properties of transition metal atoms on surfaces. We will conclude with our recent measurements of electron spin resonance in an STM on individual Fe atoms supported on an insulating thin film, offering unprecedented energy resolution on the atomic scale.

O 2: Symposium Interfacial Challenges in Solid-State Li Ion Batteries

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

Invited Talk O 2.1 Mon 9:30 HSZ 02

Interfacial challenges in solid- state Li ion: some perspectives from theory — •Alan Luntz[1], Saskia Stegmaier[1], Johannes Voss[1], and Karsten Reuter[2] — [1]Stanford University, Stanford, CA, USA — [2]Technical University of Munich, Munich, Germany

Unfortunately, interfacial challenges severely limit power and cycle life in all solid- state Li ion batteries. We use theory to investigate some of the origins of these limitations with both continuum theory and DFT. The obvious ones are electrochemical stability of the electrolyte at the anode/cathode interfaces and mechanical issues relating to maintaining interfacial contact during cycling while inhibiting Li dendrite growth. We are especially trying to understand if any fundamental limitations exist from the structures of the double layers that form at the solid electrolyte- electrode or other interfaces in the solid-state stack. These can be quite different than in conventional liquid Li ion batteries. We use Li3OCl as a prototypical Li ion superionic conductor and discuss its properties and discuss its interface with model electrode interfaces.

Invited Talk O 2.2 Mon 10:00 HSZ 02

Will solid electrolytes enable lithium metal anodes in solid state batteries? — •Jürgen Janek, Dominik Weber, and Wolfgang Zeier — Institut für Physikalische Chemie, Justus Liebig-Universität, Gießen, Germany

In order to achieve solid state lithium batteries with higher energy densities [1], lithium metal anodes are one of the primary options. However, reversible and morphologically stable plating of thick lithium metal films is difficult, as void formation and dendrite growth may occur - leading to impedance growth and/or short-circuits. Ceramic electrolytes are considered as a potential solution to this problem. In this lecture the interface between solid electrolytes and lithium metal anodes will be discussed in depth, and the occurrence of both thermodynamic and kinetic instabilities will be highlighted. In particular, the existence of SEI (”solid electrolyte interphases”), forming between lithium metal and the solid electrolyte, will be demonstrated for a number of solid electrolytes. It will also be shown that the growth of these SEI layers follows a typical square-root law-type behavior in SEI formation in liquid electrolytes.

[1] J. Janek and W. Zeier, Nat. Energy 1 (2016) 16141

Invited Talk O 2.3 Mon 10:30 HSZ 02

Hybrid Electrolytes for Solid-State Batteries — •Hans-Dieter Wiemhöfer — Inst. Inorganic & Analyt. Chem., WWU Münster — Helmholtz-Institute Münster

Rechargeable lithium batteries with largely increased energy and power densities are a primary goal at present world wide. At the same time, enhanced safety concerns cause the need to replace current liquid electrolytes by new high performance electrolytes combining higher mechanical, thermal and electrochemical stability. Finally, this leads to the development of hybrid electrolytes. The primary idea is to construct electrolytes fulfilling a multitude of requirements based on a combination of components and phases, often coupled with approaches to achieve stable meso or micro porous networks down to chemically designed nanostructures. Starting from ion conducting inorganic solids and glasses, the combination with polymers and salt-in-polymer systems opens a wide range for possibilities for chemical design, tailoring and fine tuning of electrolyte properties of such hybrid systems. The concept will be illustrated with a number of examples, for instance, self organized block-copolymer networks acting as porous containers for fast ion conducting channels. Future all solid state batteries are expected to profit from hybrid concepts as well. For instance, volume changes during charging/discharging of active electrodes need an elastic polymer network acting as a glue and stabilizing a good contact and charge transfer kinetics of solid electrolyte/solid electrode interfaces.

15 min. break

Invited Talk O 2.4 Mon 11:15 HSZ 02

Neutron diffraction on solid-state battery materials — •Helmut Ehrenberg[1], Anatoliy Senyshyn[2], Mykhailo Monchak[1], Sylvio Indris[1], and Joachim Binder[1] — [1]Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM) — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universitaet Muenchen, Garching, Germany

Solid-state batteries are a promising approach to safer electrochemical energy storage and higher energy densities. Bottle necks are interface reactions and transport limitations in the solids. Advanced and optimized materials must provide dedicated properties, for example a good Li-ion conductivity for sufficiently high current densities and only small volume changes to preserve mechanical integrity. Neutron diffraction offers unique features to elucidate the underlying structure-property relationships, which determine the resulting performance parameters on cell level. Selected examples are shown, which demonstrate the capabilities of neutron diffraction to reveal Li-ion diffusion pathways as in the $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ (LATP) superionic conductor, Li occupation numbers at intermediate states of charge as for $LiCoPO_4$ or a comparison of volume changes between commercial and alternative zero-strain electrode materials. The capabilities of solid-state batteries are discussed.

Invited Talk O 2.5 Mon 11:45 HSZ 02

Sulfate-based Solid-State Batteries — •Yuki Katoh — Toyota Motor Europe NV/SA, Hoge Wei 33, Zaventem, Belgium

Large-scale batteries are in high demand for applications such as plug-in electric hybrid or electric vehicles, and smart electric power grids. The all-solid-state battery is the most promising candidate for future battery systems, due to the high energy density obtaining by direct-series-stacking of the battery cells. However, the poor electrochemical characteristics of the all-solid-state battery, due to higher cell-resistivity than conventional liquid electrolyte batteries, still remain as an unsolved issue. We will demonstrate an all-solid-state battery with extremely high power performance that employs the superionic conductors having the Li10GeP2S12-type crystal structure. The battery can operate over a wide temperature range with extremely high current drains of 3 mAcm-2 (-30 C), 100 mAcm-2 (25 C), and 1000 mAcm-2 (100 C). Careful electrochemical examination of the all-solid-state battery with the same battery configuration as a liquid electrolyte system revealed that the rate characteristics are simply dependent on the difference in state of electrolyte. The vert high power characteristics of solid state battery comes from intrinsic ion transportation mechanism of solid electrolyte.

O 3: Scanning Probe Techniques: Method Development I

Time: Monday 10:30–13:00 Location: TRE Phy

O 3.1 Mon 10:30 TRE Phy

Characterization and Optimization of High Frequency STM — •Gregory McMurtie[1,2], Max Hänze[1,2], Jacob Burgess[1,2], and Sebastian Loth[1,2,3] — [1]Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart — [3]Institut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart

Injecting coherent pulses (pump-probe[1]) or continuous wave signals (spin-resonance[2]) into a tunnel junction has shown promising results for the characterization of fast magnetic surface dynamics using STM. When pushing into the sub-nanosecond time domain, the transmission line characteristics of the instrument strongly modify the signals reaching to the tunnel junction. This is caused by impedance mismatches in the cabling that express as reflections, resonant cavities, or low-pass filtering. We present an in-situ technique for the quantitative measurement of transmission line characteristics. Both amplitude and phase information are detected and generate a more accurate picture of the tunnel junction than conventional high frequency characterization methods. This information is used to compensate for imperfections in the transmission lines, resulting in a greatly increased effective bandwidth. By improving the time resolution of the STM, the door is opened to observe a wide range of ultra-fast phenomena at the atomic scale. Additionally, the access to phase information hints at the possibility of observing coherent excitation's.

[1] S. Loth, A. J. Heinrich et. al, Science 329 1628 (2010). [2] S. Baumann, W. Paul, A. J. Heinrich et al., Science 350 6259 (2015)

O 3.2 Mon 10:45 TRE Phy

Tip-induced vs. thermal dehalogenation of 4-bromo-3”-iodo-p-terphenyl on Cu(111) — •Qigang Zhong[1,2], Daniel Ebeling[1], Tobias Schlöder[3], Sebastian Ahles[4], Lifeng Chi[2], Doreen Mollenhauer[3], Hermann A. Wegner[4], and André Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig University, Giessen, Germany — [2]Institute of Functional Nano & Soft Materials, Soochow University, Suzhou, P. R. China — [3]Institute of Physical Chemistry, Justus-Liebig University, Giessen, Germany — [4]Institute of Organic Chemistry, Justus-Liebig University, Giessen, Germany

Dehalogenation is an important step in Ullmann reaction, which is widely used in on-surface synthesis of various functional polymers. Controlled stepwise dehalogenation will help to build more refined and customized molecular structures. However, there are few investigations on the sequential dehalogenation process so far, especially at the atomic scale. Here, we evaporated 4-bromo-3”-iodo-p-terphenyl (BITP) molecules onto a cold Cu(111) surface (Tsam < 150 K). Subsequently, single-molecule deiodination and debromination reactions were triggered either by applying different voltage pulses above iodine and bromine substituents or by heating the sample substrate. The adsorption structures of the obtained radicals were characterized via low temperature non-contact atomic force microscopy (LT-NC-AFM) with sub-molecular resolution. The distinct pulse voltages needed for deiodination and debromination coincide with the difference in bond cleavage temperatures for iodine and bromine substituents.

O 3.3 Mon 11:00 TRE Phy

Design and Realization of a Variable-Temperature Scanning-Tunneling-Microscope for the Liquid-Solid Interface — •Oliver Ochs[1,2,3] and Markus Lackinger[1,2,3] — [1]Physik-Department - Technische Universität München, Munich, Germany — [2]Deutsches Museum, Munich, Germany — [3]Center for Nanoscience, Munich, Germany

Scanning-Tunneling-Microscopy (STM) at the liquid-solid interface is a widespread experimental technique in the field of nanoscience to investigate self-assembly of supramolecular monolayers. Most liquid-solid STMs work under ambient conditions at room temperature. However, to clarify relevant and fundamental scientific questions concerning the kinetics and thermodynamics of self-assembly, it is desirable to carry out experiments at variable temperatures. Yet, the common approach of just heating the sample inside an STM normally causes temperature gradients that result in thermal drift. Furthermore, increased solvent evaporation at higher temperatures leads to unwanted concentration changes of the solution. As a new strategy for instrument design, we propose an STM that operates fully immersed into solution. Therefore the STM is integrated in a heatable, hermetically closed container with precise temperature control and stability. This minimizes temperature gradients, facilitates rapid thermalization upon temperature changes, and completely avoids solvent evaporation. First tests and measurements proved the functionality and suitability of the instrument for variable temperature experiments in liquids up to 100°C without any limitation of experimental duration due to solvent evaporation.

O 3.4 Mon 11:15 TRE Phy

Electrochemistry at the Nanoscale: Theoretical and Practical Aspects of Electrochemical Strain Microscopy — •Valon Lushta[1], Stephan Bradler[2], Bernhard Roling[2], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig-University Gießen, D-35392 Gießen, Germany — [2]Department of Chemistry,Philipps-University Marburg, D-35032 Marburg, Germany

The implementation of renewable energy as the main energy source is only possible with reliable energy storage techniques. Current batteries lose a significant amount of storing capacity after a few hundreds of charge-discharge cycles.

Mechanical strain is one of the main causes for degradation processes in solid-state batteries. Electrochemical Strain Microscopy (ESM) is a powerful tool to measure strain at the nanoscale [1].

Recent studies have shown that quantitative measurements of the local strain require a deeper understanding of the ESM signal formation [2]. Here, we present a theoretical model for the cantilever motion, and we use this model to evaluate experimental results. We show that quantitative ESM requires corrections of the signals with respect to the local contact stiffness and to frequency tracking errors [3].

[1] S. Kalinin et al., Materials Today 14 (2011) 548

[2] S. Jesse et al., J. Phys. D: Appl. Phys. 44 (2011) 464006

[3] S. Bradler, A. Schirmeisen, B. Roling, MJ. Appl. Phys. (2016)

O 3.5 Mon 11:30 TRE Phy

Utilizing STM and AFM simultaneously to study atomic-scale magnetism — •Nadine Hauptmann, Jan Gerritsen, Daniel Wegner, and Alexander Ako Khajetoorians — Institute for Molecules and Materials, Radboud University, 6500 GL Nijmegen, The Netherlands

Recent developments in surface and interfacial magnetism have raised the question if it is possible to realize a memory derived from single atoms or nanometer sized skyrmions. Therefore, it is important to understand how the local magnetic anisotropy driven by the crystal field symmetry, magnetic exchange, and hybridization influences the magnetization at the atomic length scale. Nevertheless, a vast majority of atomic-scale studies have utilized spin-polarized scanning tunneling microscopy (SP-STM), limiting the scope of materials which can be probed. In order to gain new insight into magnetism at the atomic scale, we combine SP-STM with magnetic exchange force microscopy (MExFM), based on a qPlus tuning fork design. We discuss our recent developments and demonstrate that our approach enables simultaneous measurement of the spin polarized current and the exchange force at the single atom level.

O 3.6 Mon 11:45 TRE Phy

Sensing complex tip-surface interactions with multifrequency AFM — •Daniel Platz[1,2], Daniel Forchheimer[2], and David B. Haviland[2] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]KTH Royal Institute of Technology, Albanova University Center, 10691 Stockholm, Sweden

In recent years multifrequency atomic force microscopy (AFM) revealed its potential to overcome limitations in the spatial and compositional resolution of conventional force microscopy methods. Conventionally tip-surface interactions are considered as functions of the tip position only, so-called force curves. However, especially for soft materials tip-surface interactions often depend on the tip velocity and the past tip trajectory. Here, we introduce a compact and general description of these interactions appropriate to dynamic AFM where the measurement of force is restricted to a narrow frequency band. We represent the tip-surface interaction in terms of a force disk in the phase space of position and velocity. Determination of the amplitude dependence of tip-surface forces at a fixed static probe height allows for a comprehensive treatment of conservative and dissipative interactions. We illuminate the fundamental limitations of force reconstruction with narrow band dynamic AFM and we show how the amplitude dependence of the Fourier component of the force at the tip oscillation frequency, gives insight into the detailed nature of the tip-surface interaction and allows for a quantitative force reconstruction.

O 3.7 Mon 12:00 TRE Phy

Observation of non-linear dynamics in ultra high vacuum Atomic Force Microscopy — •Daniel Forchheimer[1,2], Christian Wagner[3], Daniel Platz[1], and David Haviland[1] — [1]Kungliga Tekniska Högskolan, Stockholm, Sweden — [2]Intermodulation Products AB, Sweden — [3]Peter Grünberg Institute, Jülich, Germany

The tip-surface force in atomic force microscopy goes from being attractive to repulsive as the tip-surface separation change by only a few nano meters. Despite this highly nonlinear force the motion of cantilevers and tuning forks in ultra high vacuum AFMs lack many of the typical signatures of a nonlinear system, such as the the generation of higher harmonics. This is due to the extremely high quality factors of the force probes in vacuum which effectively dampen any off-resonance motion, masking the nonlinear interaction.

We have previously developed Intermodulation AFM for ambient condition, in which the AFM cantilever is excited with two frequencies near a single resonance. We applied such an excitation to a tuning fork AFM in vacuum and could observe the generation of several mixing tones, or intermodulation products, near resonance. These are clear signatures of a nonlinear interaction and by measuring the amplitude and phase at multiple such frequencies we could characterize conservative and dissipative properties of the interaction.

O 3.8 Mon 12:15 TRE Phy

Characterization and variation of a single molecule-metal bond via AFM-based manipulation — •Philipp Leinen[1,2], Matthew F. B. Green[1,2], Christian Wagner[1,2], Ruslan Temirov[1,2], and F. Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology

Mechanical manipulation of molecules with the scanning probe microscope (SPM) is a versatile technique to study single-molecule properties and create new devices. A single bond established between the SPM tip and a reactive atom within the molecule is a very precise way to apply forces in such a manipulation and its understanding is therefore crucial. We studied the prototypical bond between carboxylic oxygen atoms of perylene-tetracarboxylic dianhydride (PTCDA) and the Ag terminated tip of a non-contact AFM/STM regarding its mechanical properties as well as the deformation the molecule undergoes during contacting and slight tip retraction. We focus on molecules within a layer which are retained by their neighbors, thus facilitating controlled tip-molecule bond breaking by mechanical stress alone. The bond forming and breaking also provides a sensitive probe to study the balance between intra- and intermolecular interactions. For the two inequivalent molecules in the unit cell of PTCDA/Ag(111) we observe that the tip height at which the bond to chemically identical oxygen atoms is established varies by 0.4 Å depending on the local environment of each oxygen in the monolayer. The data thus provides a sensitive benchmark for theory beyond just adsorption energy and height.

O 3.9 Mon 12:30 TRE Phy

simultaneous high-resolution AFM/STM/IETS imaging of FePc on Au(111) . — •bruno de la torre[1,2], martin svec[1], radek zboril[2], and pavel jelinek[1] — [1]Institute of Physics of the CAS, Prague, Czech Republic. — [2]Regional Centre of Advanced Technologies and Materials, Palacký University, Olomouc, Czech Republic.

The recent progress in scanning probe microscopy provided unprecedented atomic resolution of single organic molecules on surfaces. Namely, the submolecular resolution was achieved in AFM [1], STM [2] and also IETS [3] mode employing functionalized tips. The origin of the submolecular contrast can be rationalized by a simple mechanical model introducing a lateral bending of a flexible tip apex [4,5]. However direct experimental evidence correlating the AFM/STM/IETS imaging mechanisms has been missing so far.

Here we present simultaneous high resolution AFM/STM/IETS imaging of iron(II) phthalocyanine (FePc) on Au(111) surface acquired with CO-functionalized probe. The acquired data demonstrate unambiguously the common imaging mechanism of the modes. We will show that not only renormalization of the frustrated translational mode [5], but also renormalization of the amplitude of IETS signal affect the IETS imaging.

[1] L. Gross et al., Science 325,1110 (2009). [2] C. Weiss et al., Phys. Rev. Lett. 105, 086103 (2010). [3] C.I. Chiang et al Science 344, 885 (2014). [4] P. Hapala et al., Phys. Rev. B 90, 085421 (2014). [5] P. Hapala et al., Phys. Rev. Lett. 113, 226101 (2014).

O 3.10 Mon 12:45 TRE Phy

Characterization of polycyclic conjugated hydrocarbons by means of NCAFM — •Zsolt Majzik[1], Niko Pavliček[1], Manuel Vilas-Varela[2], Nikolaj Moll[1], Dolores Pérez[2], Enrique Guitián[2], Gerhard Meyer[1], Diego Peña[2], and Leo Gross[1] — [1]IBM Research-Zurich, 8803 Rüschlikon, Switzerland — [2]CIQUS and Departamento de Química Orgánica, Universidade de Santiago de Compostela. Santiago de Compostela 15782, Spain.

The development of organic field effect transistors (OFETs) and organic photovoltaics (OPVs) triggered a strong interest for synthesizing and characterizing conjugated polycyclic hydrocarbons. Anti-aromatic and open-shell systems received recently a special attention because of their distinct electronic and magnetic behavior. The strong reactivity of pristine molecules creates a challenge for probing their structural and electrical properties. Until now, the fundamental analyses of these reactive compounds have been limited to theoretical works or the lifetime of a molecule was increased by careful attachment of protecting ligands for experimental investigations. Advances in atomic force microscopy, particularly resolving and modifying the structure of molecules at the atomic scale opened new routes for studying highly reactive compounds. Here we present an alternative route for the synthesis and characterization of conjugated systems. We deposited custom synthesized precursor molecules and carried out the final synthesis step in UHV environment via atomic manipulation. We used combined AFM/STM analyses supported by DFT calculations to determine the aromatic configuration of a molecule.

O 4: Plasmonics and Nanooptics I: Light-Matter Interactions

Time: Monday 10:30–13:00 Location: TRE Ma

O 4.1 Mon 10:30 TRE Ma

Nanoplasmonics from large-scale ab initio calculations: opposite trends in Ag and Na clusters — •Marc Barbry[1], Peter Koval[2], Natalia E. Koval[1], Javier Aizpurua[1], and Daniel Sánchez[1,2] — [1]Material Physics Center, San Sebastián, Spain — [2]Donostia International Physics Center, San Sebastián, Spain

An accurate description of electronic excitations is indispensable for understanding material properties and designing nanoscale devices. For instance, using large-scale TDDFT calculations, we have recently demonstrated the importance of taking into account the details of the atomic-scale structure [1] and the quantization of electron transport [2] in metal nanostructures in order to accurately describe their plasmonic properties. In this contribution we will compare the surface plasmon resonance of sodium and silver clusters within the same framework of *iterative* TDDFT [3]. Recent progress in our implementation made it possible to perform calculations of large clusters of diameters ranging from a few Å to 4–5 nm, counting up to 5000 silver atoms and using only modest computational resources (a 32-core node with 500GB RAM). With these new capabilities, we have characterized the size-scaling of the SPR frequency for both sodium and silver clusters. As expected these two materials show opposite behaviours that can be related to the different spill out of charge at the surface and to the additional screening created by the 4*d* electrons in silver.

[1] M. Barbry *et al.* *Nano Letters*, **15** (2015) 3410. [2] F. Marchesin *et al.* *ACS Photonics*, **3** (2016) 269. [3] P. Koval *et al.* *J. Phys.: Condens. Matter*, **28** (2016) 214001.

O 4.2 Mon 10:45 TRE Ma

Mueller matrix investigation of gold gratings — •Meng Wang, Anja Löhle, Bruno Gompf, Martin Dressel, and Audrey Berrier — 1. Physikalisches Institut and Research Center SCoPE, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Surface plasmon polaritons (SPPs), dispersive collective electron excitations propagating along metal-dielectric interfaces leading to strong field confinement, are powerful ways to control the electromagnetic field. They foster promising applications, e.g., in sensing and nanophotonics. In this work, a plasmonic one-dimensional grating fabricated by evaporating gold thin films on an elastomer is investigated by Mueller Matrix (MM) spectroscopic ellipsometry, a powerful tool to characterize the interaction of nanostructured objects with polarized light. All 16 MM elements were measured in reflection. To evaluate the respective role of specific features, such as plasmonic modes, anisotropy, material absorption, or simply diffraction orders, the optical response was measured at various angles of incidence and different azimuthal orientations over a broad frequency range. Hence, the complex interactions resulting from the interplay of these excitations can be unravelled. Modelling of the optical properties based on a biaxial model completes the study. Anisotropy, SPPs, diffraction orders and inter-band transition are distinguished from their different dispersive behaviour and explain all MM features. This knowledge can help to better understand how to tailor the specific excitations and provides guidelines for the design of novel optical functionalities using nanostructured materials.

O 4.3 Mon 11:00 TRE Ma

Pump-probe nanoscopy with NIR to deep THz radiation — •F. Kuschewski[1], S.C. Kehr[1], J. Döring[1], N. Awari[2], B. Green[2], S. Kovalev[2], M. Gensch[2], and L.M. Eng[1] — [1]Institut für Angewandte Physik, TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf

Recently, scattering-type scanning near-field infrared microscopy (s-SNIM) was successfully combined with pump-probe experiments pushing the temporal resolution of s-SNIM down to a few fs [1]. That combination offers spectacular possibilities to explore the dynamics of nanoscale physical devices, but usually shows a low optical contrast due to high background signals. We analyzed the frequency spectrum in pump-probe s-SNIM finding sidebands to the main carrier frequency that provide a much higher signal-to-noise ratio, as proven both by simulations and recent experiments [2]. Experimentally a greatly increased contrast in the 1st order sideband was found [2], that now has been extended up to the 5th order, applying s-SNIM to a structured gold/semiconductor sample. Note that our approach is applicable to the broad spectral range from visible to THz wavelengths.

[1] M. Wagner et al. *Nano Lett.* **14**, 894 (2014).
[2] F. Kuschewski et al. *Sci. Rep.* **5**, 12582 (2015).

O 4.4 Mon 11:15 TRE Ma

Photon emission from plasmonic tunnel junctions including a microscope tip and metallic quantum wells — •Tomoki Sueyoshi, Peter-Jan Peters, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, CAU Kiel, Germany

Radiative decay processes involving tunneling electrons are studied by probing light emission from metallic quantum-well (QW) junctions in a scanning tunneling microscope. The electronic states of Pb QWs on Ag(111) are controlled with the number of Pb layers and identified by scanning tunneling spectroscopy. The luminescence from the tip-QW-metal junctions involves radiative decay of tip-induced localized plasmons excited by inelastic tunneling electrons. The observed optical spectra reflect the plasmon density of states in the junctions. In addition, intense emission is observed from transitions of tunneling electrons between unoccupied QW states. These results demonstrate plasmon-assisted luminescence induced by tunneling electrons in the QW tunnel junctions.

O 4.5 Mon 11:30 TRE Ma

Temporal dynamics of nanowire based lasers — •Robert Röder[1], Themistoklis Sidiropoulos[2], Rupert F. Oulton[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Germany — [2]Imperial College London, UK

Reinforced work in the field of nanophotonics for on-chip integrated optical components is urgent to provide novel approaches for optical data processing which can circumvent the forthcoming limitations of conventional electronic circuits. Here, II-VI compound semiconductor nanowires (NW) provide robust high optical gain and show beneficial Fabry-Pérot resonator properties allowing low threshold NW lasing at room temperature [Geburt et al, Nanotechnology 23, 365204 (2012)] and even continuous wave emission [Röder et al, Nano Letters 13, 3602 (2013)]. Yet, optical confinement in semiconductor NWs, and thus there size, is diffraction limited. However, plasmonic lasers using semiconductor NWs as gain medium have generated significant interest, since the optical mode size in these systems is far below the vacuum wavelength. By exploiting the natural non-linearity of the laser process itself, we investigate the laser dynamics of both photonic [Röder et al, Nano Lett. 15, 4637 (2015)] and plasmonic NW lasers [Sidiropoulos et al., Nat. Phys. 10, 870 (2014)], which are of high interest for concepts of ultrafast optical switching, nanosensing and nanospectroscopy.

O 4.6 Mon 11:45 TRE Ma

Using plasmonic nanoantennas to read out the orbital angular momentum of light — •Richard M. Kerber[1], Jamie M. Fitzgerald[2], Sang Soon Oh[2], Ortwin Hess[2], and Doris E. Reiter[1,2] — [1]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — [2]Department of Physics, The Blackett Laboratory, Imperial College London, South Kensington Campus, London SW7 2AZ, United Kingdom

The orbital angular momentum of light has recently been recognized as a new degree of freedom to encode information in communication technology. One way to determine the orbital angular momentum of light is to destroy the helical wavefront of the light beam. We here propose an alternative way to read out the orbital angular momentum of light using plasmonic nanoantennas by converting the phase information into spectral information without losing the phase properties of the beam. Using the excitation of bright and dark modes of a plasmonic nanoantenna, which exhibit different resonant wavelengths, the determination of the value of orbital angular momentum of the light beam becomes possible. Exemplary considering rotation-symmetrical nanorod antennas we show that their scattering cross-section is sensitive to the value of orbital angular momentum combined with the polarization of an incident orbital angular momentum light beam. For the simulation of the scattering cross-section we use the boundary element method and further predict the orbital angular momentum dependence of the excited modes with an analytical line antenna model.

O 4.7 Mon 12:00 TRE Ma

Temporal characteristics of intense tunable pulses from an infrared free-electron laser — •Riko Kiessling, Sandy Gewinner, Wieland Schöllkopf, Martin Wolf, and Alexander Paarmann — Fritz-Haber-Institut der MPG, Berlin

For the generation of coherent radiation in the infrared region, the free-electron laser (FEL) posseses unique properties regarding intensity, wavelength tunability and short pulse durations. Covering the spectral range from 3 to 50 μm, the IR FEL at the Fritz Haber Institute is dedicated to (non-)linear spectroscopy of vibrational resonances in molecules, clusters and solid matter.

Here, we present the first cross-correlation measurements of the ps FEL pulses with a synchronized fs fiber oscillator via sum-frequency generation in nonlinear media. The observed FEL pulse intensity envelope confirms a lasing behavior typical for oscillator-type FELs [1]. Also, the influence of the FEL cavity detuning on the temporal shape, duration and fluctuation of the IR pulse is discussed. Using a differential cross-correlation scheme [2] will allow the exact determination of the absolute timing between accelerator-based and table-top optical pulses, which enables time-resolved studies of FEL-induced transient processes in solid-state systems.

[1] Knippels et al., PRL 83, 1578 (1999)
[2] Schulz et al., Nat. Commun. 6, 5938 (2015)

O 4.8 Mon 12:15 TRE Ma

Tip modified fluorescence — •Jonas Albert and Markus Lippitz — Experimental Physics III, University of Bayreuth, Germany

In Near Field Microscopy the near field interaction is used to overcome the diffraction limit. We utilise the near-field interaction to modify fluorescence of our samples by the presence of the near-field probe, a metal coated AFM-tip. First experiments on CdSe nanocrystals show significant changes in the fluorescence lifetime dependent on the distance between crystal and a gold-tip.

Furthermore the optical fields at the near-field probe are confined in a space much smaller than the wavelength and therefore showing a high field gradient on the nanometer scale. We are using the optical field gradients to enhance dipole forbidden transitions in coherent excitonic systems, such as wire-like molecular aggregates.

O 4.9 Mon 12:30 TRE Ma

Strongly Enhanced Mid-Infrared Second Harmonic Generation from Weak Optical Phonon Modes — •Alexander Paarmann, Ilya Razdolski, Sandy Gewinner, Wieland Schöllkopf, and Martin Wolf — Fritz-Haber-Institut, Berlin, Germany

Mid-infrared second harmonic generation (SHG) spectroscopy [1] provides a unique access to optical phonon resonances in the nonlinear-optical response of polar dielectrics, representing an alternativ spectroscopic approach to established techniques like infrared or Raman spectroscopy. Specifically, the SHG signal is sensitive not only to resonances in the nonlinear susceptibility, but also to the local electromagnetic fields determined by the linear optics. Here, we demonstrate how this intertwined sensitivity can be exploited for enhancement of the SHG specfically for weak oscillators.

Our experiments employ intense, tunable and narrowband mid-infrared pulses from a free-electron laser to acquire SHG excitation spectra from 4H-SiC with the c-axis of the uniaxial crystal in the surface plane [2]. Depending on the crystal azimuthal angle, we observe sharp enhancement of the SHG yield at the frequency of a weak zone-folded mode that exists in 4H-SiC due to the layer stacking along the c-axis. Perspectives are discussed on how to use this effect to detect periodic lattice distortions in strongly correlated insulators.

[1] Paarmann et al., Appl. Phys. Lett. 107, 081101 (2015), [2] Paarmann et al., Phys. Rev. B 94, 134312 (2016)

O 4.10 Mon 12:45 TRE Ma

A near field study on the transition from localized to propagating plasmons on 2D nano-tips — •Thorsten Weber[1,2], Thomas Kiel[3], Stephan Irsen[2], Kurt Busch[3,4], and Stefan Linden[1] — [1]Physikalisches Institut, Universität Bonn, Nußallee 12, D-53115 Bonn, Germany — [2]Electron Microscopy and Analytics, Center of Advanced European Studies and Research, Ludwig-Erhard-Allee 2, D-53175 Bonn, Germany — [3]Institut für Physik, Humboldt-Universität Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [4]Max-Born-Institut, Max-Born-Straße 2A, D-12489 Berlin, Germany

Plasmonic nano-structures have the unique capability to concentrate light in nanometric volumes. One approach to use this capability is based on resonant plasmonic nanostructures like rod nanoantennas or split ring resonators. In these resonant structures, hot spots of the electromagnetic field are created by localized particle plasmons. Another approach is utilizing non-resonant structures, such as nano-tips, on which propagating surface plasmons are excited at the wider end and travel towards the tip's apex.

Here, we report on a near field study of two-dimensional plasmonic gold nano-tips using electron energy loss spectroscopy in combination with scanning transmission electron microscopy, as well as discontinuous Galerkin time-domain calculations. With increasing nanotip size, we observe a transition from localized particle plasmons on resonant nano-tips to non-resonant propagating surface plasmons on large nano-tips. Furthermore we demonstrate that nano-tips with a groove cut can support both localized and propagating plasmons.

O 5: Organic-Inorganic Hybrid Systems and Organic Films I

Time: Monday 10:30–13:00 Location: WIL A317

O 5.1 Mon 10:30 WIL A317

The Impact of Doping on the Interface Structure and Level Alignment of ZnO/F6TCNNQ Interfaces from First Principles — •Simon Erker and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

In inorganic/organic heterostructures the interface decisively determines the performance of a device. However, in particular for materials such as ZnO, which is commonly employed in organic electronics, the surface composition is often not well known. Indeed, experimentally the polar (000-1) surface shows a wide variety of different structures, even under notionally similar conditions. Recent work indicates that doping, that is often not systematically controlled, may be responsible for the observed diversity. However, so far a theoretical verification was impeded by the lack of a computational first-principles approach that allows dealing with long-ranged band bending and charged surfaces. We present an extension of the recently introduced charged-reservoir electronic sheet technique (CREST) [PRB 91, 075311 (2015)] to incorporate band-bending effects directly into our calculations. Using DFT in combination with ab-initio thermodynamics we determine a doping dependent surface phase diagram of O-terminated ZnO. We find that the surface preferably adsorbs hydrogen to achieve a stable surface, but that its coverage becomes smaller with increasing doping concentration. We proceed to show how the different surface terminations and the corresponding band-bending affects the level alignment and the adsorption energy for the deposition of the strong electron acceptor F6TCNNQ.

O 5.2 Mon 10:45 WIL A317

Extended Space Charge Region and Unoccupied Molecular Band Formation in Epitaxial F4TCNQ Films — •David Gerbert and Petra Tegeder — Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Germany

The generation of well-defined molecular structures at inorganic/organic interfaces and within thin molecular films is crucial for charge carrier transport and thus the performance of organic-molecule-based (opto)electronic devices. In this talk we show by means of low-energy electron diffraction that F4TCNQ grows in an epitaxial fashion on Au(111) surfaces. These well-ordered crystalline films feature an extended space charge region and a dispersing unoccupied electronic molecular state as it was demonstrated using energy- and angle-resolved two-photon photoemission. The latter finding is a clear proof for band formation in epitaxial grown F4TCNQ films on Au(111). From our perspective the high electron affinity of F4TCNQ and a band-like charge transport from the interface into the molecular film are responsible for the formation of the space charge region. Our presented results suggest the application of epitaxial F4TCNQ films as hole injection layer to manipulate the hole injection barrier in organic electronic devices in a controlled way via the F4TCNQ layer thickness.

O 5.3 Mon 11:00 WIL A317

Photoemission Tomography of NiTPP on Cu(100) — •Daniel Lüftner[1], Giovanni Zamborlini[2], Zhijing Feng[3], Carlo Dri[3], Vitaly Feyer[2], and Peter Puschnig[1] — [1]Institut für Physik, Universität Graz, 8010, Graz, Austria — [2]Peter Grünberg Institut (PGI-6), Forschnungszentrum Jülich GmbH, 52425, Jülich, Germany — [3]CNR-IOM Laboratorio Nazionale TASC, 34012 Trieste, Italy

In this work we present a comprehensive characterization of the geometrical and electronic structure of self assembled Nickel-tetraphenylporphyrin (NiTPP) films on Cu(100) utilizing various experimental techniques, supported by theoretical calculations using density functional theory (DFT). In particular we make use of scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and photoemission tomography (PT), where the results of angle resolved photoemission spectroscopy (ARPES) measurements are systematically compared to the Fourier Transform of molecular orbitals, obtained in DFT. On the basis of STM and LEED measurements, we find, that NiTPP can arrange in two different geometrical configurations. In terms of electronic structure, PT allows for a direct assignment of peaks in the angle integrated ARPES spectrum to individual molecular orbitals and as such we observe a strong interaction of NiTPP with the metallic substrate resulting in occupation of LUMO/LUMO+1 and the LUMO+3 of the gas phase molecule. Our work emphasizes that a multi technique approach is essential in order to have a complete picture of the adsorption behavior and electronic properties of the metal/molecule interface.

O 5.4 Mon 11:15 WIL A317

Metastable tautomers — tuning the lifetime with an STM tip — •Andreas Krönlein[1], Jens Kügel[1], Aimee Sixta[1,2], Markus Böhme[1], and Matthias Bode[1,3] — [1]Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany — [2]University of Texas at Austin, 78712 Austin, Texas, United States — [3]Wilhelm Conrad Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, 97074 Würzburg, Germany

Although the influence of an scanning tunneling microscopy tip is often considered to be negligible, there are many examples where the tip is strongly affecting the physical properties of the probed system, as, for example, shown for the excitation spectra of Fe-OEP-Cl molecules [1].

Here, we present a detailed study of the tautomerization of dehydrogenated phthalocyanine molecules on a Ag(111) surface by means of scanning tunneling microscopy and STM-based pump-and-sample experiments [2]. Our data reveal that the molecule can switch between four different tautomeric forms. Whereas two of tautomers exhibit a very long lifetime, the lifetime of the other two tautomers amounts to seconds only. Current- and bias-dependent studies indicate that the presence of the STM tip modifies the potential barrier, thereby allowing for a controlled tuning of the metastable tautomer's lifetime.
[1] B. W. Heinrich *et al.*, Nature Physics **9**, 765 (2013)
[2] J. Kügel *et al.*, ACS Nano in press

O 5.5 Mon 11:30 WIL A317

Breaking Degeneracy of Tautomerization - Influence of the substrate — •Markus Böhme[1], Jens Kügel[1], Aimee Sixta[1,3], Andreas Krönlein[1], and Matthias Bode[1,2] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Wilhelm Conrad Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]University of Texas at Austin, Austin, Texas 78712, United States

We present a detailed study of the tautomerization, i.e., the switching of hydrogen protons, between different sites in the molecular frame of phthalocyanine (H_2Pc) on Ag(111) by means of scanning tunneling microscopy (STM) [1]. Our data reveal that the symmetry mismatch between the substrate and the molecular frame lifts the energetic degeneracy of the two H_2Pc tautomers. Their energy difference is so large that only one tautomer can be found in the ground state. Tip-induced tautomerization was triggered at sufficiently high bias voltages. By the controlled removal of a hydrogen proton from the molecule, a four-level system was created, consisting of two stable and two metastable states .
[1] J. Kügel *et. al.*, ACS Nano **Article ASAP** DOI: 10.1021/acsnano.6b05924

O 5.6 Mon 11:45 WIL A317

Excited states dynamics in TIPS-Pentacene on Au(111) — •Arnulf Stein and Petra Tegeder — PCI Universität Heidelberg, Heidelberg, Deutschland

Singlet fission is a promising approach to overcome the theoretical Shockley Queisser - Limit in organic semiconductor solar cells and is so far only obtained in a limited number of molecules [1]. One representative compound is the triisopropylsilylethynyl-pentacene (TIPS-Pn) which stands out because it combines solubility, self-assembly into π-stacked arrays to enhance intermolecular orbital overlap [2] and vacuum processability [3]. We studied TIPS-Pn adsorbed on Au(111) using two-photon-photoemission spectroscopy (2PPE). We determined the electronic structure and the dynamics of optically excited states at interfaces and within thin films.
[1] M.B. Smith and J. Michl, Chem. Rev. 110, 6891 (2010)
[2] J.E. Anthony *et al.*, JACS, 123, 9482 (2001).
[3] A. Gnoli *et al.* J. Phys. Chem. C, 118, 22522 (2014).

O 5.7 Mon 12:00 WIL A317

Interaction of free-base tetraphenylpoprhyrin with magnesium oxide: Inluence of MgO morphology on metalation — •Gianluca Di Filippo, Andrej Classen, Rebecca Pöschel, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058, Erlangen, Germany

Using x-ray photoemission spectroscopy we investigated the self-metalation of free-base tetraphenylporphyrin (2HTPP) on thin MgO(100) films on Ag(100). The deposition of one monolayer 2HTPP on MgO results in the formation of magnesium(II) tetraphenylporphyrin (MgTPP) at room temperature. We demonstrate that the efficiency of the reaction drastically depends on the morphology of the oxide layers. A thin MgO/Ag(100) film grown at 393 K presents a high island density [1]. Partial metalation of 1 ML 2HTPP onto this surface is already observed at a nominal MgO thickness well below 1 ML. The increase of the MgO amount leads to the progressive increase of the number of metalated molecules. Larger islands are obtained at a growth temperature of 573 K [1]. On such a substrate the metalation efficiency is consistently reduced so that partial metalation is only observed for a MgO nominal thickness above 1 ML. We ascribe these results to the fact that MgTPP formation takes place through the hydroxilation of steps and defects on the MgO surface [2], as confirmed by the increase of the OH signal in the O 1s line.
[1] A. Ouvrard *et al.*, J. Phys. Chem. C **115**, 8034 (2011)
[2] J. Schneider *et al.*, Chem. Eur. J. **22**, 1744 (2016)

O 5.8 Mon 12:15 WIL A317

Controlled On-Surface Synthesis of Organic and Organometallic Macrocycles — •Qitang Fan[1], Cici Wang[2], Tao Wang[2], Junfa Zhu[2], Min Chen[1], Malte Zugermeier[1], Claudio K. Krug[1], Julian Kuttner[1], Gerhard Hilt[1], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]National Synchrotron Radiation Laboratory, University of Science and Technology of China

Macrocycles and cyclic polymers have properties distinctly different from those of their linear counterparts. While effective approaches for their synthesis in solution remain scarce, on-surface synthesis has proven to be a viable alternative due to the inherent template effects. The controlled formation of hyperbenzene and organometallic macrocycles has been achieved on metal surfaces from 4,4"-dibromo-m-terphenyl (DBMTP) precursor molecules. Hyperbenzene, a hexagon consisting of 18 phenyl rings, forms on Cu(111), Ag(111) and Au(111) with different yields, which are maximized under pseudo-high dilution conditions. On clean Cu(110), DBMTP reacts to form zigzag organometallic chains linked with C-Cu-C bonds. However, with a template based on a Cu(110)-(2 * 1)O supergrating, cyclic organometallic tetragons (MTP-Cu)4 and hexagons (MTP-Cu)6 are obtained on the Cu stripes (with width from 2.6 nm to 3.6 nm). These methods may pave the way for the synthesis of other macrocycles.

O 5.9 Mon 12:30 WIL A317

Electronic Properties of the Potential Organic Superconductor 1,2;8,9-Dibenzopentacene on Ag(111) — •Felix Otto, Maximilian Schaal, Christian Udhardt, Tobias Huempfner, Lennart Vorbrink, Bernd Schröter, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Research on superconductivity in doped polycyclic aromatic hydrocarbons has attracted strong interest in the last few years. Among the investigated molecules potassium-doped 1,2;8,9-dibenzopentacene (DBPen, $C_{30}H_{18}$) was reported to exhibit one of the highest critical temperatures (33 K) [1]. Nevertheless, there are only few studies regarding its electronic properties. We deposited thin films of DBPen on Ag(111) in the range up to a few monolayers and investigated their behavior after several annealing procedures. Thickness dependent measurements with ultraviolet and x-ray photoelectron spectroscopy (UPS, XPS) were combined with low-energy electron diffraction (LEED) to elucidate the relationship between structural and electronic properties. We observed molecular signatures in the UP spectra which have their origin in different electronic structures of the molecules. These are analyzed under consideration of the LEED patterns that show one rather stable highly ordered phase. The influence of the molecule-substrate interaction on the results will also be discussed.

O 5.10 Mon 12:45 WIL A317

Work function tuning by electron irradiation of aromatic self-assembled monolayers — •Eric Sauter[1], Can Yildirim[1], Andreas Terfort[2], and Michael Zharnikov[1] — [1]Applied Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — [2]Institut für Anorganische und Analytische Chemie, Universität Frankfurt, Max-von-Laue-Straße 7, 60438 Frankfurt, Germany

Self-assembled monolayers are frequently used to manipulate injection barriers in organic electronics by introduction of a specific dipole moment at the interfaces between the electrodes and adjacent organic layers. This is usually achieved by the selection of a proper dipolar terminal tail group comprising the SAM-ambient interface, which was recently complemented by embedding such a group into the molecular backbone. Here we demonstrate that the work function of SAMs can also be adjusted by electron irradiation in a quite broad range and in controlled fashion, as far as these films contain pyridine or pyrimidine group. This effect is demonstrated by the example of several representative aromatic SAMs with either embedded pyrimidine group or terminal pyridine group. The observed behavior is presumably related to specific chemical transformations involving the nitrogen atom in these moieties. The SAMs with the embedded pyrimidine group are then especially attractive since this moiety is decoupled from the SAM-ambient interface. The effect is especially pronounced as far as it is monitored in situ but is partly quenched upon exposure of the irradiated films to ambient which is attributed to the enhanced reactivity of these films to airborne molecules, above all water.

O 6: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - I

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

O 6.1 Mon 10:30 GER 38

DFT wants U: Embedded-cluster calculations of surface oxygen vacancies at TiO_2 with Hubbard-corrected DFT — •Matthias Kick, Karsten Reuter, and Harald Oberhofer — Technische Universität München

Surface oxygen vacancies, in particular their nature as charge trapping centers, play an inportant role for many oxide materials properties. However, addressing them with first-principles density-functional theory (DFT) computations remains a challenge. At least Hubbard corrected DFT+U is required to achieve an appropriate electron localization. At the same time, the large dielectric constant of polarizable oxides like TiO_2 leads to a strong polarization response. As a result supercells of increasing size are necessary in order to avoid spurious interactions between periodic images in case of charged defects, rendering the conventional periodic boundary condition supercell approach impractical.

Full DFT+U functionality has been implemented in the all-electron electronic structure code FHI-aims. Combined with the solid state (QM/MM) embedding functionality in FHI-aims, this yields a numerically most efficient approach to treat aperiodic aspects at oxide surfaces. We illustrate this by calculating neutral and charged states of the surface oxygen vacancy at rutile TiO_2 (110). We systematically assess the reliability and computational efficiency by comparing to hybrid-level DFT calculations and calculations performed in conventional supercells.

O 6.2 Mon 10:45 GER 38

Hubbard interactions from density-functional perturbation theory — •Iurii Timrov, Matteo Cococcioni, and Nicola Marzari — Theory and Simulation of Materials (THEOS), and NCCR-MARVEL, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

DFT+U, together with its V and J extensions, is a simple and powerful tool to model systems containing partially-filled manifolds of localized states [1]. However, the Hubbard parameters are often - and in our view incorrectly - treated semi-empirically. Conceptual and practical methods to determine e.g. the Hubbard U parameter have nevertheless been introduced long ago, based either on the constrained random-phase approximation (cRPA) or on linear-response theory [2]. These approaches make DFT+U a fully first-principles and self-contained method, but are often overlooked due to their cost or complexity. Here, we introduce a computationally inexpensive and straightforward approach to determine the linear-response U, hitherto obtained from the difference between bare and self-consistent inverse electronic susceptibilities evaluated from supercell calculations. By recasting these calculations in the language of density-functional perturbation theory we remove the need of supercells, and allow for a fully automated determination of susceptibilities and Hubbard parameters. Such developments open the way for deployment in high-throughput studies, while providing the community with a simple tool to calculate consistent values of U for any system at hand. [1] V. Anisimov et al., PRB 44, 943 (1991), [2] M. Cococcioni et al., PRB 71, 035105 (2005).

O 6.3 Mon 11:00 GER 38

Time-evolution using full configuration interaction quantum Monte Carlo — •Kai Guther[1], Werner Dobrautz[1], Olle Gunnarsson[1], and Ali Alavi[1,2] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, United Kingdom

We report on a new method to perform real-time quantum evolution of a fermionic system using the full configuration interaction quantum Monte Carlo method [1]. To stabilize the algorithm, a slow simultaneous imaginary-time evolution is performed, yielding properties for times slightly rotated into the complex plane.

We employ this technique to compute Green's functions and therefore by means of analytic continuation also spectral weight functions. We demonstrate the applicability of the algorithm using the examples of the 2D-Hubbard model and the carbon dimer, showing that the algorithm can in principle be used as an Anderson solver for DMFT and is capable of obtaining photoemission spectra of ab-initio systems.

[1] G.H. Booth, A.J.W. Thom and A. Alavi, J. Chem. Phys. 131, 054106 (2009)

O 6.4 Mon 11:15 GER 38

Laplace-transformed MP2 with localized Resolution of Identity for molecular and periodic systems — •Arvid Ihrig, Igor Ying Zhang, and Matthias Scheffler — Fritz-Haber-Institut, Berlin, Germany

The self-interaction error is a well-known problem in (semi)local functionals in density-functional theory (DFT) and to a lesser extend also in hybrid functionals. It leads to a quantitatively and sometimes even qualitatively wrong description. One possible remedy is the 2nd order Moller-Plesset perturbation theory (MP2) and the double-hybrid DFT methods based on it. However, the time and memory requirements prevent their routine-usage for large molecular and condensed-matter systems.

In this work we combine our localized Resolution of Identity (RI-LVL) [1] and its favourable memory requirements with the low-order scaling of the Laplace-transformed MP2 (LT-MP2) [2]. Our highly parallelizable LT-MP2 implementation in a numeric atom-centered orbital (NAO) framework allows us to treat both cluster and periodic models in the same computational environment. We demonstrate the accuracy and other features of our implementation for examples of water clusters and TiO_2 surfaces with small absorbed molecules. We furthermore present a way how the distance-dependent integral screening [3] from the Ochsenfeld group can be generalized to periodic systems.

[1] Ihrig et al., New J. Phys. 17, 093020 (2015)
[2] P. Ayala et al., J. Chem. Phys. 110, 3660 (1999)
[3] S. Maurer et al., J. Chem. Phys. 136, 144107 (2012)

O 6.5 Mon 11:30 GER 38

Bond Disproportionation in Rare-Earth Nickelates: Describing Lattice Distortions within DFT+DMFT — •Alexander Hampel and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

Perovskite rare-earth nickelates, $R\text{NiO}_3$, display a rich and only partially understood phase diagram, where all compounds with R from Pr to Lu undergo a metal-insulator transition (MIT), that is accompanied by a structural distortion. This distortion breaks the symmetry between formerly equivalent Ni sites and can (in the simplest picture) be understood as a charge disproportionation of the Ni^{3+} cations into Ni^{2+} and Ni^{4+}. Here, we use density functional theory (DFT) and its extensions (DFT+U, DFT+DMFT) combined with symmetry-based distortion mode analysis to explore the interplay between lattice distortions, magnetic order and electronic correlation effects in rare-earth nickelates. Thereby, we want to explore the capabilities of the DFT+DMFT method to describe complex materials with coupled electronic and structural degrees of freedom by comparing with DFT+U results and available experimental data.

O 6.6 Mon 11:45 GER 38

Density matrix embedding theory for coupled fermion-boson systems — •Teresa E. Reinhard[1], Uliana Mordovina[1], Heiko Appel[1], Joshua S. Kretchmer[2], Garnet K. L. Chan[2], and Angel Rubio[1,3] — [1]Max Planck Institut für Struktur und Dynamik der Materie, Hamburg — [2]Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian

We analyze strongly correlated fermion-boson systems by extending Density Matrix Embedding Theory (DMET) from the purely electronic case [1] to coupled fermion-boson systems. DMET is a novel embedding theory which uses the Schmidt decomposition to divide the treated system into an impurity and a bath part. We project the bath part into the part of the Fock space that contains the entanglement with the impurity region and then solve this much smaller entangled system with exact diagonalization and DMRG.

With this technique, we treat lattice systems of Hubbard-Holstein type, where fermions and bosons are coupled by a bilinear Froehlich coupling. As we choose coherent states for the bosonic basis set, it is convenient to apply our approach to electron-phonon as well as to electron-photon systems.

By using a DMRG solver for the DMET algorithm, an accurate treatment of 2 dimensional systems becomes feasible.

[1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012)

O 6.7 Mon 12:00 GER 38

Vertex function of homogeneous electron gas — •Yaroslav Pavlyukh — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, P.O. Box 3049, 67653 Kaiserslautern, Germany — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

We present a systematic study of the vertex function correction in homogeneous electron gas at metallic densities [1]. Contrary to a popular belief the vertex function not only provides corrections to the well known plasmon or particle-hole pair scatterings, but also gives rise to new physical processes such as generation of two plasmon excitations or the transformation of the initial one-particle state into a two-particles-one-hole state. Using a merger of the many-body perturbation and scattering theories, which is a distinct feature of our method, it is shown that additional scattering channels are responsible for the bandwidth reduction (as observed in photoemission experiments on bulk sodium), appearance of the secondary plasmonic satellite below the Fermi level and lead to a substantial modification of the electron spectral function.

[1] Y. Pavlyukh, A.-M. Uimonen, G. Stefanucci, R. van Leeuwen, Phys. Rev. Lett. **117**, 206402 (2016)

O 6.8 Mon 12:15 GER 38

Coupled-Cluster approaches for molecules and solids in the numeric atom-center orbital framework — •Tonghao Shen, Igor Ying Zhang, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, DE

As a well-established and successful wave-function theory hierarchy in quantum chemistry, the coupled-cluster (CC) ansatz is attracting increasing attention in computational materials science [1]. However, compared to traditional density-functional approximations, CC approaches face much greater challenges regarding numerical implementation, bassis-set accuracy and efficiency, in particular for solids [2]. In this report, we present a highly parallel implementation of the CC approaches with singles, doubles and perturbative triples, CCSD(T), in the numeric atom-center orbital (NAO) framework. This implementation allows CCSD(T) simulations to be carried out using both cluster and periodic models in a single computational environment. Taking some popular quantum-chemistry test sets (S22, ISO34, and CYCONF), we demonstrate that CCSD(T) with correlation-consistent NAO basis sets [3] can provide accurate reference data for molecular properties. Our solid-state examples include elemental and binary crystals, as Ne (fcc), C, Si (diamond), LiF, MgO (rocksalt), and BN (zincblende).

O 6.9 Mon 12:30 GER 38

Implementation of the SU(2) Symmetry in FCIQMC using the Graphical Unitary Group Approach — •Werner Dobrautz[1] and Ali Alavi[1,2] — [1]Max-Planck-Institut für Festkörperforschung — [2]Department of Chemistry, University of Cambridge

The Full Configuration Interaction Quantum Monte Carlo (FCIQMC) algorithm [1] is a projector QMC method, previously formulated in the total anti-symmetric space of Slater Determinants, based on the imaginary-time Schrödinger equation to obtain the ground state of a system in the long-time limit.

By formulating the method in eigenfunctions of the $\hat{S}^2$ spin-operator via the Graphical Unitary Group Approach [2] we can make use of the block-diagonal form of spin-preserving, non-relativistic Hamiltonians for different values of the total spin. This allows us to lift possible near degeneracies of low-lying excitations of different spin sectors, calculate spin-gaps more easily and obtain the physical correct groundstate, without spin-contamination, and identify its total spin quantum number.

Our method does not rely on expanding the spin-eigenfunctions in linear combinations of Slater Determinants and thus does not hit an exponential bottle neck and can be applied to system sizes larger than previously reachable with similar approaches.

[1] G. Booth, A. Thom and A. Alavi, J. Chem. Phys. **131**, 054106 (2009)

[2] I. Shavitt, Int. J. Quantum Chem. Symp., **11:** 131 (1977); Int. J. Quantum Chem. Symp., **12:** 5 (1978)

O 6.10 Mon 12:45 GER 38

A study of the dense uniform electron gas with high orders of coupled cluster — •Verena Andrea Neufeld and Alex James William Thom — University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, United Kingdom

We used the recently developed stochastic coupled cluster method [Phys. Rev. Lett. (2010) 105, 263004 and J. Chem. Phys. (2016) 144, 084108] to benchmark the dense uniform electron gas (UEG). The aim was to make predictions about what truncation level of coupled cluster is needed to reach sufficient accuracy in electronic correlation energies for a range of electron densities. This will aid our future studies of solids with stochastic coupled cluster.

We take advantage of sparsity in wavefunctions by doing coupled cluster stochastically. In this study, we used coupled cluster truncation levels up to CCSDTQ5, that includes single, double, triple, quadruple and quintuple excitations directly. We considered the 14 electron UEG with Wigner-Seitz radius in the range 0.5 to 5.0 a.u.. We applied coupled cluster truncations from CCSD to CCSDTQ5 and extrapolated to the complete basis set size limit. By comparing the differences in energy calculated with CCSD to CCSDTQ5, we learn what truncation level is necessary for sufficient accuracy. What truncation level is needed, is dependent on the level of correlation, which decreases with electron density. We are therefore able to relate the degree of correlation linked to electron density to the level of coupled cluster needed for accuracy. This information will prove valuable when tackling periodic solids that can be approximated by the UEG.

O 7: Electronic Structure of Surfaces: Magnetism and Spin Phenomena

Time: Monday 10:30–12:45 Location: WIL C107

O 7.1 Mon 10:30 WIL C107

Magnetic properties of rare earth single atoms on metal substrates. — •Aparajita Singha[1], Romana Baltic[1], Fabio Donati[1], Christian Wäckerlin[1], Jan Dreiser[1,2], Luca Persichetti[3], Sebastian Stepanow[3], Pietro Gambardella[3], Stefano Rusponi[1], and Harald Brune[1] — [1]Ecole Polytechnique Fédérale de Lausanne — [2]Paul Scherrer Institute — [3]ETH Zürich

Surface-supported rare earths (RE) single atoms have been recently shown to have unprecedented magnetic stability [Science 318, 352 (2016)]. However to further benefit from their intriguing properties requires an in-depth understanding of the interaction between RE atoms and the surface which defines the energy spectrum of their magnetic quantum levels. Here we show a systematic study of several REs (Dy, Ho, Er,and Tm) on different metal substrates (Pt(111), Cu(111), Ag(100), and Ag(111)). Using x-ray absorption spectroscopy and magnetic circular dichroism we reveal that only $4f^n$ and $4f^{n-1}$ configurations are possible for these RE atoms where n corresponds to the free atom occupation. Moreover, we identify that the ionization potential of the $4f$ elements and the substrate density of states at the Fermi level are the two key factors governing the $4f$ occupation of the REs. All magnetization loops at 2.5 K show no hysteresis indicating that magnetic relaxation is faster than about 10 s. The comparison of our experimental spectra with multiplet calculations provides the identity and energy splitting of the magnetic quantum levels of these RE adatoms.

O 7.2 Mon 10:45 WIL C107

Superlattice of single atom magnets on graphene — •Romana Baltic[1], Marina Pivetta[1], Fabio Donati[1], Christian Wäckerlin[1], Aparajita Singha[1], Jan Dreiser[1,2], Stefano Rusponi[1], and Harald Brune[1] — [1]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland — [2]Swiss Light Source, Paul Scherrer Institute, Switzerland

Regular arrays of single atom magnets represent the model systems for information storage at the ultimate length scales. In this regard, individual rare-earth atoms on decoupling layers have recently received great attention for showing extraordinary magnetic stability [F. Donati et al., Science 352, 318 (2016)]. However, they lack spatial order.

Here we show that the spatial arrangement of Dy atoms on graphene/Ir(111) can be controlled by the substrate temperature during their deposition. Deposition at 40 K leads to the formation of a regular array of Dy atoms with the periodicity defined by the graphene moiré pattern, while deposition at lower temperatures results in disordered systems. In addition, the Dy atoms in both configurations show magnetic hysteresis up to 5.6 T and spin lifetime of 1000 s at 2.5 K. The observed magnetic stability of Dy atoms is a consequence of the low intrinsic electron and phonon densities of graphene, the six-fold adsorption site, and the $J_z = \pm 7$ ground state [R. Baltic et al., Nano Lett. (2016), DOI: 10.1021/acs.nanolett.6b03543].

O 7.3 Mon 11:00 WIL C107

Tailoring the hysteresis of Dy single atom magnets with $4f$ orbital filling — •Fabio Donati[1], Stefano Rusponi[1], Aparajita Singha[1], Romana Baltic[1], Luca Persichetti[3], Christian Wäckerlin[1], Jan Dreiser[2], Pietro Gambardella[3], and Harald Brune[1] — [1]Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland — [2]Swiss Light Source, Paul Scherrer Institute, Switzerland — [3]Department of Materials, ETH Zürich, Switzerland

Individual rare earth atoms adsorbed on a MgO surface are intensively investigated as they were recently found to preserve magnetic remanence up to 40 K [F. Donati et al., Science **352**, 318 (2016)]. Their magnetic properties are directly related to the occupation of the $4f$ orbitals, which determines the multiplicity of the lowest multiplet and the integer/half-integer character of the total angular momentum J. Therefore, tuning the $4f$ occupation offers a direct way to control the behavior of these single atom magnets. Using x-ray magnetic circular dichroism, we show that the magnetism of Dy atoms on MgO/Ag(100) can be controlled with the thickness of the MgO film. The occupation of the $4f$ orbitals changes from 9 to 10 by increasing the number of MgO layers from 3 to 6. Magnetization loops at 2.5 K exhibit hysteresis with characteristic shape and opening that depend on the electronic configuration of the Dy atoms. Our results highlight the role of the proximity of the metal substrate in determining the magnetism of single atoms on insulating layers.

O 7.4 Mon 11:15 WIL C107

Inelastic Electron Tunneling: Selection Rules and Orbital Exchange — •Jindrich Kolorenc — Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

We investigate tunneling of electrons from an STM tip to a substrate through a magnetic adatom by means of the Anderson impurity model. We employ an approximation analogous to the cotunneling theory [1] and concentrate on f-electron adatoms with large spin-orbital coupling. We compare the obtained inelastic electron tunneling spectra (IETS) with predictions of the spin model that has been very successful in the case of transition-metal adatoms [2]. When the spin model is applied to f electrons, the adatom spin $\mathbf{S}$ is replaced with its angular momentum $\mathbf{J}$ [3,4]. The spectra calculated in the two models differ, and we trace this difference to the exchange interaction between the adatom and the tunneling electrons. The bilinear (Heisenberg) exchange $\mathbf{J}\cdot\mathbf{s}$, assumed in the spin model [3,4], implies a selection rule $\Delta m_J = 0, \pm 1$ for single-electron scatterings, whereas the Anderson model indicates a larger number of allowed scattering channels. The less restrictive selection rule originates in the orbital exchange that is active for the orbital contribution to the magnetic moment of the adatom. This more general exchange influences also the lifetime of the magnetic states since they are destabilized, among other mechanisms, by the exchange with substrate electrons [4]. [1] F. Delgado and J. Fernández-Rossier, Phys. Rev. B **84**, 045439 (2011), [2] M. Ternes, New. J. Phys. **17**, 063016 (2015), [3] T. Schuh *et al.*, Phys. Rev. B **84**, 104401 (2011), [4] T. Miyamachi *et al.*, Nature **503**, 242 (2013).

O 7.5 Mon 11:30 WIL C107

Orbital Picture of Yu-Shiba-Rusinov Multiplets — •Benjamin W. Heinrich[1], Michael Ruby[1], Yang Peng[2], Felix von Oppen[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin — [2]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin

Magnetic impurities on an s-wave superconductor induce Yu-Shiba-Rusinov (YSR) bound states within the excitation gap of the superconductor. Here, we investigate single manganese (Mn) atoms adsorbed on different surface orientations of superconducting lead (Pb) and the nature of their YSR states. Depending on the adsorption site and surface, we detect a distinct number and characteristic patterns of YSR states around the Mn atoms. We show that the YSR states inherit their properties from the Mn d levels, which are split by the surrounding crystal field [1]. The periodicity of the long-range YSR oscillations allows us to identify a dominant coupling of the d states to the outer Fermi sheet of the two-band superconductor Pb. The long-range and directional nature of the states are promising for the design of coupled adatom structures, which could bear topological phases.

[1] M. Ruby *et al.*, Phys. Rev. Lett. **117**, 186801 (2016).

O 7.6 Mon 11:45 WIL C107

Proximity coupled Co chains on Pb(110) — Michael Ruby, Benjamin W. Heinrich, Yang Peng, Felix von Oppen, and •Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin

Proximity-coupled ferromagnetic chains on a superconductor with strong spin-orbit coupling have been predicted as a nearly universal system for topological superconductivity and for hosting Majorana zero modes [1]. Experiments on Fe chains on Pb(110) indeed exhibit signatures of Majorana end states [2]. Here, we test the universality prediction by growing Co chains on a Pb(110) surface. Using Co-coated STM tips, we detect spin-polarized d-bands reflecting ferromagnetic coupling along the chain. The Yu-Shiba-Rusinov bands inside the superconducting energy gap also exhibit spin contrast. However, the rich subgap structure does not provide evidence of Majorana end states. In a simple model of tight-binding calculations, we ascribe the absence of Majorana end states to an even number of d-band crossings of the Fermi level. This is the crucial difference to the case of Fe chains.

[1] J. Li, et al., Phys. Rev. B 90, 235433 (2014).

[2] S. Nadj-Perge, et al., Science 346, 602 (2014).

O 7.7 Mon 12:00 WIL C107

Magnetic character of holmium atom adsorbed on platinum surface — Alexander Shick[1], Dmitry Shapiro[2], Jindrich Kolorenc[1], and •Alexander Lichtenstein[3] — [1]Institute of Physics ASCR, Prague, Czech Republic — [2]Institute of Radio Engineering and Electronics RAS, Moscow, Russia — [3]University of Hamburg, Hamburg, Germany

We address recent controversy concerning the magnetic state of holmium adatom on platinum surface. Within a combination of the density functional theory (DFT) with the exact diagonalization (ED) of Anderson impurity model, the $\langle J_z \rangle = 0$ paramagnetic ground state is found. In an external magnetic field, this state is transformed to a spin-polarized state with $\langle J_z \rangle = 6.6 - 6.8$. We emphasize the role of $5d$-$4f$ interorbital exchange polarization in modification of the $4f$ shell energy spectrum. It is further suggested that when an external magnetic field is removed, the spin-polarized state relaxes back to the paramagnetic state through an intermediate quasi-degenerate and magnetically unstable state overruling the existence of long living magnetic moment, and the magnetic remanence for Ho adatom on Pt surface.

O 7.8 Mon 12:15 WIL C107

Spin-spirals in bottom-up fabricated Fe chains induced by Dzyaloshinskii-Moriya interaction — •Manuel Steinbrecher[1], Khai Ton That[1], Jan Hermenau[1], Alexander Ako Khajetoorians[2], Jens Wiebe[1], and Roland Wiesendanger[1] — [1]Department of Physics, Hamburg University, 20355 Hamburg, Germany — [2]IMM, Radboud University, 6525 AJ Nijmegen, The Netherlands

Magnetic atoms adsorbed on the surface of strong spin-orbit coupling materials experience indirect Dzyaloshinskii-Moriya interaction (DMI) [1]. DMI is an exchange interaction responsible for the stabilization of spin-spirals or Skyrmions by favoring perpendicular orientation of neighboring spins. By depositing single magnetic atoms on a surface and using the tip of a scanning tunneling microscope as a tool, those atoms can be moved to build bottom-up fabricated nanostructures [2]. Spin-sensitive measurements of such bottom-up fabricated chains enable the observation of the spin-state of each atom within the chain. So far, only collinear ferromagnetic [3] or antiferromagnetic [4] ground states have been observed. Here, we were able to measure DMI induced non-collinear ground states on chains of Fe atoms on Pt(111) of different lengths. By fixing the magnetization of the outermost atom in a 16 atoms long chain, we were able to stabilize a spin-spiral and investigate its properties by spin-polarized tunneling spectroscopy. [1] Khajetoorians *et al.*, Nat. Commun. **7**, 10620 (2016), [2] Khajetoorians *et al.*, Nat. Phys. **8**, 497 (2012); [3] A. Spinelli *et al.*, Nat. Mat. **13**, 782 (2014); [4] Khajetoorians *et al.* Science 332, 1062 (2011).

O 7.9 Mon 12:30 WIL C107

Electronic and magnetic properties of the GdAu$_2$ surface alloy probed by SP-STM — •Maciej Bazarnik[1], Emil Sierda[1], Mikel Abadia[2], Micha Elsebach[1], Jens Brede[2], and Ronald Wisendanger[1] — [1]Department of Physics, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany — [2]Centro de Física de Materiale, P Manuel de Lardizabal 5, Donostia - San Sebastián, Gipuzkoa E-20018, Spain

In light of recent developments in spintronics it is essential to develop interfaces between magnetic materials and superconductors, topological insulators or organic structures. Tailoring magnetic properties of structurally robust and chemically inert systems is therefore of high importance. In this respect, there has recently been a lot of interest in novel kinds of systems such as intercalated graphene, h-BN, or thin oxide films. Lately a new class of 2D systems has been discovered that is very promising to fulfill all requirements, namely GdAu$_2$ and GdAg$_2$ surface alloys. Those systems are confined to one bilayer of the material grown on Au(111) or Ag(111) surface respectively. The 2D structure exhibits magnetic properties very different from its bulk counterpart, ie. while GdAu$_2$ alloy is antiferromagnet in bulk it is in fact a ferromegnet as a 2D film. In this presentation we will focus on the GdAu$_2$ surface alloy on Au(111) as examined by SP-STM. We will first address the local electronic and magnetic properties and compare our results to investigations by complementary surface science techniques. Then we will prove that the GdAu$_2$ surface alloy acts as a catalyst for the on-surface Ullmann reaction.

O 8: 2D Materials Beyond Graphene I

Time: Monday 10:30–13:00 Location: REC/PHY C213

O 8.1 Mon 10:30 REC/PHY C213

Transfer of a 2D silica sheet — •Christin Büchner[1], Kristen M. Burson[2], Markus Heyde[1], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Hamilton College, Clinton, NY, USA

Two-dimensional (2D) materials hold immense technological potential for creating nanoelectronic devices. Highly conductive materials such as graphene are combined with insulators but the library of 2D materials with large band gap is effectively limited to h-BN. 3D insulators can compromise the electronic properties of graphene due to structural defects and surface roughness.

We present a 2D SiO$_2$ bilayer film, prepared on a Ru(0001) substrate via CVD. The atomic structure has been investigated using scanning probe microscopy.[1] Extended honeycomb structures and glass-like network structures were identified, while DFT calculations and STS measurements indicate a band gap larger than 6.5 eV.[2,3]

Recently, we transferred the bilayer from the growth substrate to a new substrate using a modified mechanical exfoliation procedure. The film maintains its atomically flat structure on the mm-scale after being transferred to a foreign substrate [4]. Low energy electron diffraction, Auger electron spectroscopy, scanning tunneling microscopy and environmental scanning electron microscopy indicate that the structure is maintained throughout the transfer procedure.

[1] DOI: 10.1002/anie.201107097 [2] DOI: 10.1063/1.4939279 [3] DOI: 10.1088/0953-8984/24/35/354010 [4] DOI: 10.1021/acsnano.6b03929

O 8.2 Mon 10:45 REC/PHY C213

Photocarrier dynamics and interaction effects of interlayer excitons in WSe$_2$/MoSe$_2$ heterostructures — •Philipp Nagler, Gerd Plechinger, Alexey Chernikov, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Regensburg, Germany

Atomically thin transition metal dichalcogenides (TMDCs) such as WSe$_2$ or MoSe$_2$ have lately emerged as a promising platform to study the physics of excitons in strongly confined systems. Thereby, the use of transfer techniques allows for the fabrication of van der Waals heterostructures by deterministic stacking of individual monolayers. It is expected that type-II band alignment of the individual monolayers results in the formation of spatially indirect excitons. Here, we present a detailed study of the optical properties of interlayer excitons in a WSe$_2$/MoSe$_2$ heterostructure using static and time-resolved photoluminescence measurements. At low temperatures, we observe the emergence of an energetically separated (1.4 eV) and spectrally sharp (FWHM $<$ 20meV) feature, which we attribute to the emission of interlayer excitons. Power-dependent measurements show a considerable blue shift of the interlayer exciton peak position due to dipolar exciton-exciton interaction effects. Finally, we employ a streak camera system in order to reveal the photocarrier dynamics of interlayer excitons for varying temperatures. The lifetime at low temperatures amounts to several nanoseconds, which is a consequence of the reduced oscillator strength of the interlayer exciton.

O 8.3 Mon 11:00 REC/PHY C213

Electronic and atomic structure of the honeycomb lattice of Sn/Au(111) reconstruction — •Dominik Jungkenn[1], Maniraj Mahalignam[1], Sebastian Emmerich[1], Lyu Lu[1], Jobinson Kollamana[1], Zheng Wei[1], Wujun Shi[2], Binghai Yan[2], Benjamin Stadtmüller[1], Mirko Cinchetti[3], Stefan Mathias[4], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Str 46, 67663 Kaiserslautern — [2]Max-Planck-Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden — [3]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund — [4]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Motivated by recent prediction of Stanene, a honeycomb structure of Sn atoms on a Au substrate [1], we investigated the structure formation of Sn on Au(111) using LEED and STM. In the sub monolayer regime, Sn forms a variety of ordered surface reconstructions depending on Sn coverage and post annealing temperature. One of the most stable structures is the (Sqrt3 x Sqrt3)R30° reconstruction which is characterized by a hexagonal super lattice. Angle resolved photoemission revealed a rich band structure with a Rashba type split band in the vicinity of the Gamma point, in agreement with band structure calculations based on density functional theory. Our results will be compared to the predicted fingerprints of stanene [1]. [1] S. Nigam, et al. Phys. Chem. Chem. Phys., 2015,17, 6705-6712

O 8.4 Mon 11:15 REC/PHY C213

Electronic properties of single-layer antimony crystals from a tight-binding description: hopping integrals, spin-orbit coupling, and Coulomb interactions — •Alexander Rudenko — Radboud University, Nijmegen, The Netherlands

Single-layer antimony (Sb) crystals have recently been produced using different methods, including mechanical [1] and liquid-phase [2] exfoliation. Excellent environmental stability and a moderate band gap ($\sim$1.5 eV) make this material promising for electronic and optical applications. Here, we present an analytical tight-binding model for single-layer Sb, derived on the basis of relativistic first-principles calculations within the density functional theory. Significant corrections due to the strong ($\lambda = 0.34$ eV) intraatomic spin-orbit coupling are taken into account perturbatively. The model offers an efficient and accurate description of single-particle electronic states in a wide spectral region up to the mid-UV. The problem of the Coulomb interactions in 2D Sb is also addressed. We find that the screening effects originate predominantly from the $5p$ states, and thus fully captured by the proposed model. The results presented here provide an essential step toward the understanding and rational description of a variety of electronic properties of the novel 2D material.

[1] P. Ares *et al.*, Adv. Mater. **28**, 6332 (2016).

[2] C. Gibaja *et al.*, Angew. Chem. Int. Ed. **55**, 14345 (2016).

O 8.5 Mon 11:30 REC/PHY C213

Realization of stanene on the surface of Au(111) — •Mahalingam Maniraj[1], Benjamin Stadtmüller[1], Wujun Shi[2], Dominik Jungkenn[1], Sebastian Emmerich[1], Johannes Stöckl[1], Lu Lyu[1], Jobynson Kollamana[1], Zheng Wei[1], Anatol Jurenkow[1], Sebastian Jakobs[1], Yongli Gao[3], Mirko Cinchetti[4], Binghai Yan[2], Stefan Mathias[5], and Martin

Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Department of Physics and Astronomy, University of Rochester, Rochester, NY 14627 — [4]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany — [5]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Stanene was recently predicted and has subsequently triggered intense research on Sn-based graphene-like 2D materials. Combining LEED, STM, spin- and angle-resolved photoemission (ARPES) and DFT calculation, we present clear evidence for the formation of a stanene-like superstructure on the surface of Au(111). Our ARPES results show the existence of Dirac-cone-like bands around the $\bar{\Gamma}$ point with an electron velocity of $1{\times}10^6$ m/s, which originates from the admixture of Sn p and Au d states. Spin-resolved ARPES measurements reveal a topological insulator-like spin texture. Our realization of a Stanene-like superstructure lays the foundation for the easy fabrication and investigation of stanene as a potential next generation 2D material.

O 8.6 Mon 11:45 REC/PHY C213

Localized defect states in $\mathbf{MoS_2}$ monolayers: Electronic and optical properties — •Jens Kunstmann, Tsegabirhan B. Wendumu, and Gotthard Seifert — Theoretische Chemie, TU Dresden, Germany

Defects usually play an important role in tuning and modifying various properties of semiconducting or insulating materials. Here we study the impact of point and line defects on the electronic structure and optical properties of MoS_2 monolayers using density-functional methods. The different types of defects form electronic states that are strongly localized on the defect. The electronic structure of the monolayer system is quite robust and it is well preserved for point defect concentrations of up to 6%. The impact of point defects on the optical absorption for concentrations of 1% and below is found to be very small. For higher defect concentrations, molybdenum vacancies were found to quench the overall absorption and sulfur defects lead to sharp absorption peaks below the absorption edge of the ideal monolayer. For line defects, we did not find a considerable impact on the absorption spectrum. These results support recent experiments on defective transition metal chalcogenides. [Kunstmann, Wendumu, Seifert, phys. stat. sol. (b) (2016), doi:10.1002/pssb.201600645]

O 8.7 Mon 12:00 REC/PHY C213

Chemical and Electronial Repair of Defective $\mathbf{MoS_2}$ Monolayers Through Thiols- — •Anja Förster[1,2], Sibylle Gemming[3,4], Gotthard Seifert[2], and David Tománek[1] — [1]Physics and Astronomy Department, Michigan State Unversity, East Lansing, Michigan 48824, USA — [2]TU Dresden, Center for Advancing Electronics Dresden (cfaed), 01062 Dresden, Germany — [3]Institute of Ion Beam Physics and Material Research, Helmholtz-Zentrum Dresden Rossendorf, Center for Advancing Electronics Dresden (cfaed), Bautzner Landstr. 400, 01328 Dresden, Germany — [4]Insitute of Physics, TU Chemnitz, 09107 Chemnitz, Germany

Molybdenum disulfide (MoS_2) monolayers are promising candidates for new low-power electronic circuits and sensors. In order to ensure their usability for mass-production, it is necessary to heal the defects that significantly affect the electronic properties of MoS_2.

For this purpose, we focus on two defect types: sulfur monovacancies and sulfur-adatoms. We show their effect on the density of states (DOS) of MoS_2 and show how thiols can be used to heal these defects.

In detail, the sulfur mono-vacancies introduce defective states near the Fermi-energy to the DOS of MoS_2. Thiols are able to cure those defective states by re-inserting the missing sulfur atoms.

In the case of sulfur adatoms, the Fermi-level of MoS_2 is shifted by 0.7 eV, bring the conducting band very close to ther Fermi-energy. Thiols are able to remove the sulfur adatoms by forming hydrogen sulfide and disulfides. The latter are adsorbed on the MoS_2 surface.

O 8.8 Mon 12:15 REC/PHY C213

Ion-beam mediated patterning of MoS2 monolayers — •Mahdi Ghorbani-Asl[1], Silvan Kretschmer[1], Douglas Spearot[2], and Arkady Krasheninnikov[1,3] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Department of Mechanical and Aerospace Engineering, University of Florida, Gainesville, Florida 32611, USA — [3]Department of Applied Physics, Aalto University School of Science, P.O. Box 11100, 00076 Aalto, Finland

Using analytical potential molecular dynamics combined with first-principles calculations, we study the production of defects in free-standing MoS2 monolayers under ion irradiation for a wide range of ion energies when nuclear stopping dominates. The probabilities of defect production have been studied for various types of defects. We show that depending on the incident angle, ion type and energy, sulfur atoms can be sputtered away predominantly from the top or bottom layers, providing unique opportunities for ion-beam mediated patterning of MoS2. As an example, we study the stability and electronic properties of mixed MoSX compounds where X are chemical elements from group V or VII. We demonstrate that such systems can show metallic character (e.g. MoSF) and further be used to design metal/semiconductor/metal junctions, which exhibit negative differential resistance.

O 8.9 Mon 12:30 REC/PHY C213

Van der Waals Epitaxy of Single Layer Transition Metal Dichalcogenides — •Joshua Hall[1], Borna Pielić[2], Tobias Wekking[1], Marko Kralj[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicherstr. 77, D-50937 Köln — [2]Center of Excellence for Advanced Materials and Sensing Devices, Institute of Physics, Bijenička 46, HR-10000 Zagreb

We employ molecular beam epitaxy on van der Waals substrates to grow epitaxial mono- to bilayer samples of transition metal dichalcogenides (TMDC). The scalability of the method allows for subsequent investigations such as angle resolved photo emission spectroscopy.

As substrates for our two step synthesis of the TMDC we use in situ fabricated graphene or a monolayer of hexagonal boron nitride. In the first synthesis step, at temperatures in the range from 100 K to 400 K, we expose the substrate to a metal vapor in the background of a sulfur pressure. As signified by low energy electron diffraction, already after this step, the TMDC forms. We find that the ratio of metal to sulfur flux is crucial for the growth mode of the TMDC. As a second step, the sample is annealed in the range of 800 K to 1100 K in a sulfur background. Annealing decreases epitaxial orientation scatter and enlarges domain sizes. It is limited in time and temperature by the onset of TMDC decomposition and intercalation of the educts under the van der Waals substrate monolayer. Our scanning tunneling microscopy studies document the versatility of the two step synthesis by providing examples for excellent quality monolayers of MoS_2, WS_2, TaS_2 and VS_2.

O 8.10 Mon 12:45 REC/PHY C213

Investigation of 2D hBN after ion irradiation — •Lara Bröckers, Henry Bohnen, and Marika Schleberger — Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany

Ion irradiation is a useful tool for the controlled modification of two-dimensional (2D) materials. Previous experiments have revealed characteristic, structural modification of graphene and other 2D materials created by swift heavy ion (SHI) irradiation [1,2]. We could show that the size of these modification, called foldings, vary depending on the irradiation parameters. Typically, the foldings are 50-80 nm in width and more than a micron in length, depending on the angle of incidence of the ions and on the substrate [3]. The main channel for energy deposition in solids by SHIs is the excitation of the target electrons. Therefore, a comparison between 2D materials with different electronic properties can help to reveal the physical mechanisms of defect creation. Comparing the folding of graphene (semiconductor) with the folding of hBN (insulator) we found significant differences. We determine the so-called efficiency, i.e. the number of ions needed to create one folding one average. For graphene this number equals one only for single layer graphene, otherwise it decreases rapidly down to zero with increasing number of layers. In the case of hBN however, also thicker layers are folded with a high efficiency. In addition, we have studied how the efficiency is influenced by the substrate.

[1] Akcöltekin S. et al. *Applied Physics Letters*, 98 (2011) 103103

[2] Ochedowski O. et al. *NimB*, 340 (2014) 39.

[3] Ochedowski O. et al. *Nanotechnology*, 26 (2015) 465302

O 9: Solid-Liquid Interfaces: Structure, Spectroscopy I

Time: Monday 10:30–13:00 Location: WIL C307

O 9.1 Mon 10:30 WIL C307

Self-Diffusion Mechanisms of Surface Defects at Copper-Water Interfaces — •Suresh Kondati Natarajan and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr Universität Bochum, Germany

The self-diffusion mechanisms of surface defects at metal-water interfaces have to be studied for understanding heterogeneous catalysis, electrochemistry and corrosion. Although a number of studies in the literature have been dedicated to the investigation of these mechanisms at metal-vacuum interfaces, there are hardly any studies for metal-water interfaces. Here, we unravel the surface adatom and vacancy diffusion mechanisms at several copper-water interfaces using a high dimensional neural network potential based on density functional theory [1]. In case of the low index surfaces such as (111), (100) and (110), the adatom diffusions by means of a simple hop and an exchange with a surface atom are investigated and we find that the free energy barrier to the hopping mechanism is much smaller than the barrier to the exchange mechanism. We find that the interfacial water molecules assist in the adatom diffusion processes. The adatoms at stepped surfaces like (311) and (211) hop along the step edge more frequently compared to the hop across the step edge. Finally, the vacancy hop at (100) surface is found to be twice as probable as the hop at (111) and (110) surfaces in the presence of water.

[1] S. K. Natarajan and J. Behler, Phys. Chem. Chem. Phys. 18, 28704 (2016).

O 9.2 Mon 10:45 WIL C307

Force Implementation for the Modified Poisson-Boltzmann Solvation Model in FHI-aims — •Christoph Muschielok, Stefan Ringe, Harald Oberhofer, and Karsten Reuter — Technische Universität München, Germany

Implicit solvation approaches represent a numerically appealing route to account for solvation effects in first-principles electronic structure calculations. These effects comprise both energetic and structural changes induced by the surrounding medium. Among a plethora of implicit solvation methods, the size-modified Poisson-Boltzmann (MPB) approach thereby combines an account of the dielectric solvent response with a mean-field description of solvated finite-sized ions.

Using a function-space based solution scheme MPB implicit solvation functionality has recently been implemented into the all-electron, numeric-atomic-orbital based density-functional theory (DFT) package FHI-aims.[1] This implementation fully exploits the specialised atom-centered integration grids of FHI-aims. To also allow for structural relaxation under the electrolyte influence, we now derived analytic nuclear derivatives for this MPB functionality. In this contribution we will present the individual terms and their efficient numerical implementation. As a showcase application we investigate conformer stabilities of biomolecules in electrolytes.

[1] S. Ringe *et al.*, J. Chem. Theory Comput. **12**, 4052 (2016).

O 9.3 Mon 11:00 WIL C307

Towards the Understanding of the Water/Zinc Oxide Interface Employing Artificial Neural Networks — •Vanessa Quaranta, Matti Hellström, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Bochum, Germany

The interaction of liquid water with zinc oxide (ZnO) is important in different fields like corrosion protection, electrochemistry and heterogeneous catalysis. To date, theoretical studies have mainly addressed single water monolayers while the reactivity of this material in presence of water multilayers is still poorly investigated due to the required large simulation cells which strongly limit the applicability of *ab initio* techniques. Here a reactive DFT-based neural network potential (NNP) for the liquid water/ZnO interface will be presented. We demonstrate that this potential allows to perform extended simulations enabling to unravel the properties of the interfacial water molecules and the proton transfer (PT) events occurring at the non-polar ZnO surfaces.

O 9.4 Mon 11:15 WIL C307

Optical fingerprints of solid-liquid interfaces: a joint ATR-IR and *first principles* investigation — •Lei Yang[1], Fang Niu[1], Stefanie Tecklenburg[1], Marc Pander[1], Simantini Nayak[1], Andreas Erbe[1], Stefan Wippermann[1], Francois Gygi[2], and Giulia Galli[3] — [1]MPI Eisenforschung — [2]UC Davis — [3]U Chicago

Despite the importance of understanding the structural and bonding properties of solid-liquid interfaces for a wide range of (photo-)electrochemical applications, there are presently no experimental techniques available to directly probe the microscopic structure of solid-liquid interfaces. To develop robust strategies to interpret experiments and validate theory, we carried out attenuated total internal reflection (ATR-IR) spectroscopy measurements and *ab initio* molecular dynamics (AIMD) simulations of the vibrational properties of interfaces between liquid water and well-controlled prototypical semiconductor substrates. We show the Ge(100)/H_2O interface to feature a reversible potential-dependent surface phase transition between Ge-H and Ge-OH termination. The Si(100)/H_2O interface is proposed as a model system for corrosion and oxidation processes. We performed AIMD calculations under finite electric fields, revealing different pathways for initial oxidation. These pathways are predicted to exhibit unique spectral signatures. A significant increase in surface specificity can be achieved utilizing an angle-dependent ATR-IR experiment, which allows to detect such signatures at the interfacial layer and consequently changes in the hydrogen bond network. Funding from DOE-BES Grant DE-SS0008939 and the DFG (RESOLV, EXC 1069) are acknowledged.

O 9.5 Mon 11:30 WIL C307

Influence of lithium ions onto water structures on Au(111) — •Irene Weber and Karina Morgenstern — Chair of Physical Chemistry I, Ruhr-Universität Bochum

Providing information about solvation effects near the liquid-solid interface is of tremendous importance for the understanding of electrochemical processes, i.e. in electrocatalysis. However, the understanding of ions influencing water structures and dynamics near metal surfaces on the atomic scale is far from complete. In our study amorphous water and lithium ions are used to mimic fluid water and circular cations, respectively. We found that lithium ions do not adsorb at specific sites on Au(111) during adsorption at around 215 K and that water nucleation starts predominantly at the elbow sites of the herringbone reconstruction. Contrary to the weak interaction of water with Au(111), water molecules bind strongly to lithium ions on Au(111). Depending on the water-lithium ions-ratio, several types of interactions between water, lithium ions and the Au(111) substrate were determined. In this contribution we will review our recent variable-temperature Scanning Tunneling Microscopy (STM) studies of the influence of lithium ions onto amorphous ice structures on Au(111).

O 9.6 Mon 11:45 WIL C307

Stability and Structure of TiO_2 Rutile (011) Surface Exposed to Liquid Water — •Jan Balajka, Martin Setvín, Martin Čalkovský, Zdeněk Jakub, Matthias Müllner, Stijn Mertens, Michael Schmid, and Ulrike Diebold — Institute of Applied Physics, TU Wien, Austria

Understanding the interface between titanium dioxide (TiO_2) and liquid water is important for many practical applications such as photocatalytic water splitting.

The (011) termination of TiO_2 rutile is the second lowest energy facet and exhibits a (2x1) reconstruction when prepared in UHV. Based on DFT predictions [1] the (2x1) structure should no longer be favorable in a liquid water environment.

A TiO_2 rutile (011) sample, prepared and characterized in UHV, was exposed to liquid water and consequently analyzed with STM, XPS, LEIS and LEED. For this purpose a dedicated UHV system was used that allows controlled and clean transfer of the samples between the UHV and an electrochemical cell.

The results indicate a surface restructuring upon contact with liquid water. An overlayer of dissociated water is formed with a c(2x1) symmetry. As the splitting of the LEED spots corresponding to the (2x1) structure was observed while the bulk (1x1) spots did not change it is likely that the (2x1) substrate is also affected by the presence of liquid water. By combining XPS and LEIS the possibility of contaminant-induced restructuring was excluded.

[1] U. Aschauer, A. Selloni, PRL **106** (2011), 166102.

O 9.7 Mon 12:00 WIL C307

Understanding water relaxation at interfaces — •Dominika Lesnicki and Marialore Sulpizi — Department of Physics, Johannes Gutenberg University, Staudingerweg 7, 55128 Mainz, Germany

Advances in ultrafast spectroscopy allow to study vibrational energy transfer of water molecules at interfaces. In the case of water-air interface, it has been shown that the vibrational energy relaxation dynamics is significantly different from that of bulk water.

Here we propose a method to understand vibrational energy relaxation time scales and pathways of the OH stretching mode of water, which is based on the calculation of vibrational response function and the direct simulation of the energy relaxation processes using density functional theory based molecular dynamics (DFTMD) simulations, where a consistent treatment of the electronic structure of solvent and surface is provided.

We apply our method to the fluorite/water interface as function of pH. This system shows a fast relaxation, at low pH, similar to that of bulk water, and a slow relaxation at hight pH. Direct comparison to the experimental results is also possible thanks to the collaboration with the molecular spectroscopy group of E. Backus at MPIP.

O 9.8 Mon 12:15 WIL C307

Ions at hydrophobic interfaces — •Yury Forov[1], Michael Paulus[1], Susanne Dogan[1], Paul Salmen[1], Christopher Weis[1], Mirko Elbers[1], Simon Egger[2], Elena Zwar[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, GER — [2]Physikalische Chemie, TU Dortmund, 44221 Dortmund, GER

The investigation of the microscopic structure of water is one of the important areas of modern research [1]. In particular, the understanding of the behavior of water at interfaces is essential for the explanation of interfacial phenomena in several natural and technological environments [2]. Hereby, one important research area is the behavior of ions at hydrophobic interfaces [3]. Much pioneer work has been done to describe the interactions between ions and hydrophobic surfaces, but a complete description of the physical mechanism of the hydrophobic interaction is still pending [4]. We investigated the adsorption behavior of ions of aqueous salt solutions at hydrophobic interfaces as a function of different ionic radii and concentrations by means of x-ray reflectivity at ambient conditions. The use of high energy x-rays allows the analysis of buried interfaces in-situ and thus can be used for studying the properties of multilayer systems, such as layer thickness, roughness, and electron density. We observed changes in the shape of the hydrophobic interface both with rising salt concentrations and ion radii for different salt types. [1] A. Nilsson and L.G.M. Pettersson, Chem. Phys. 389, 1 (2011); [2] D. Chandler, Nature 437, 640-647 (2005); [3] P. Jungwirth and B. Winter, Annu. Rev. Phys. Chem. 59, 343-366 (2008); [4] S. H. Donaldson et al., Langmuir 31, 2051-2064 (2015)

O 9.9 Mon 12:30 WIL C307

Calcium-Silicate Phases Explained by High Temperature Resistant Phosphate-Probe Molecules — •Nicolas Giraudo and Peter Thissen — Karlsruher Institut für Technologie (KIT), Institut für Funktionelle Grenzflächen (IFG), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

In this work, high temperature resistant phosphate molecules are applied to characterize ultrathin (100 nm) Calcium-Silicate (C-S) phases. These C-S phases are synthetized on silicon wafers, and the interaction of phosphates with the C-S phases is studied by means of in-situ transmission Fourier Transform Infrared (FTIR) spectroscopy. At room temperature the chemistry of the system is dominated by the formation of Calcium-Phosphates (C-P). In case of temperatures rising up to 1000 °C, the C-S phases are regenerated. FTIR results are analyzed on the basis of first-principles calculations and further supported by complementary Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) experiments. This study provides a detailed and self-consistent picture of the chemical and structural properties of interfaces like the one between the atmosphere and ultrathin C-S phases (gas/C-S) and the one between them and silicon wafers (C-S/Si bulk). The material combination of ultrathin C-S phases grown on silicon wafers might in the future have great potential in selective chemistry, catalysis and sensing technology as well as in the semiconductors manufactory.

O 9.10 Mon 12:45 WIL C307

Characterization of anion layering and steric anion hydration repulsion on positively charged surfaces in aqueous media — •Qingyun Hu[1] and Markus Valtiner[1,2] — [1]Max-Planck-Institut fuer Eisenforschung, Duesseldorf, Germany — [2]TU Bergakademie Freiberg, Freiberg, Germany

How anions influence the structure at positively charged solid/liquid interfaces is much less understood. Here we measured force versus distance profiles on mica using Atomic Force Microscopy with SiO2 terminated tips. We characterized steric anion hydration forces for a set of common anions at pH = 1 in 100 mM concentration, where protons are the only positive counter ion. Steric anion hydration effects strongly depend on the anion type and their structuring within the Stern layer. Anions with low hydration energies such as Cl- and NO3- strongly structure within the first 1-2 nm of a positively charged surface due to specific adsorption effects leading to full charge screening within the Stern layer. In contrast strongly hydrated ions such as multivalent anions do not lead to significant structural forces at distances below 1-2 nm showing thermally disordered structuring in accordance with expected Debye screening lengths. In contrast, in perchlorate based electrolytes interfacial protonation of the anionic species leads to an effective increase of the Debye length. In summary, this work highlights that anion structuring in the inner double layer is very ion specific and correlates with hydration free energies, which may play a vital role in understanding processes where positive charge is screened by anions within an electrolyte, including protein folding or colloidal stability.

O 10: Overview Talk: Jascha Repp

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

Invited Talk O 10.1 Mon 15:00 TRE Phy

Overview of the development of ultrafast scanning tunneling microscopy — Dominik Peller, Tyler L. Cocker, Ping Yu, Rupert Huber, and •Jascha Repp — Department of Physics, University of Regensburg, 93040 Regensburg, Germany

Since the early days of scanning tunneling microscopy (STM) people have tried to combine atomic-scale resolution with an ultrafast temporal resolution [1]. Recently time-dithering optical pulse pairs has minimized the deleterious effect of light-induced heating [2] and hot-electron transfer has been demonstrated with sub-molecular resolution [3]. An all-electronic pump-probe scheme [4] has allowed for a direct observation of the relaxation of individual spins at the nanosecond timescale. Cocker et al. [5] were the first to use terahertz (THz) pulses acting analogously to voltage pulses accessing much shorter timescales. Recently, THz-STM enabled a novel, state-selective regime, in which a single electron can be selectively removed from a specific molecular orbital at combined sub-Ångstrom and sub-picosecond resolution [6].

[1] Hamers and Cahill, Appl. Phys. Lett. 57, 2031 (1990); Nunes and Freeman, Science 262, 1029 (1993) [2] Terada, Yoshida, Takeuchi and Shigekawa, Nature Photon. 4, 869 (2010); Yoshida et al., Nature Nano. 9, 588 (2014) [3] Wu and Ho, Phys. Rev. B 82, 085444 (2010) [4] Loth et al., Science 329, 1628 (2010) [5] Cocker et al., Nature Photon. 7, 620 (2013) [6] Cocker et al., Nature 539, 263 (2016).

O 11: Plasmonics and Nanooptics II: Light-Matter Interaction

Time: Monday 15:00–16:45 Location: TRE Ma

O 11.1 Mon 15:00 TRE Ma

Three-electron photon interaction mediated by localized plasmons — Peter-Jan Peters and •Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel

The light emission from a scanning tunneling microscope operated on Ag(111) surfaces at 5 K is analyzed from low conductances G to values approaching the conductance quantum. Optical spectra reveal emission due to localized plasmons with photon energies exceeding the applied bias more than twice ($h\nu > 3eV$). The emission intensity varies in a non-monotonic fashion with G. An empirical model reproduces the scaling of the photon yield and the optical spectra near the thresholds for two-electron and three-electron processes. While some heating of the electron gas occurs, the predominat part of the light emission is due to coherent processes.

O 11.2 Mon 15:15 TRE Ma

AlN/GaN multilayer interface phonons studied with mid-IR second-harmonic phonon spectroscopy — •Christopher J. Winta[1], Nikolai Passler[1], Ilya Razdolski[1], D. Scott Katzer[2], Ioannis Chatzakis[3], Neeraj Nepal[2], David J. Meyer[2], Chase T. Ellis[2], Joseph G. Tischler[2], Alexander J. Giles[2], Sandy Gewinner[1], Wieland Schöllkopf[1], Martin Wolf[1], Joshua D. Caldwell[2], and Alexander Paarmann[1] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4–6, 14195 Berlin — [2]U.S. Naval Research Laboratory, Washington, D.C. 20375 — [3]NRC Postdoctoral Fellow (residing at NRL, Washington D.C. 20375)

Combining multiple atomic-scale layers of polar crystals allows for active modification of phonon lifetimes, frequencies and hence engineering of Reststrahlen band spectral positions. Specifically, new interface optical phonon modes emerge in these so-called crystalline hybrids (XHs). The atomic-scale layer thicknesses allow for tuning of these modes, opening up a new class of engineered materials [1].

In our experiments, we study the nonlinear response of an AlN/GaN 27-layer superlattice material on a SiC substrate with varying layer thicknesses ranging from ∼2 to 4 nm independently for both constituents by means of mid-IR second-harmonic phonon spectroscopy [2]. The higher spectral resolution of SHG as compared to reflectivity allows us to uniquely assign peaks to specific modes. In consequence, we are able to identify interface phonons by their layer thickness dependent behavior. [1] Caldwell et al., Nat. Nanotechnol. **11**, 9–15 (2016); [2] Paarmann et al., Phys. Rev. B **94**, 134312 (2016)

O 11.3 Mon 15:30 TRE Ma

Second Harmonic Generation from Surface Phonon Polaritons in Silicon Carbide — •Nikolai Christian Passler, Ilya Razdolski, Martin Wolf, and Alexander Paarmann — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin

Surface Phonon Polaritons (SPhP) have recently emerged as novel building block for mid-infrared (MIR) nanophotonic applications, promising to possibly overcome the intrinsic loss problem of plasmonics [1]. SPhPs arise in polar dielectrics due to optical phonon resonances leading to negative permittivity between transverse and longitudinal optical phonon frequencies. Furthermore, SPhPs exhibit tremendous field enhancements, driving the lattice atoms into a strongly nonlinear regime. Hence, SPhPs might grant a frequency-tunable access to vibrational-driven transient transitions of material phases.

Here, we use linear and nonlinear MIR spectroscopy [2], revealing the resonant second harmonic generation (SHG) arising from propagating SPhPs in SiC in the Otto geometry. Our experiments employ intense, tunable and narrowband MIR pulses from a free-electron laser. Corresponding to the absorption dip in our reflectivity spectra, we observe a strongly enhanced SHG yield at the SPhP resonance. Furthermore, we develop a matrix formalism for anisotropic multilayer wave propagation, allowing for precise prediction of the linear and non-linear properties of SPhPs.

[1] Caldwell et al., Nano Letters (2014) [2] Paarmann et al., APL (2015)

O 11.4 Mon 15:45 TRE Ma

Charge dynamics in organic materials imaged with nanosecond and nanometer resolution. — •Anna Rosławska[1], Pablo Merino[1], Christoph Grosse[1,2], Markus Etzkorn[1], Klaus Kuhnke[1], and Klaus Kern[1,3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]NanoPhotonics Centre, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — [3]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The dynamics of charges and bound pairs of charge carriers (excitons) determines the performance of organic optoelectronic devices, such as light emitting diodes or solar cells. Precise nanoscale characterization of light emission at the nanosecond timescale can help to improve the efficiency of such devices. Here, by using low-temperature Scanning Tunneling Microscopy-induced Luminescence (STML) we probe the charge dynamics on defect-related light emission centers in C_{60} thin films. We apply 100 ns long square voltage pulses [1] to the tunnel junction and record transients of the emitted light with sub-nanosecond resolution as a function of injection current and lateral distance from the emission center. Analysis of luminescence transients discloses time constants ranging from 5 ns to 50 ns depending on the position in space. They can be attributed to hole and electron injection rates to the defect state. Our approach allows mapping the transients on a grid and therefore obtaining light intensity videos with sub-nanosecond time resolution at the ultimate molecular scale.

[1] C. Große, *et al.*, Appl. Phys. Lett., 103, 183108 (2013)

O 11.5 Mon 16:00 TRE Ma

Single solid state quantum emitter coupled to a resonant plasmonic antenna array — •Markus Pfeiffer[1,2,3], Paola Atkinson[4], Armando Rastelli[4], Oliver G. Schmidt[4], Harald Giessen[3], Markus Lippitz[5,2,3], and Klas Lindfors[1,2,3] — [1]Department of Chemistry, University of Cologne, Luxemburger Str. 116, 50939 Köln, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [3]Fourth Physics Institute and Research Center SCOPE, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [4]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [5]Experimental Physics III, University of Bayreuth, Universitätsstrasse 30, 95447 Bayreuth, Germany

Plasmon resonant arrays or meta-surfaces shape optical fields and the local density of states. They provide large regions of enhanced emission from emitters and greater design flexibility than single nanoantennas. This makes them of great interest for engineering optical absorption and emission. Here we study the coupling of single self-assembled semiconductor quantum dots to plasmonic meta-surfaces. We investigate the influence of spectral properties of the nanoantenna array and the position of the emitter in the unit cell of the structure. We observe a resonant enhancement due to emitter-array coupling in the far-field regime and find a clear difference from the interaction of an emitter with a single antenna.

O 11.6 Mon 16:15 TRE Ma

Plasmon-exciton coupling in microcavities — •Igor Shavrin[1], Mario Hentschel[2], Daniel E. Gómez[3,4], Dirk Hertel[1], Klaus Meerholz[1], Timothy J. Davis[3,4], Harald Giessen[2], and Klas Lindfors[1] — [1]Department of Chemistry, University of Cologne, Luxemburger Str. 116, 50939 Köln, Germany — [2]4th Physics Institute and Research Center SCOPE, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [3]CSIRO, Materials Science and Engineering, Private Bag 33, Clayton, Victoria, 3168, Australia — [4]Melbourne Centre for Nanofabrication, Australian National Fabrication Facility, Clayton VIC 3168, Australia

Strong interactions between plasmons and excitonic states are interesting due to the extreme field confinement in plasmon resonant structures [1]. So far strong plasmon-exciton coupling has been achieved by placing the excitonic material in the near-field of a metal nanostructure. This however results in strong quenching of fluorescence.

Here we study the plasmon-exciton coupling mediated by a microcavity mode. We fabricate gold nanorod antennas in a wavelength-thick thin-film microcavity with the antennas positioned at one of the field anti-nodes using dielectric spacer layers. At the other anti-node we deposit a thin film of merocyanine molecules. These molecules form large J-aggregates that exhibit excitons with a strong dipole moment and therefore resulting in enhanced light-matter coupling. We observe three avoided crossings in reflection spectra that are well explained by a model with three coupled oscillators.

[1] J. Bellessa *et al.*, Phys. Rev. Lett. **93**, 036404 (2004).

O 11.7 Mon 16:30 TRE Ma

Double Modematching for Metal Nanoantennas — •Thorsten Feichtner[1], Silke Christiansen[2,3], and Bert Hecht[1] — [1]Nano-Optics & Biophotonics Group, Department of Experimental Physics 5, Röntgen Research Center for Complex Material Research (RCCM), Physics Institute, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [3]Max Planck Institute for the Science of Light, Günther-Scharowsky-Straße 1, 91058 Erlangen, Germany

The efficient coupling of photons from propagating far-fields to nanoscale volumes is a fundamental problem in quantum optics and at the heart of light-matter interaction. A common model system is the coupling between a point-like two-level quantum emitter (QE) and the continuum of radiative modes, which can be expressed in terms of the frequency-dependent partial local density of states (LDOS) at the QE position. Resonant plasmonic nanoantennas can be designed to strongly localize fields into a small volume leading to a LDOS enhanced by a factor of 10^5 and possibly beyond.

Here a description of power transfer between a QE and an optical antenna resembling a three-dimensional mode matching formalism is developed[1]. After introducing a second dipole in the far-field, another mode-matching step leads to a set of novel optical antenna design guidelines for QE emission enhancement. Accordingly a plasmonic cavity antenna (PCA) geometries is devised and compared to an established dipolar two-wire antenna geometry.

[1] T. Feichtner, S.H. Christiansen, and B. Hecht; arXiv:1611.05399

O 12: Organic-Inorganic Hybrid Systems and Organic Films II

Time: Monday 15:00–16:45 Location: WIL A317

O 12.1 Mon 15:00 WIL A317

Promoted exchange reaction between alkanethiolate self-assembled monolayers and an azide-bearing substituent — Rui Yan[1], Loïc Le Pleux[2], Marcel Mayor[2], and •Michael Zharnikov[1] — [1]Applied Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — [2]University of Basel, Department of Chemistry, St. Johannsring 19, CH-4056 Basel, Switzerland

The possibility of ultraviolet (UV) light promoted exchange reaction (UVPER) between the primary alkanethiolate (AT) self-assembled monolayers (SAM) and an azide-functionalized substituent (12-Azido-1-dodecanethiol, C12N3), capable of click reaction with ethynyl-bearing species, is demonstrated. This reaction resulted in the mixed AT/C12N3 films, with the portion of C12N3 precisely controlled by selection of a suitable UV dose. As the primary matrix, either non-substituted or oligo(ethylene glucole) (OEG) substituted AT SAMs were used, targeting mixed SAMs of chemical and biological significance. To demonstrate the flexibility of the approach, UV light with two different wavelengths (254 and 375 nm) was used, applied to the non-substituted and OEG-substituted AT SAMs, respectively. The surface density of the chemically active azide groups embedded in the non-reactive primary matrix could be varied according to the composition of the mixed SAMs. For the OEG-AT/C12N3 films, this resulted in the preparation of templates for specific protein adsorption, comprising biotin-bearing moieties embedded in the protein-repelling OEG-AT matrix.

O 12.2 Mon 15:15 WIL A317

The effect of different anchoring groups on immobilized Ruthenium (II) Bipyridine complexes for dye sensitised solar cells: A computational study — •Anik Sen and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

There is a currently a growing interest in the development of dye sensitized solar cells (DSSC) based on the p-type inorganic semiconductors such as NiO. The working principle is based on hole injection into the valence band of the p-type semiconductor from the photo excited semiconductor. We have performed density functional theory (DFT) calculations in order to understand the influence of different anchoring groups and spacer molecules attached to a photoactive Ruthenium polypyridine dye molecule on the physical and chemical properties of the DSSCs. The conversion efficiency of the dye molecules is assessed using time-dependent DFT. The NiO substrate is modeled within the cluster approach, and implicit solvent model calculations are performed to take the influence of the liquid environment into account.

The immobilized photo-active complexes bind to the NiO-substrate through the anchoring groups in mono-, bi- and tri-dentate forms. In our discussion of the computational results, we will in particular discuss the correlation between the adsorption geometry and the electronic structure of the complexes which is critical for the overall performance of the DSSC.

O 12.3 Mon 15:30 WIL A317

Spin-dependent dispersion of the hybrid band structure of the Alq3/Co interface — •Johannes Stöckl[1], Anatol Jurenkow[1], Nicolas Grossmann[1], Benjamin Stadmüller[1], Mirko Cinchetti[2], and Martin Aeschlimann[1] — [1]1 Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

Extensive studies in the last decade revealed that the spin polarization of ferromagnetic surfaces can be strongly altered by the adsorption of organic molecules. This effect is usually attributed to the formation of hybrid interface states across the metal-organic interface. Here we use spin- and angle-resolved photoemission (SR-ARPES) performed with VUV radiation to reveal changes in the spin dependent surface band structure of a thin cobalt film upon adsorption of the prototypical molecule Alq3. For the bare Co(100) surface, we find clearly dispersing d-bands along Γ-X in the vicinity of the Fermi energy, leading to an overall negative spin polarization at EF. The dispersion of the d-bands, and hence the corresponding spin polarization, change upon adsorption of Alq3. In particular, the effective mass of the Co d-bands increases significantly for both majority- and minority bands leading to an almost flat band dispersion and a uniform spin polarization for electron momenta at the Alq3/Co interface. Our findings will be discussed in the framework of a final state diffraction effect at the metal-organic interface and the formation of hybrid interface states.

O 12.4 Mon 15:45 WIL A317

Competition of surface-assisted organometallic and dehydrogenation reactions of non-functionalized porphyrin on Cu (111) — •Feifei Xiang, Anja Gemeinhardt, and M. Alexander Schneider — Solid State Physics, Friedrich-Alexander-University Erlangen-Nürnberg, 91058, Erlangen, Germany

The adsorption properties, self-assembly and surface assisted reactions of 5,15-diphenylporphyrin (2H-DPP) on Cu(111) are studied by low-temperature scanning tunneling microscopy in ultra-high vacuum. When deposited at room temperature and imaged at 80 K, well-ordered chain-like 2H-DPP structures along Cu [11-2] and equivalent directions are found that are stabilized by a weak interaction between the phenyl and pyrrole rings of neighboring molecules. At elevated annealing temperatures, an intramolecular dehydrogenation reaction is first triggered along with the Cu metalation of the DPP core producing a new planar Cu-DPP species on the surface. After that, two types of oligomer reaction products are formed, one of which consists of the planar Cu-DPP species linked by C-Cu-C bonds and the other by C-C covalent bonds. The latter product is the dominant species on the surface. We argue that is due to much faster reaction rates of the covalent bonded species than of the Cu linked species on Cu (111).

O 12.5 Mon 16:00 WIL A317

Structural, electronic and optical properties of K-doped PTCDA monolayer domains on Ag(111) — •M. Gruenewald[1], C. Zwick[1], F. Otto[1], A. Baby[2,3], E. Verwüster[2], O. T. Hoffmann[2], R. Forker[1], B. Stadtmüller[4], G. P. Brivio[3], G. Fratesi[3,5], C. Kumpf[6], E. Zojer[2], and T. Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena — [2]Institute of Solid State Physics, Graz University of Technology — [3]Department of Materials Science, University of Milano-Bicocca — [4]Fachbereich

Physik and Research Center OPTIMAS, University of Kaiserslautern — [5]Dipartimento di Fisica, Università degli Studi di Milano — [6]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich

Here we report the influence of potassium doping on highly ordered ultrathin layers of the dye molecule 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on Ag(111). The doped thin films have been characterized by LEED, STM, PES, x-ray standing wave (XSW), and differential reflectance spectroscopy (DRS). The experimental results are consistently interpreted with the help of density functional theory (DFT) calculations. We find that potassium doping induces a structural reordering of the commensurate PTCDA herringbone phase into point-on-line structures comprising charge-transfer complexes. Their stoichiometries are determined to K_2PTCDA and K_4PTCDA with potassium adsorption sites nearby the anhydride groups. PTCDA appears doubly negatively charged in both complex geometries; metal-organic hybridization becomes weaker with increasing potassium concentration.

O 12.6 Mon 16:15 WIL A317

Self-assembly and metal coordination of surface-adsorbed Pyrphyrin molecules — •Jingyi Li[1], Christian Wäckerlin[1], Stephan Schnidrig[2], Evelyne Joliat[2], Roger Alberto[2], and Karl-Heinz Ernst[1,2] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, 8600 Dübendorf, Switzerland — [2]Institut für Chemie, Universität Zürich, CH-8057 Zürich, Switzerland

The pyrphyrin molecule, which in contrast to porphyrin consists of four fused pyridine groups instead of pyrrol groups in its macrocycle, has been predicted to be a potential molecular catalyst. Using thermal desorption and X-ray photoelectron spectroscopy, we demonstrate that in monolayer coverage on Cu(111), the core of pyrphyrin is metalated with Cu adatoms at 377 K. Scanning tunneling microscopy reveals different self-assembly patterns before and after metalation. 2D honeycomb and 1D linear arrangements of pyrphyrin molecules are formed by linking the the cyano groups of pyrphyrin to Cu adatoms. Dehydrogenation at the periphery of the molecule after annealing at 520 K leads to the disappearance of self-assembled layers.

O 12.7 Mon 16:30 WIL A317

Comparison of various approaches to van der Waals interactions for anthracene and pentacene on Ag(111) — •Juliana Morbec and Peter Kratzer — Faculty of Physics, University of Duisburg-Essen, Germany

Anthracene and pentacene molecules have great potential for optoelectronic applications due to their high carrier mobility and excellent electroluminescence and photoluminescence. In this work we performed density-functional theory calculations to investigate the effects of the van der Waals (vdW) interactions on the structural and electronic properties of anthracene and pentacene adsorbed on the Ag(111) surface [1]. Our results show that vdW interactions strongly affect the stability and structural properties of both anthracene/Ag(111) and pentacene/Ag(111), but have little effect on the electronic properties of these systems. In particular, we found that the inclusion of vdW corrections is crucial to correctly describe the flat adsorption geometry of anthracene/Ag(111) observed in experiments. Moreover, we found that the adsorption of anthracene induces a larger reduction in the work function of the Ag(111) surface than pentacene, which is consistent with the stronger physisorption character observed in anthracene/Ag(111). The vdW interactions were treated using both the pairwise density-dependent vdW$^{\mathrm{surf}}$ approach [2] and many-body dispersion (MBD) method [3].

[1] Juliana M. Morbec and Peter Kratzer, submitted (2016). [2] V. G. Ruiz et al., Phys. Rev. Lett. 108, 146103 (2012). [3] A. Ambrosetti et al., J. Chem. Phys. 140, 18A508 (2014).

O 13: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - II

Time: Monday 15:00–18:15 Location: GER 38

Invited Talk O 13.1 Mon 15:00 GER 38

Towards efficient orbital-dependent density functionals for weak and strong correlation — •Igor Ying Zhang[1], Patrick Rinke[1,2], John P. Perdew[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Aalto University, Finland — [3]Temple University, USA

We present a new paradigm for the design of exchange-correlation functionals in density-functional theory [1]. Electron pairs are correlated explicitly by means of the recently developed second order Bethe-Goldstone equation (BGE2) approach [2]. Here we propose a screened BGE2 (sBGE2) variant that efficiently regulates the coupling of a given electron pair. sBGE2 correctly dissociates H_2 and H_2^+, a problem that has been regarded as a great challenge in density-functional theory for a long time [3]. The sBGE2 functional is then taken as a building block for an orbital-dependent functional, termed ZRPS, which is a natural extension of the PBE0 hybrid functional. While worsening the good performance of sBGE2 in H_2 and H_2^+, ZRPS yields a remarkable and consistent improvement over other density functionals across various chemical environments from weak to strong correlation. [1] IY Zhang et al., Phys. Rev. Lett. 117, 133002 (2016); [2] IY Zhang et al., New J. Phys. 18 073026 (2016); [3] AJ Cohen et al., Chem. Rev. 112 289 (2011).

O 13.2 Mon 15:30 GER 38

Towards a functional for strong correlation via semiclassical model for the indirect energy and local interpolation along the adiabatic connection — •Stefan Vuckovic and Paola Gori-Giorgi — Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling, FEW, Vrije Universiteit, De Boelelaan 1083, 1081HV Amsterdam, The Netherlands

Finding an approximate XC functional that is able to capture strong correlation effects is a big, unsolved DFT challenge. Even a bigger challenge is to find a functional able to treat any correlation regime successfully. We attempt to construct an XC functional that has no bias towards a particular correlation regime by using a local interpolation along the adiabatic connection between the weak and the strong coupling limit of DFT. [1] In addition to this approach, I will also present our semiclassical model for accurate indirect energies. I will discuss how this model can be used for a construction of XC functionals, exploiting its XC energy density in the conventional gauge, the one of the electrostatic potential of the XC hole.

1. Stefan Vuckovic, Tom J. P. Irons, Andreas Savin, Andrew M. Teale, and Paola Gori-Giorgi, Journal of Chemical Theory and Computation 2016, 12 (6), 2598-2610

O 13.3 Mon 15:45 GER 38

Benchmark of *GW* approaches for the *GW*100 test set — •Patrick Rinke[1], Matthias Dauth[2], Fabio Caruso[3], and Michiel van Setten[4] — [1]COMP Centre of Excellence, Aalto University, Finland — [2]University of Bayreuth, Germany — [3]University of Oxford, England — [4]Université Catholique de Louvain, Belgium

Many-body theory in the *GW* approach has become the method of choice for calculating charged excitations in solids. Now it is increasingly being applied to molecules, but fundamental questions regarding its *modus operandi* and its accuracy remain. To address both of these aspects, we present a comprehensive assessment of different *GW* methodologies for the recent *GW*100 test set [1] of molecular ionization energies [2]. We compare our *GW* calculations to coupled-cluster singles, doubles, and perturbative triples [CCSD(T)] reference data for *GW*100. We find ionization energies of fully self-consistent *GW* and quasiparticle self-consistent *GW* in excellent agreement with CCSD(T), with discrepancies typically smaller than 0.3 eV and 0.2 eV, respectively. For partially self-consistent and perturbative *GW* the deviation from CCSD(T) is strongly dependent on the starting point. An optimal starting point is found by minimizing the deviation from the straight-line error [3], which concomitantly yields a systematic improvement of the ionization energies. [1] M. J. van Setten, P. Rinke, *et al.*, J. Chem. Theory Comput. **11**, 5665 (2015), [2] F. Caruso, M. Dauth, M. J. van Setten, and P. Rinke, J. Chem. Theory Comput. **12**, 5076 (2016), [3] M. Dauth, F. Caruso, S. Kümmel, and P. Rinke, Phys. Rev. B **93**, 121115(R) (2016).

O 13.4 Mon 16:00 GER 38

Addressing electron-hole correlation in core excitations of solids: A first-principles all-electron approach based on many-body perturbation theory — •Christian Vorwerk, Caterina Cocchi, and Claudia Draxl — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

In the framework of an all-electron implementation of many-body perturbation theory, we investigate K, $L_{2,3}$, and M_4 absorption edges of three exemplary solids, spanning a broad range of transition energies from a few hundred to several thousands eV. We find that transitions from deep core states, such as the Ti 1*s* states in TiO_2 and the Pb 3*d* states in PbI_2, are ruled by the long-range electron-hole attraction. Spin-orbit coupling and local fields play only a minor role for these excitations, which occur at several keV. The exchange interaction between the excited electron and the core hole becomes more relevant for smaller transition energies, as exemplified with the Ca $L_{2,3}$ edge in CaO. The overlap between Ca 2*p* and 3*d* states calls for a careful treatment of local field effects in order to describe these excitations. Our results, in good agreement with the available experimental data, are thoughtfully analyzed with advanced visualization tools in order to further gain insight into the electronic contributions and the spatial extension of the resulting electron-hole pairs.

O 13.5 Mon 16:15 GER 38

Non-linear-screening contributions to photoemission spectra — •Marilena Tzavala[1,2], Claudia Rödl[1,2,3], and Lucia Reining[1,2] — [1]Laboratoire des Solides Irradiés, École polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF) — [3]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The state-of-the-art approach to calculate photoemission spectra of a broad range of materials is many-body perturbation theory in the *GW* approximation, sometimes combined with a cumulant expansion. The effective interaction that appears in these approaches is screened within the linear-response approximation. However, the photoemission of a core electron or a localized valence electron may be a strong perturbation, which suggests that non-linear screening effects could be important. We propose a formulation of the functional relations between the one-body Green's function and the screened interaction which is an alternative to Hedin's equations and which explicitly displays non-linear screening. Using a simple model, we show that exchange-correlation contributions are crucial in order to capture the non-linear effects. We also discuss how to apply the scheme to real materials using time-dependent density-functional theory (TDDFT).

O 13.6 Mon 16:30 GER 38

Dynamic LDA for electronic excitations — •Marco Vanzini[1,2], Matteo Gatti[1,2,3], and Lucia Reining[1,2] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF) — [3]Synchrotron SOLEIL, L'Orme des Merisiers, BP 48 Saint-Aubin, 91192 Gif sur Yvette, France

Density Functional Theory is an extremely useful tool for dealing with ground state properties such as the density or total energy. Kohn–Sham eigenvalues are often considered as approximated electronic excitations, but the resulting spectra are poor.

We propose a generalization of the Kohn–Sham approach to address in an exact framework electron addition and removal spectra. They can be measured by photoemission experiments, and can be evaluated using a computationally expensive non–local Self Energy. Our method is instead based on a frequency–dependent *local* potential [1], which significantly reduces the computing time of an ab–initio calculation.

To find this spectral potential in practice, we propose a jellium–based *dynamical* local density approximation (dynLDA): it relates the unknown potential to its homogeneous counterpart, via a non–trivial connector in space and frequency, which is based on physical insight.

In this talk, I will discuss the achievements and the limits of dynLDA, using models and real solids.

[1] M. Gatti et al., Phys. Rev. Lett. **99**, 057401 (2007).

O 13.7 Mon 16:45 GER 38

Recent developments of the Sternheimer-GW method — •Martin Schlipf[1], Henry Lambert[1,2], and Feliciano Giustino[1] — [1]Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom — [2]Department of Physics, King's College London, London WC2R 2LS, United Kingdom

The GW many-body perturbation method is an important tool to access accurate band gaps from first principles calculations. The conventional implementation determines the Green's function and the screened Coulomb interaction by a summation over unoccupied states tedious to converge. Giustino et al. demonstrated an alternative method to obtain these quantities by solving Sternheimer linear response equations. In this poster, we present our Sternheimer-GW software implemented in the Quantum Espresso framework and highlight some recent advances regarding the precision and stability of the method. We present our results for a small set of semiconducting materials and compare these to results obtained with conventional GW codes. We illustrate on selected examples the complete frequency dependent self energy, which is a natural product of the Sternheimer-GW method, and can be directly compared to experimental angle-resolved photoemission spectroscopy (ARPES) experiments.

O 13.8 Mon 17:00 GER 38

Calculating electronic correlations in the CASTEP ab initio code — •Vincent Sacksteder[1] and Evgeny Plekhanov[2] — [1]W155 Wilson Building, Royal Holloway University of London, Egham Hill, Egham, TW20 0EX, — [2]Kings College London

We present new DMFT and GW features in the CASTEP DFT code. These features are designed to provide more accurate treatment of correlations between localized orbitals, of electronic screening, and of excited states. In present benchmarks on Cerium Oxide, the gamma phase of Cerium, and Silicon. We discuss the calculation of atomic forces within the GW framework.

O 13.9 Mon 17:15 GER 38

Efficient G_0W_0 using localized basis sets: a benchmark for molecules — •Peter Koval[1,2], Mathias Per Ljungberg[1], and Daniel Sánchez Portal[1,2] — [1]Donostia International Physic Center, San Sebastian, Spain — [2]Centro de Fisica de Materiales, San Sebastian, Spain

Electronic structure calculations within Hedin's *GW* approximation are becoming increasingly accessible to the community. In particular, as it has been shown earlier and we confirm by calculations using our **MBPT_LCAO** package [1], the computational cost of the so-called G_0W_0 can be made comparable to the cost of a regular Hartree-Fock calculation. In this work, we study the performance of our new G_0W_0 implementation based on a contour deformation technique to reproduce the ionization potentials of all 117 closed-shell molecules belonging to the G2/97 test set, using a pseudo-potential starting point provided by the popular density-functional package **SIESTA** [2]. Moreover, the ionization potentials and electron affinities of a set of 24 acceptor molecules [3] are compared to experiment and to reference all-electron calculations.

[1] `http://mbpt-domiprod.wikidot.com`; [2] Soler J. M., *etal* J. Phys.: Condens. Matter **14** (2002) 2745; [3] Knight J. W., *etal* J. Chem. Theory Comput., **12** (2016) 615.

O 13.10 Mon 17:30 GER 38

A dynamic exchange correlation kernel derived from recent results for the homogeneous electron gas — •Martin Panholzer, Matteo Gatti, and Lucia Reining — Laboratoire des Solides Irradies UMR 7642, CNRS-CEA/DSM, Ecole Polytechnique, Palaiseau, France

Time-Dependent Density Functional Theory (TDDFT) is a method of choice to calculate the dynamic structure factor of a wide range of materials. Even in the simplest Adiabatic Local Density Approximation (ALDA), plasmon spectra are generally well described. However, several shortcomings remain. In particular, the onset energy of the spectrum is underestimated [1], and dynamical effects such as lifetime damping and double plasmon excitations are absent [2].

In this work we investigate recent results for the dynamic response of the homogeneous electron gas (HEG)[3] to extract an exchange correlation kernel for TDDFT. In order to get an estimate of the validity of such an approach we compare our results for the dynamic kernel $f_{xc}(q, \omega)$ for the HEG with different kernels and known exact properties. We implemented this kernel with the simplest connection between the HEG and the real material, the mean density approximation. We compare results on simple metals, such as Na and Al, with experiments and ALDA. In order to explore the validity of such an approach we also applied the kernel to Si.

[1] G. Onida et al., Rev. Mod. Phys. 74, 601 (2002)

[2] M. Cazzaniga et al., Phys. Rev. B 84, 075109 (2011)

[3] H. M. Böhm et al., Phys. Rev. B 82, 224505 (2010)

O 13.11 Mon 17:45 GER 38

Benchmark calculations of the electronic structure for molecules from the second-Born self-energy — •Michael Schüler[1] and Yaroslav Pavlyukh[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany — [2]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, P.O. Box 3049, 67653 Kaiserslautern, Germany

The non-equilbrium Green's function (NEGF) formalism provides a state-of-the-art tool for modeling modern spectroscopic experiments. In particular, time-dependent problems can be treated based on the Kadanoff-Baym equations. The underlying approximation to the self-energy has to be consistent with the treatment of the initial state - as captured by the Matsubara formalism - in order to guarentee the basic conservation laws. One of simplest non-trivial approximation to the self-energy is the second-Born approximation (2BA), which has been employed in numerous time-dependent studies. Systematic tests on the accuracy of the 2BA for various molecules has, however, been lacking so far. In our contribution we fill this gap by benchmark calculations for the 2BA for small molecules from the well established G2 test set. We demonstrate that the accuracy of the 2BA for predicting ionization potentials and electron affinities can compete with accurate quantum chemistry methods such as the Møller-Plesset perturbation theory and the coupled-cluster method. We also apply our method to a class of larger molecules, the diamonoids, which are in the focus of recent experiments and theoretical studies.

O 13.12 Mon 18:00 GER 38

Performance of the GW approximation at reproducing key features in exact Kohn-Sham potentials — •Jack Wetherell[1], Leopold Talirz[1], Matt Hodgson[2], and Rex Godby[1] — [1]University of York, York, United Kingdom — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

One of the major goals of the GW method is to improve the accuracy of charge densities produced by density functional theory (DFT). In this work we test the applicability of one-shot GW from various DFT starting Kohn-Sham orbitals. Also we implement and test the fully self-consistent GW method. We test the applicability of these methods by using them to compute densities for simple model 1D systems from which the exact density can be obtained by the direct solution of the Schrodinger Equation. We choose a set of test systems that are either dominated by exchange or correlation, or contain non-local steps in the exact exchange-correlation potential. Also we analyse systems dominated by electronic interaction. We can also investigate how accurate the exchange-correlation potentials associated with the GW densities are, using our reverse-engineering algorithm.

O 14: Electronic Structure of Surfaces: Magnetism and Spin Phenomena II

Time: Monday 15:00–17:30 Location: WIL C107

O 14.1 Mon 15:00 WIL C107

Exchange Splitting above the Curie Temperature in EuO — •Timm Gerber[1], Markus Eschbach[1], Tristan Heider[1], Ewa Mlynczak[1], Patrick Lömker[1], Pika Gospodaric[1], Mathias Gehlmann[1], Moritz Plötzing[1], Okan Köksal[2], Rossitza Pentcheva[2], Lukasz Plucinski[1,2], Claus M. Schneider[1,2], and Martina Müller[1,2] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, Germany — [2]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Germany

The ferromagnetic semiconductor europium monoxide (EuO) is an efficient spin filter and, therefore, an attractive material for fundamental research in the field of spintronics [1,2]. Although EuO is considered to be a Heisenberg ferromagnet, a Stoner-like vanishing of the conduction band's exchange splitting is typically observed [3].

We investigated the electronic structure of EuO by means of spin- and angle-resolved photoemission spectroscopy (spinARPES) complemented by DFT + U calculations. Our spin-resolved data reveals a complex temperature dependence of the occupied density of states which can not be accessed by spin-integrated ARPES measurements [4]. We show that the exchange splitting of the O $2p$ band persists up to the Curie temperature and even above. Our findings indictate that sizeable short range magnetic order in EuO is present above T_C.

[1] M. Müller et. al., J. Appl. Phys. 105, 07C917 (2009)

[2] A. Schmehl et. al., Nat. Mater. 6, 882 (2007)

[3] M. Freiser et al., Helv. Phys. Acta 41, 832 (1968).

[4] H. Miyazaki et. al., Phys. Rev. Lett. 102, 227203 (2009)

O 14.2 Mon 15:15 WIL C107

Impurity states and ferromagnetic superexchange interactions in the magnetic topological insulator V:(Bi,Sb)$_2$Te$_3$: a combined resonant photoemission and x-ray magnetic circular dichroism study — •Thiago R. F. Peixoto[1], Hendrik Bentmann[1], Sonja Schatz[1], Steffen Schreyeck[2], Martin Winnerlein[2], Charles Gould[2], Karl Brunner[2], Kai Fauth[3], Arthur Ernst[4], Laurens W. Molenkamp[2], and Friedrich Reinert[1] — [1]EP VII, Uni-Würzburg, Germany — [2]EP III, Uni-Würzburg, Germany — [3]EP II, Uni-Würzburg, Germany — [4]Max Planck Institute of Microstructure Physics, Halle, Germany

Recently we have demonstrated the impurity character of the V $3d$ density of states (DOS) at V:(Bi,Sb)$_2$Te$_3$ magnetic topological insulator thin films [1], a newly reported quantum anomalous Hall system (QAHS), by resonant photoemission spectroscopy (resPES). Here we used resPES at the Cr $L_{2,3}$ edges to extract the Cr $3d$ DOS of Cr:(Bi,Sb)$_2$Te$_3$ thin films, another QAHS, and compare with the V $3d$ states. In addition, we probed x-ray magnetic circular dichroism (XMCD) of the V $3d$ states, showing a persistent ferromagnetic character up to 50 K. A small opposite XMCD signal was observed at the Sb M_5 edge, evidencing an induced antiparallel magnetic moment at the Sb atom, as recently reported for Cr:(Bi,Sb)$_2$Te$_3$ [2]. The $3d$ impurity states are expected to mediate a ferromagnetic superexchange interaction, thus contributing to the ferromagnetism in these systems.

[1] T. R. F. Peixoto *et al.*, Phys. Rev. B **94**, 195140 (2016).

[2] M. Ye *et al.*, Nat. Commun. **6**, 8913 (2015).

O 14.3 Mon 15:30 WIL C107

Switchable spin - orbit gaps in a prototypical ferromagnet — •Ewa Mlynczak[1], Markus Eschbach[1], Stephan Borek[2], Jan Minar[2], Jürgen Braun[2], Irene Aguilera[1], Gustav Bihlmayer[1], Sven Döring[1], Mathias Gehlmann[1], Pika Gospodaric[1], Shigemasa Suga[1], Lukasz Plucinski[1], Stephan Blügel[1], Hubert Ebert[2], and Claus M. Schneider[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [2]Department Chemie, Ludwig-Maximilians-Universität München, Butenandtstrasse 5-13, 81377 München, Germany

In this contribution we will present results of a recent study of the influence of spin-orbit interaction (SOI) on the electronic properties of a prototypical ferromagnet, Fe(001) [1]. Using high resolution angle-resolved photoemission spectroscopy we demonstrate openings of the SOI - induced electronic band gaps, spin-orbit gaps (SOG), near the Fermi level. The SOG and thus the Fermi surface can be manipulated by changing the remanent magnetization direction. The experimental results are compared with the first-principles calculations and one-step photoemission calculations.

By pinpointing the regions in the electronic band structure where the switchable band gaps occur, we demonstrate the significance of SOI even for elements as light as 3d ferromagnets.

[1].E. Mlynczak et al. 'Fermi surface manipulation by external magnetic field demonstrated for a prototypical ferromagnet' Phys. Rev. X (2016), accepted

O 14.4 Mon 15:45 WIL C107

Spin texture manipulation in the multiferroic Rashba semiconductor GeMn$_x$Te — Juraj Krempasky[1], Stefan Muff[1,2], Jan Minar[3], Nicolas Pilet[1], Peter Warnicke[1], Vladimir Strocov[1], Gunther Springholz[4], and •Hugo Dil[1,2] — [1]Swiss Light Source, Paul Scherrer Institut, Switzerland — [2]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland — [3]Department of Chemistry, Ludwig Maximillian Universität, Germany — [4]Institut für Halbleiter-und Festkörperphysik, Johannes Kepler Universität, Austria

The search for materials with novel functional spin properties has received a prominent place in modern condensed matter physics because of the promise they bear in spinorbitronics and topological quantum phenomena. Multiferroic Rashba semiconductors are expected play an important role in this aspect because they combine a large Rashba-type spin splitting and ferromagnetic order in a manipulatable environment. By using a combination of spectroscopic techniques we could determine the electronic structure and spin properties of Mn-doped GeTe thin films[1,2]. The 3D Fermi surface takes the shape of a gapped spindle torus with just one spin-polarised Fermi sheet. Furthermore, it will be shown that the spin properties can be manipulated by either an electric field, a magnetic field, or optical stimuli. The films remain superconducting even after Mn doping, thus providing all the ingredients for the formation and manipulation of Majorana fermions.

[1,2] J. Krempasky et al. PRB 94, 205111 (2016); J. Krempasky et al. Nature Commun. 7, 13071 (2016).

O 14.5 Mon 16:00 WIL C107

Controlling the Rashba spin texture by adsorption of inorganic molecules — •Rico Friedrich, Vasile Caciuc, Gustav Bihlmayer, Nicolae Atodiresei, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, D-52425 Jülich

We demonstrate from first principles that the spin texture of a surface Rashba system can be controlled by the adsorption of molecules. By making use of physisorbed and chemisorbed inorganic molecules on the BiAg$_2$/Ag(111) surface alloy [1] we show that both the spin-orbit splitting and the spin direction of Rashba-split surface states can be manipulated selectively.

The physisorption of NH$_3$ gives rise to a slightly enhanced outward buckling of the surface Bi which enlarges the magnitude of the Rashba splitting. On the contrary, the weak chemisorption of BH$_3$ defines a strong inward relaxation of the surface Bi. This causes the occupied Rashba split state to shift into Ag bulk states. In addition a new Rashba splitting is created in an unoccupied state upon BH$_3$ adsorption. Most importantly, in contrast to the clean surface [1,2] in case of the BH$_3$-BiAg$_2$/Ag(111) system the out-of-plane spin polarization is significantly larger than the in-plane one.

[1] C. R. Ast *et al.*, Physical Review Letters **98**, 186807 (2007).
[2] G. Bihlmayer *et al.*, Physical Review B **75**, 195414 (2007).

This work is supported by the Volkswagen-Stiftung through the Optically Controlled Spin Logic project and by DFG through SFB 1238 (Project C01).

O 14.6 Mon 16:15 WIL C107

Spin crossover molecules on ferromagnetic FeN layer — •Jinjie Chen and Wulf Wulfhekel — Physikalisches Institut, Karlsruhe Institute of Technology (KIT)

Organic spintronics has become an attractive research field combining spin-based functional devices with the benefits of organic materials. A promising candidate to build organic electronic switches at nanoscale are spin crossover molecules, which display a transition between a low- and a high-spin state upon various external stimuli. Unlike a frozen spin state when deposited on metallic surfaces (Cu(111), Cu(100), Au(111), Ag(111) and Co/Cu(111)), Fe-(phenanthroline)2-(NCS)2 complexes (short Fe-phen) deposited on single ferromagnetic layer of FeN on Cu(100) can be switched between the two spin states at low temperatures. By switching the spin states, also the exchange interaction between individual Fe-phen molecule and FeN layer can be tuned. This work indicates a potential route to manipulating the magnetic properties of a hybrid system.

O 14.7 Mon 16:30 WIL C107

Spin polarization and attosecond time delay in photoemission from spin-degenerate states of Copper, Graphene and BSCCO — •Mauro Fanciulli[1,2], Stefan Muff[1,2], Andrew P. Weber[1,2], Ulrich Heinzmann[3], and Hugo Dil[1,2] — [1]École Polytechnique Fédérale de Lausanne, Switzerland — [2]Paul Scherrer Institut, Villigen, Switzerland — [3]University of Bielefeld, Germany

During the photoemission process from spin-degenerate states of solids, the photoelectron beam can present a spin polarization which originates from the phase of the photoelectron wavefunction and can be measured by spin-resolved photoemission spectroscopy. The binding energy dependence of the spin polarization can then be related to an attosecond time delay of the photoemission process via the Eisenbud-Wigner-Smith half-scattering model.

Our study involves three different solid state physics benchmark materials: Cu(111), quasi-free-standing graphene, and the cuprate superconductor BSCCO. Without any time resolution, our photoemission experiments on Cu(111) with full angular, energy and spin resolution show an attosecond time delay of the sp bulk-derived band. In the experimentally more complicated cases of graphene and BSCCO a sizeable spin polarization is still observed and can be related to the phase and time information.

These results open the way for new developments in spin- and time-resolved photoemission theory and experimental setups, and could help in the understandings of the physics of many different systems of interest.

O 14.8 Mon 16:45 WIL C107

Application of the Ir(100) surface as a spin-filter usingthe azimuthal characteristics of its scattering properties — •Keisuke Hatada[1], Stephan Borek[1], Jürgen Braun[1], Jan Minar[1,2], Erik Schäfer[3], Hans-Joachim Elmers[3], Gerd Schönhense[3], and Hubert Ebert[1] — [1]Ludwig-Maximilians-Universität München — [2]University of West Bohemia Pilsen — [3]Johannes-Gutenberg-Universität Mainz

It has been shown recently that the Ir(100) surface is a promising candidate for the application as spin filter [1]. In our theoretical study we investigated a semi-infinite Ir(100) system with a structural relaxed surface. Using the fully relativistic Korringa-Kohn-Rostoker method we are able to characterize the scattering of spin polarized electrons [2]. The calculations have been done for an energy range from 6 to 15 eV, i.e. for the energy regime of SPLEED (Spin Polarized Low Energy Electron Diffraction). With respect to experimental applications the diffraction patterns have been calculated using a polar angle of incidence of 45 deg. Considering the azimuthal degree of freedom we calculated so-called rotation diagrams beginning at a high symmetry direction of the Ir surface. The use of the azimuthal angle provides an additional possibility to construct spin-filter applications. In combination with external magnetic fields the detection of all components of the spin polarization is possible. Results of our corresponding calculations will be compared to experimental data.

[1] D. Kutnyakhov et al. Ultramicroscopy **130**, 63 (2013)
[2] H. Ebert et al., The Munich SPR-KKR package, version 7.2, 2016

O 14.9 Mon 17:00 WIL C107

Potential Energy Driven Spin Manipulation via a Controllable Hydrogen Ligand — •Peter Jacobson[1], Matthias Muenks[1], Gennadii Laskin[1], Oleg Brovko[2], Valeri Stepanyuk[3], Markus Ternes[1], and Klaus Kern[1,4] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy — [3]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120, Halle(Saale), Germany — [4]Institut de Physique, École Polytechnique Fédérale de Lausanne, CH-1015, Lausanne, Switzerland

Spin-bearing molecules can be stabilized on surfaces and in junctions with desirable properties such as a net spin that can be adjusted by external stimuli. Using scanning probes, initial and final spin states can be deduced from topographic or spectroscopic data, but the transition mechanism between these states is largely unknown. We address this question by manipulating the total spin of cobalt complexes on a h-BN surface with a H-functionalized scanning probe tip by simultaneously tracking force and conductance. When the additional H ligand is brought close to the CoH, switching between a correlated S = 1/2 Kondo state and a S = 1 state with anisotropy is observed. We show that the total spin changes when the system is transferred onto a new potential energy surface defined by the position of the H in the junction. These results show how and why chemically functionalized tips are an effective tool to manipulate adatoms and molecules, and a promising new method to selectively tune spin systems.

O 14.10 Mon 17:15 WIL C107

Vectorial Multichannel Spin-Polarimetry Using an Ir(001) Imaging Spin Filter — •Erik Schaefer[1], Stephan Borek[2], Jürgen Braun[2], Ján Minár[2,3], Hubert Ebert[2], Katerina Medjanik[1], Gerd Schönhense[1], and Hans-Joachim Elmers[1] — [1]Institut of Physics, Johannes Gutenberg-Universität Mainz, Staudingerweg 7, 55128 Mainz, Germany — [2]Department Chemie, Ludwig-Maximilians-Universität München, Butenandtstraße 5-13, 81377 München, Germany — [3]New Technologies-Research Centre, University of West Bohemia, Univerzitni 8, 306 14 Pilsen, Czech Republic

A newly developed high-performance imaging spin filter system based on a large Ir(001) scattering crystal tackles the issue of previously inefficient spin-resolving photoemission spectrometers. An increase of the effective figure of merit by a factor of over 10^3 in contrast to standard single-channel detectors is presented together with a detailed characterization of the experimental setup. The spin filter efficiency is analyzed by mapping a broad range of scattering energy and azimuthal angle. A high sensitivity to spin-components parallel and perpendicular to the scattering plane is observed under certain scattering conditions. An additional spin rotator element allows the independent determination of the two in-plane components of the spin vector. By combining three or six scattering conditions a vectorial spin analysis becomes possible for both, magnetic and non-magnetic samples.

O 15: Solid-Liquid Interfaces: Structure, Spectroscopy II

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

O 15.1 Mon 15:00 WIL B321

Traceable chemical analyses of new liquid and solid battery components by X-ray spectrometry in UHV environment — •Claudia Zech[1], Olga Grätz[2], Ivan Raguzin[2], Svetlozar Ivanov[3], Markus Börner[4], Marco Evertz[4], Marcelina Pyschik[4], Daniel Grötzsch[5], Wolfgang Malzer[5], Manfred Stamm[2], Sascha Nowak[4], and Burkhard Beckhoff[1] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany, — [2]Leibniz-Institut für Polymerforschung, Dresden, Germany — [3]Technische Universität Ilmenau, Germany — [4]Münster Electrochemical Energy Technology, Germany — [5]Technische Universität Berlin, Germany

The decomposition of the electrolyte solution, the degradation of the active material and the deposition of impurities are among the main aspects that worsen the performance of a battery so that the elemental composition and the species of the single components need to be studied. The determination of these properties is the challenge for most analytical methods due to a lack of reference materials. With reference-free X-ray fluorescence spectrometry (XRF) we can determine the mass deposition of elements and with X-ray absorption spectrometry (XAS) we get access to the oxidation state of single elements. With these techniques we investigated the cathodes of lithium-sulfur batteries, the anodes of NCM based Li-Ion batteries and Ionic Liquids. All measurements are done with synchrotron radiation under UHV environment at BESSY II in Berlin.

O 15.2 Mon 15:15 WIL B321

Unraveling water structuring on Nafion-like sulfonate-based model surfaces with increasingly hydrophobic character using force spectroscopy — •Laila Moreno Ostertag[1], Xiao Ling[2], Thomas Utzig[1], Philipp Stock[1], Sapun Parekh[2], Katrin Domke[2], and Markus Valtiner[1,3] — [1]Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf - Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz - Germany — [3]Institut für Physikalische Chemie der TU Bergakademie Freiberg, 09599 Freiberg - Germany

Nafion membranes are an essential component of fuel cells, providing an effective medium to separate cathode and anode while facilitating proton conduction. Specifically, Nafion is a porous material with 1-2 nm pore diameters. The way water is structured across a pore is essential to understand the mechanism of proton transport. Here, we used atomic force microscopy to measure interaction forces between Nafion-like model surfaces emulated via self-assembled monolayers (SAM) where SO3- groups were gradually substituted by hydrophobic groups. The resulting interaction force profiles can be fitted to extended DLVO models depending on hydrophobic or charged content, in order to gain insight into the molecular surface structure that gives rise to the measured forces. Our data indicates a non-linear trend of the solvent structure at the surface as a function of the hydrophobic-to-sulfonate group ratio, indicating that small changes in stoichiometry can significantly alter water layering. We will discuss how our results relate to proton conductivity and how they may help to optimize membrane properties.

O 15.3 Mon 15:30 WIL B321

STM investigation on the adsorption of water on Ru(0001) - Influence of temperature and coadsorbed CO — •Martin Schilling, Laura Friedrich, Sylvain Brimaud, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, 89069 Ulm, Germany

The interaction of water with metal surfaces is of particular interest as model for the solid-liquid interface, and has therefore been studied intensely [1]. Besides adsorbate-metal interactions, also intermolecular interactions were found to play an important role. The situation becomes even more complex for the coadsorption of two adsorbing species.

Here we present results of a low temperature scanning tunnelling microscopy (STM) study on the structure of adsorbed water and water co-adsorbed with CO on Ru(0001), which was performed under ultra-high vacuum (UHV) conditions. For the adsorption of water we found distinctly different adsorbate arrangements, depending on the adsorption temperature (100 - 150 K). For deposition temperatures of 120 - 150 K, well-ordered stripe structures can be formed.

Post-exposure of such surfaces to CO revealed that only little CO was adsorbed in the areas between the stripes formed by adsorbed water, indicating that these areas are not bare Ru(0001) but (partly) covered by a dilute adsorbate layer that is not resolved in STM images. Different possibilities are discussed. Finally we investigated the influence of the dosing sequence on the structure of the resulting adlayer.

[1] J. Carrasco *et al., Nat. Mater.* **11** (2012) 667

O 15.4 Mon 15:45 WIL B321

In-situ tracking of the dynamic structure evolution in nanometer confined liquids by combining X-Ray Reflectivity and white light interferometry in a surface forces apparatus — •Sadhanaa Buvaneswaran[1], Henning Weiss[2], Hsiu-Wei Cheng[1], Claudia Merola[1], Julian Mars[2], Markus Mezger[2], and Markus Valtiner[1] — [1]Max-Planck-Institut fur Eisenforchung GmbH — [2]Max-Planck-Institut fur Polymerforchung

Nanometer confined liquids between solids exhibit molecular ordering and find importance in friction and energy conversion. How this structuring reacts to external triggers such as sliding of surfaces against each other, or changing applied stresses is notoriously hard to measure in experiment. Here, we experimentally obtain the structural information under precisely controlled liquid confinement with dynamically changing conditions. For this, we combine the Surface Force Apparatus which allows quantification of applied forces between two opposing surfaces based on optical interference and XRR that determines crystallographic structure on a molecular scale. A pore(mm2 area) with controlled height of only 100s of nm of a model liquid crystal 8CB could be realized. When no force is applied, X-Ray scattering (probed horizontal direction) showed a sharp peak at q=2nm-1 which agreed well with the calculated molecular length established in previous literature. In XRR (investigated vertical liquid layering) similar intensities at identical q indicated isotropic behavior. However, during dynamic straining, the scattering intensities were 180 degree out-of-phase to the reflectivity intensity pointing towards anisotropic behavior.

O 15.5 Mon 16:00 WIL B321

Self-Assembly of Imidazolium Based Ionic Liquids at Mica Interfaces is Induced by Confinement and the Presence of Water — •Hsiu-Wei Cheng, Jan-Niklas Dienemann, Philipp Stock, Claudia Merola, Ying-Ju Chen, and Markus Valtiner — Max-Planck Instut für Eisenforschung

Tuning chemical structure and molecular layering of ionic liquids (IL) at solid interfaces offers leverage to tailor performance of ILs in applications such as super-capacitors, catalysis or lubrication. Recent experimental interpretations suggest that ILs containing cations with long hydrophobic tails form well-ordered bilayers at interfaces. Here we demonstrate that interfacial bilayer formation is not an intrinsic quality of hydrophobic ILs. In contrast, bilayer formation is triggered by boundary conditions including confinement, surface charging and humidity present in the IL. Therefore, we performed force versus distance profiles using atomic force microscopy and the surface forces apparatus. Our results support models of disperse low-density bilayer formation in confined situations, at high surface charging and/or in the presence of water. Conversely, interfacial structuring of long-chain

ILs in dry environments and at low surface charging is disordered and dominated by bulk structuring. Our results demonstrate that boundary conditions such as charging, confinement and doping by impurities have decisive influence on structure formation of ILs at interfaces. As such, these results have important implications for understanding the behavior of solid/IL interfaces as they significantly extend previous interpretations.

O 16: SYLI: Interfacial Challenges in Solid-State Li Ion Batteries - Interface-dominated behaviour

Time: Monday 15:45–16:45 Location: IFW A

O 16.1 Mon 15:45 IFW A

Interfacial double layers in all-solid-state Li-ion batteries: theoretical insights — •Johannes Voss[1], Saskia Stegmaier[2], Karsten Reuter[3], and Alan Luntz[1,2] — [1]SLAC National Accelerator Laboratory, Menlo Park, CA, USA — [2]Stanford University, Stanford, CA, USA — [3]Technische Universität München, Germany

Neglecting potential electrochemical and mechanical stability issues of the interface between battery electrode and solid Li-ion conducting electrolyte, we present a theoretical study of charge double layers at ideal solid-solid interfaces. Based on DFT calculations for Li_3OCl, we discuss ionic charge carrier stabilities and interactions in the bulk and at interfaces to electrodes. We furthermore employ continuum models parametrized with DFT energies to understand charging at both the anode and cathode interfaces, respectively, and discuss how spacer materials could mitigate related potential interfacial issues.

O 16.2 Mon 16:00 IFW A

Separation of Intra Grain and Grain Boundary Processes in Solid Electrolytes by High-Resolution Impedance Spectroscopy — •Andreas Mertens, Shicheng Yu, Deniz Guenduez, Hermann Tempel, Roland Schierholz, Hans Kungl, Rüdiger-A. Eichel, and Josef Granwehr — Forschungszentrum Jülich, Institute of Energy and Climate Research, IEK-9, D-52425 Jülich, Germany

Solid electrolytes are intensively researched for the next generation lithium-ion batteries. Yet their ion transport mechanisms must be better understood to improve their still too low ionic conductivity. Especially distinguishing between contributions from intra grain and grain boundary processes proved to be particularly challenging. This is mainly due to similar time constants of both processes at room temperature, leading to a strong overlap of their impedance contributions.

In this work we use a distribution of relaxation times analysis (DRT) in two dimensions (2D-DRT) to increase the resolution of impedance data measured at Li1.3Al0.3Ti1.7(PO4)3 (LATP) solid electrolyte samples sintered between 950°C and 1100°C. The second dimension of the 2D-DRT is given by data measured at varying temperatures between 10°C and 50°C. With the 2D-DRT it is possible to quantify the resistances and thus the activation energies of the intra grain and the grain boundary ionic charge transport processes under realistic battery operation conditions. Moreover, the ionic conductivity within the grain and the grain boundary could be determined.

O 16.3 Mon 16:15 IFW A

Microstructural Properties of Li1.3Al0.3Ti1.7(PO4)3 Solid-State Electrolyte — •Deniz Cihan Gunduz[1,2], Roland Schierholz[1], Shicheng Yu[1,2], Andreas Mertens[1,2], Hermann Tempel[1], Hans Kungl[1], and Rüdiger-A Eichel[1,2,3] — [1]Forschungszentrum Jülich, Institute of Energy and Climate Research, IEK-9, 52425 Jülich, Germany — [2]RWTH Aachen University, Institute of Physical Chemistry, 52074 Aachen, Germany — [3]Jülich-Aachen Research Alliance, Section JARA-Energy, Germany

Lithium-ion batteries are important in daily life. One task is to replace liquid electrolytes by solid ones and Li1.3Al0.3Ti1.7(PO4)3 (LATP) is a promising candidate exhibiting high ionic conductivities. For further development it is important to understand the influence of the microstructure on the ionic conductivity. Solid state electrolytes have been mainly investigated via means of electron microscopy (Scanning Electron Microscopy as well as Transmission Electron Microscopy). Here we combine these techniques with Laser Scanning Microscopy (LSM) to study the microstructure, such as grain size, grain boundary width, porosity and secondary phase content and distribution of LATP pellets sintered at different temperatures; and draw a relation to impedance measured on these pellets.

O 16.4 Mon 16:30 IFW A

Development of Bulk-type All-Solid-State Lithium-ion Battery Based on Phosphate Backbone Materials — •Shicheng Yu, Hermann Tempel, Andreas Mertens, Deniz Cihan Gunduz, Svenja Benning, Roland Schierholz, Florian Hausen, Hans Kungl, and Rüdiger-A Eichel — Forschungszentrum Jülich, Institute of Energy and Climate Research, IEK-9, D-52425 Jülich, Germany

Considerable efforts have been devoted to the development of thick-film solid-state batteries while less achievement has been published owing to the poor interfacial compatibility between electrodes and electrolytes as well as low lithium ion transfer kinetics in solid materials. Here, we demonstrate the fabrication and performance of thick-film monolithic all-phosphate ceramic solid-state Li-ion batteries with high power density and cycling stability at ambient temperature based on LiTi2(PO4)3/C//Li1.3Al0.3Ti1.7(PO4)3//Li3V2(PO4)3/C. Theoretically, due to the crystal structure matchup of LiTi2(PO4)3, Li1.3Al0.3Ti1.7(PO4)3 and Li3V2(PO4)3, the solid-solid interface between Li1.3Al0.3Ti1.7(PO4)3 electrolyte and LiTi2(PO4)3 anode is expected to facilitate smooth contact while partially matched on the other side for the solid-solid contact of solid electrolyte and Li3V2(PO4)3 cathode. Besides, the operation voltage of the electrode pair is highly matched with the electrochemical window of solid electrolyte. Excitingly, by optimizing the morphology of electrode materials and composition of each layer, the all-solid-state lithium-ion battery, which has a controllable thickness from 0.7 up to 2 mm, showed high capacity and more than 300 stable cycles.

O 17: Scanning Probe Techniques: Method Development II

Time: Monday 15:45–18:00 Location: TRE Phy

O 17.1 Mon 15:45 TRE Phy

Imaging adatoms, rest atoms and defects on Si(111)-7x7 with a CO terminated metal tip — •Daniel Meuer and Franz Josef Giessibl — University of Regensburg, D-93055 Regensburg, Germany

The surface of Si(111)-7x7 exposes adatoms at the top surface layer and rest atoms that are approximately 100 pm below the adatom layer [1]. We show that a CO tip of an AFM resolves both adatoms and rest atoms as roughly Gaussian protrusions, which is in agreement with charge density calculations using Slater-type-orbitals. Both the experimental and calculated data do not show apparent artifacts. In this contribution we also present that we can resolve the atomic structure inside surface defects. This is possible due to the fact that the CO molecule at the metal tip apex is a very sharp probe with a thin apex compared to metal cluster tips.

The previous work was done in a force regime, where CO bending artifacts do not occur. For distance regimes with CO bending one would expect a non-Gaussian shape of the adatoms. In 2014 Sweetman et al showed data, where they observe a non-Gaussian shape of the adatoms with a unknown tip termination. They relate this subatomic features of the adatoms of the Si(111)-7x7 surface to the back bonding of the surface atoms [2]. We show data with a CO terminated tip, which clearly show CO bending in preferred directions.

References:

[1] K. D. Brommer et al - Jpn. J. Appl. Phys. 32, 1360 (1993)

[2] A. Sweetman et al.- Nano Lett. 14, 2265-2270 (2014)

O 17.2 Mon 16:00 TRE Phy

Measurement of Nano Particle Adhesion by Atomic Force Microscopy — •Daniel Geiger[1], Irina Schrezenmeier[1], Matthias Roos[3], Tobias Neckernuss[1], Michael Lehn[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Institute of Numerical Mathematics, Ulm University, Helmholtzstrasse 20, 89081 Ulm, Germany — [3]Carl Zeiss SMT GmbH, Rudolf-Eber-Strasse 2, 73447 Oberkochen, Germany

The adhesiveness of nanoparticles on surfaces is of interest for many applications. This includes processes that are intended to deposit particles on a surface as well as processes that aim to remove nanoparticles from a surface.

We present a method to measure the adhesiveness of nanoparticles by means of lateral force measurements using an atomic force microscope. The measurement protocol is based on conventional contact, constant force mode scanning of a sample decorated with nano beads. By moving the particles laterally their adhesive forces are given as the lateral force acting on the cantilever. Geometry related measurement errors are compensated by statistical analysis. For that reason a model based on probability theory was derived that allows reconstruction of the actual pushing force distribution acting on the beads. The model is applied to measurement data of 50 nm silica nano beads on a silicon substrate.

O 17.3 Mon 16:15 TRE Phy

Controlled Nanometer Layer Ablation by Diamond AFM tips in a hybrid SEM/AFM — •Frank Hitzel[1] and Jason Kilpatrick[2] — [1]Semilab Germany GmbH, Braunschweig, Germany — [2]Adama Innovations, Dublin, Ireland

Combined Scanning Electron Microscope / Focused Ion Beam (SEM/FIB) systems are nowadays an established and stable technology for precise nanometer manipulation / cutting and in-depth analysis of structures. Nevertheless, the electrical properties of the areas manipulated by FIB strongly change because of implanted Gallium atoms.

In such situations, another technique has been recently evolving, often called "scalpel AFM". Here, typically a diamond tip is scanned with predefined force over a sample surface, removing in a controlled way a few atomic layers of the sample material. Like FIB treatment, this gives access to the layers buried below the surface. But in contrast to FIB treatment, these layers are not contaminated by Ga atoms opening up the possibility for electrical characterization.

The hybrid SEM/AFM enables live imaging of the modified area and gives exceptional control of the ablation process, which is to some extend similar to scratching with a screw driver in a clay layer. Similar to FIB tomography, the combination enables the possibility to switch between SEM imaging and the ablation process, resulting in a 3 dimensional image of the manipulated surface.

O 17.4 Mon 16:30 TRE Phy

Atomic Force Microscopy with stiff qPlus sensors in liquid environments — •Korbinian Pürckhauer, Alfred J. Weymouth, and Franz J. Giessibl — University of Regensburg, Germany

We set up a custom-built AFM with qPlus sensors to operate in ambient conditions as well as in liquid environments [1]. For measurements in liquids we immerse the sample in liquid and use long tips, only submerging the tip apex. We discuss the decrease of the Q-factor as a function of the penetration depth of the tip in liquid. The high stiffness of our qPlus sensors ($k \geq 1800$ N/m) allows us to keep this Q value above 140 during measurements.
Atomic resolution of muscovite mica was achieved both in ambient conditions and in liquid. Beside H_2O we used Tris-HCl buffer and a culture medium, which contains salts, a mineral solution, Resazurin, Na_2S and other solutes.

[1] Wastl, D. S., Weymouth, A. J., & Giessibl, F. J. (2013). Optimizing atomic resolution of force microscopy in ambient conditions. Physical Review B, 87(24), 245415.

O 17.5 Mon 16:45 TRE Phy

Imaging successive intermediate states of the on-surface Ullmann reaction — •Daniel Ebeling[1], Sören Zint[1], Tobias Schlöder[2], Sebastian Ahles[3], Doreen Mollenhauer[2], Hermann A. Wegner[3], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Germany — [2]Institute of Physical Chemistry, Justus Liebig University Giessen, Germany — [3]Institute of Organic Chemistry, Justus Liebig University Giessen, Germany

Recently, different bottom-up approaches have been developed for the on-surface synthesis of covalently bonded organic frameworks. In order to use these structures for future applications, such as nanoelectronic or -optical devices, in-depth knowledge about the underlying reaction mechanisms has to be gained. This is crucial for establishing a basis for the design of new functional devices with tailor-made properties. Here, we are using low temperature atomic force microscopy (AFM) with CO functionalized tips together with density functional theory (DFT) calculations with dispersion correction to study the complete reaction pathway of the on-surface Ullmann-type coupling between bromotriphenylene molecules on a Cu(111) surface. All steps of the Ullmann reaction, i.e., bromotriphenylenes, triphenylene radicals, organometallic intermediates, and bitriphenylenes could be imaged with submolecular resolution. We can unambiguously identify the chemical structure and the adsorption geometry of each individual species and therewith provide deeper insight into the reaction process.

O 17.6 Mon 17:00 TRE Phy

AFM investigation on CaF2(111) with atomically characterized tips — •Alexander Liebig, Angelo Peronio, Daniel Meuer, Alfred J. Weymouth, and Franz J. Giessibl — Universität Regensburg, Germany

In contrast to ionic crystals of the rock salt structure, the surface ions of CaF2(111) are all charged negatively, and AFM measurements on this surface had previously been used to identify positively- and negatively-terminated tips [1]. Similar to previous experiments on Cu2N [2], we imaged this surface with both metal- and CO-terminated tips that were characterized using the COFI method, where an adsorbed CO molecule is used to image the tip apex [3]. We simulated the AFM data with a simple electrostatic model, in which the surface atoms are represented as point charges and the tip as a dipole. For measurements acquired relatively far from the surface the electrostatic force is the dominant contribution to the AFM contrast and the model allows us to determine the sign of the net charge at the tip apex. However, this point-charge model fails to reproduce the data closer to the surface, where the bending of the CO molecule and Pauli repulsion become important [4,5]. These effects lead to a contrast inversion in the AFM images acquired with a CO-terminated tip at very close tip-sample distances.

[1] A.S. Foster et al., Phys. Rev. Lett. 86, 2373 (2001). [2] M. Schneiderbauer et al., Phys. Rev. Lett. 112, 166102 (2014). [3] J. Welker and F.J. Giessibl, Science 336, 6080 (2012). [4] L. Gross et al., Science 337, 6100 (2012). [5] M. Ellner et al., ACS Nano Letters 16, 3 (2016).

O 17.7 Mon 17:15 TRE Phy

HR-LC-AFM for detection of current paths on oxides with atomic resolution — •Christian Rodenbücher, Gustav Bihlmayer, Marcin Wojtyniak, Wolfgang Speier, and Kristof Szot — Peter-Grünberg-Institut and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich

The ongoing miniaturization of electronic devices and the introduction of novel materials such as metal oxides for memristive applications is accompanied with new challenges since the electronic transport phenomena have to be analyzed on the atomic scale. Typically, the STM method is used to obtain information about the electronic properties in nanoscale, however it cannot be successfully applied on all surfaces. For example, on surfaces with inhomogeneous conductivity any changes in the electrical properties of the surface are inseparable from changes in the sample topography. Hence, we implemented the technique of high-resolution local-conductivity atomic force microscopy (HR-LC-AFM) for the investigation of oxide surfaces and achieved, for a first time, a direct current mapping with atomic resolution. We revealed that the surface conductivity of the prototypical transition metal oxides $SrTiO_3$ and TiO_2 is confined to conducting areas on the nanoscale. Assisted by *ab initio* theory we argue that a clustering of oxygen vacancies in the surface of transition metal oxides could be responsible for the observed localization. This way we introduced LC-AFM as next scanning probe tool with true atomic resolution complementing the well-established techniques of (NC-)AFM, FFM, SKPM, and STM which may help to open up a new chapter on surface science.

O 17.8 Mon 17:30 TRE Phy

Scanning tunneling microscopy and potentiometry using a cooled JFET electrometer — •Paul Graf, Meike Flebbe, Christian A. Bobisch, Hermann Nienhaus, and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

We show that a liquid nitrogen cooled junction field effect transistor can be used to measure either small electric charges or ultra low currents in the range of 10^{-18} A [1]. The leakage current between the gate electrode and the source-drain channel of the JFET drops to several 10^{-20} A at a temperature of 80 K, so that the gate can store charge for a time of several days. The gate voltage, hence the charge, can be easily measured by the source-drain current. Here, we combine this cooled JFET electrometer with a scanning tunneling microscope connecting the gate electrode of the JFET directly to the tunneling tip. Using an AC-bias voltage, STM imaging at low current becomes possible. Since the gate voltage automatically adjust to zero average current, the dc component directly yields the electrochemical potential. Laterally resolved images show topographic features such as atomic step edges and terraces but also lateral oscillations in the electrochemical potential, i.e. thermovoltage, which can be attributed to standing electron wave patterns, e.g., of the surface state of Cu(111).

[1] Rolf Möller and Hermann Nienhaus, patent pending, *Open FET Sensor*, Provendis Ref.-Nr. 4817

O 17.9 Mon 17:45 TRE Phy

Imaging and quantification of work function variations on a nanostructured surface with scanning quantum dot microscopy — •Christian Wagner[1,2], Matthew F. B. Green[1,2], Philipp Leinen[1,2], Michael Maiworm[3], Taner Esat[1,2], Rolf Findeisen[3], Ruslan Temirov[1,2], and F. Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Institute for Automation Engineering (IFAT), Otto-von-Guericke Universität Magdeburg, Germany

The properties of a surface are crucially influenced by its electrostatic potential landscape. This landscape is formed by work function variations, e.g., due to adsorbate layers and by the local fields of edges and point-like impurities. When imaging the surface potential it is desirable to observe all these effects on equal footing. We demonstrate that scanning quantum dot microscopy (SQDM) enables precise quantification of work function variations for structures down to 10 nm in diameter and simultaneous imaging of individual atomic-scale defects. This is possible since SQDM is essentially based on a point-like probe, a molecular quantum dot, and thus avoids the averaging effects which are intrinsic to Kelvin probe force microscopy (KPFM) and which depend on tip size, shape and height. Paradoxically, in SQDM a blunter AFM tip yields sharper images due to electrostatic screening. We exemplify our method by imaging the interface dipole of islands of perylene-tetracarboxylic dianhydride (PTCDA) on Ag(111) and determining its value to be $\Delta\phi = 145 \pm 10$ mV.

O 18: Semiconductor Substrates: Structure, Epitaxy and Growth

Time: Monday 16:00–17:30 Location: WIL C307

O 18.1 Mon 16:00 WIL C307

Deconstructing silicon: can surface reconstructions emerge from global geometry screening? — •Chiara Panosetti[1], Maximilian Bauer[1], Matt Probert[2], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]University of York, GB

The $Si(111) - (7 \times 7)$ reconstruction is arguably the most complicated surface superstructure known to date. The details of its currently accepted geometry, described by the so-called Dimer-Adatom-Stacking fault (DAS) model, are the result of a 25-year long joint effort of experiments and theory. Attempting to solve such a complicated problem—with a known solution—by means of unbiased global structure optimization is therefore a suitable testbed for the performance of corresponding computational algorithms. We here specifically assess the performance of Genetic Algorithms (GA) and the Basin Hopping (BH) approach, where the generation of trial structures for canonical and grand canonical screening is applied to the surface layer in periodic boundary conditions and where different strategies are pursued to enhance the production of chemically sensible candidate geometries. Results suggests that robustness, success and speed of convergence of the employed approaches are strongly influenced by how much the trial moves tend to preserve favourable bonding patterns once they appear.

O 18.2 Mon 16:15 WIL C307

Patterning of ultra sharp dopant profiles in silicon — Simon Cooil[1,2], Federico Mazzola[1], Hagen Klemm[3], Gina Peschel[3], Yuran Niu[4], Alex Zhakarov[4], Andrew Evans[2], Thomas Schmidt[3], Michelle Simmons[5], •Jill Miwa[6], and Justin Wells[1] — [1]NTNU, Trondheim, Norway — [2]Aberystwyth University, Aberystwyth, UK — [3]Fritz Haber Institute, Berlin, Germany — [4]MAX IV Laboratory, Lund, Sweden — [5]UNSW, Sydney, Australia — [6]Aarhus University, Aarhus, Denmark

We present a method for patterning a buried two-dimensional electron gas (2DEG) in silicon. The buried 2DEG forms from placing an ultra sharp and dense profile of phosphorus dopants beneath the silicon surface; a so-called Si:P δ-layer. The composition and structure of these Si:P δ-layers have been studied down to the atomic limit by secondary ion mass spectrometry and scanning tunnelling microscopy. Both angle resolved photoemission spectroscopy and theoretical calculations have shown that these Si:P δ-layers host a 2DEG with properties desirable for atomic scale quantum electronic devices. Here, we provide a new method for patterning such buried 2DEGs using low kinetic energy electron beam lithography. Using a combination of microscopic and spectroscopic techniques, we demonstrate the formation of patterned features with dopant concentrations sufficient to create 2DEG states.

O 18.3 Mon 16:30 WIL C307

Surface Structure of MOVPE-prepared GaP(111)B — •Peter Kleinschmidt[1], Pingo Mutombo[2], Oleksandr Romanyuk[2], Marcel Himmerlich[3], Theresa Berthold[3], Xin Wen[1], Andreas Nägelein[1], Matthias Steidl[1], Agnieszka Paszuk[1], Oliver Supplie[1], Stefan Krischok[3], and Thomas Hannappel[1] — [1]Photovoltaics Group, Institute of Physics, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [2]Institute of Physics, Academy of

Sciences of the Czech Republic, Cukrovarnicka 10, 162 00 Prague 6, Czech Republic — [3]Technical Physics I, Institute of Physics and IMN MacroNano, Technische Universität Ilmenau, 98684 Ilmenau, Germany

We have characterized the structure of MOVPE-prepared GaP(111)B surfaces by STM, XPS and ab intio DFT. After deoxidation under tertiarybutylphosphine and subsequent annealing in H_2, STM images show flat terraces with an atomic surface structure which is congruent with the underlying lattice, but only locally exhibits ordered regions of (2×2), $c(4 \times 2)$ and $(\sqrt{3} \times \sqrt{3})$ reconstruction. We identify the protrusions in the images as dangling bonds of an otherwise H-terminated phosphorus face. The DFT calculations predict a (2×2)-3H and $c(4 \times 2)$-3H reconstruction under H-rich conditions, while the $(\sqrt{3} \times \sqrt{3})$-2H reconstruction is less favorable. Preparation without annealing in H leads to a P-rich surface with an additional adlayer of trimers.

O 18.4 Mon 16:45 WIL C307

In situ surface control of AlP on GaP(100) substrate during processing in MOCVD ambient — •Manali Nandy, Agnieszka Paszuk, Anja Dobrich, Oliver Supplie, Peter Kleinschmidt, and Thomas Hannappel — TU Ilmenau, Gustav-Kirchhoff-Straße 5 (Meitnerbau) 98693 Ilmenau

Epitaxial growth of III-V materials on Si substrate can be beneficial for cost-effective devices in optoelectronic applications. However the nucleation of III-V materials like AlxGa1-xP material grown on Si(100) substrate could serve as a buffer layer for other III-V materials, due to small lattice mismatch between the Si and AlxGa1-xP(from 0.36%-0.37% for x=0 to 1)[2]. Here,first we focus on the growth of AlP buffers on GaP(100) substrate. After deoxidation of GaP(100) substrates at 630°C under H2 ambient, we have grown GaP buffer layer prior to growth of AlP epilayer. The growth temperature was kept at 600°C and the reactor pressure was constant at 100 mbar throughout the process. The whole process was monitored in-situ by reflection anisotropy spectroscopy (RAS). The RAS signal taken at 300°C from the AlP surface shows a clear, distinguishable intense peak at 3.62 eV; probably corresponds to a Phosphorus-rich AlP(100) surface and in addition, we observe a continuous change in the RAS line shape with increasing temperature without phosphorus stabilization. Above 720°C we observe a second clear distinguishable RA-signal which may be corresponds to a Al-rich surface. [1] H. Kawanami, Solar Energy Materials & Solar Cells 66, 479 (2001) [2] H. Kroemer, J. Cryst. Growth, 81,193 (1987)

O 18.5 Mon 17:00 WIL C307

The structure of single-crystalline ZnO surfaces — •Jens Niederhausen[1,2], Antoni Franco-Cañellas[3], Simon Erker[4], Martin Oehzelt[2], Thorsten Schultz[1], Patrick Amsalem[1], Pardeep K. Thakur[5], Katharina Broch[6], David Duncan[5], Anton Zykov[1], Stefan Kowarik[1], Tien-Lin Lee[5], Alexander Gerlach[3], Oliver T. Hofmann[4], Frank Schreiber[3], and Norbert Koch[1,2] — [1]Institut für Physik, Humboldt-Universität, Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [3]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — [4]Institut für Festkörperphysik, TU Graz, Graz, Austria — [5]Diamond Light Source, Oxfordshire, UK — [6]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The electronic and catalytic properties of metal oxide surfaces are controlled by their atomistic details. For ZnO, ab-initio calculations predict rich phase diagrams, with the resulting structures varying significantly in terms of surface reconstruction, adsorbate species, and surface relaxation. A clear experimental identification of a predicted surface structure as well as the identification of thus far disregarded chemical species and structural effects arising from the surface preparation procedure are significantly assisted by the X-ray standing waves (XSW) technique that yields structural information with chemical sensitivity. We employed XSW to monitor how Ar^+ sputtering deteriorates the surface crystallinity and show that this effect can be largely reversed by annealing. By variation of temperature and H_2O partial pressure we determined surface structures for selected phase diagram points.

O 18.6 Mon 17:15 WIL C307

Atomic scale STM and nc-AFM study of the Hematite (012) surface — •Zdenek Jakub[1], Florian Kraushofer[1], Magdalena Bichler[2], Jan Hulva[1], Martin Setvin[1], Michael Schmid[1], Ulrike Diebold[1], Peter Blaha[2], and Gareth. S. Parkinson[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Institute of Materials Chemistry, TU Wien, Austria

For its abundance, low cost, stability and environmental benignity, hematite (α-Fe2O3) is a promising material for utilization in a wide range of fields, including as a photoanode for photoelectrochemical water splitting [1]. Although (012) is known to be one of the most stable surfaces of hematite, the atomic-scale structure remains unknown. Here we present the first-ever atomic-scale scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) study of the surface. Our data suggests that a bulk termination model for the oxidized (1x1) surface is plausible, but images of the reduced (2x1) surface are inconsistent with any of the previously proposed structural models. Based on the experimental data we propose a new model for the (2x1), whose plausibility is supported by our DFT calculations. We also present the results of H2O adsorption studies on the (2x1) surface and discuss the data in the context of previously published results [2].

[1] Parkinson, G.S., Surface Science Reports, 71, 272-365 (2016).

[2] Henderson, M.A. et al.. Surface Science, 417, 66-81 (1998).

O 19: 2D Materials Beyond Graphene II

Time: Monday 16:00–18:30 Location: REC/PHY C213

O 19.1 Mon 16:00 REC/PHY C213

2d Heterojunctions From Non-Local Manipulation of the Interactions: Single and Two-Particle Properties — •Christina Steinke[1,2], Daniel Mourad[1,2], Malte Rösner[1,2], Michael Lorke[1], Christopher Gies[1], Frank Jahnke[1], Gerd Czycholl[1], and Tim Oliver Wehling[1,2] — [1]ITP, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]BCCMS, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany

In modern optoelectronics heterojunctions are central building blocks of various applications, which commonly rely on interfaces of different materials. Here, we propose a novel scheme to induce heterojunctions within a single *homogeneous* layer of a two dimensional (2d) material based on Coulomb-interaction effects. Therefore we make use of the fact that in 2d semiconductors the Coulomb interaction can modify band gaps on an eV scale and can be drastically manipulated by external screening. This allows to spatially control the band gap by structured dielectric surroundings. We provide a proof of principle by combining a real-space tight-binding description with a many-body formalism for a model system emulating transitionmetal dichalcogenides. We find sizeable spatial band-gap modulations yielding type-II heterojunctions as needed for solar cells or quantum dots and present detailed insights into their excitation-induced two-particle properties. Utilizing the Bethe-Salpeter equation we show that Rydberg-like higher excitonic states can be strongly tuned by the dielectric surroundings. This effect may be used for efficient trapping of these excitonic states upon tailoring of the environment.

O 19.2 Mon 16:15 REC/PHY C213

Growth of Ge and Si on the monolayer silicene on Ag(111) — •Deng-Sung Lin and Han-De Chen — National Tsing Hua University, Hsinchu, Taiwan

Growth of Ge by molecular beam epitaxy on top of silicene monolayer on the Ag(111) surface results in either a dispersed adlayer or a two-dimensional ordered depending on the silicene phases. Scanning tunneling microscopy images show that the ordered adsorbed Ge atoms on the domains occupy directly on top of down-atoms in the buckled silicene layer.[1] By contrast, further growth Si on the silicene up to several MLs results in an atomic flat film with surface structure. We use low-temperature scanning tunneling microscopy to observe the chemical response of the film surface exposed to an atomic deuterium (D) beam. We find D displaces the Ag surfactant adatoms, resulting in a D-terminated (1x1) surface. The displaced Ag atoms migrate on the surface to form Ag(111) crystallites. The results confirm that the surfaces of the few-layer Si films grown on Ag(111) are Ag terminated and suggest that the films have a diamond-like structure [2].

[1]. Chen, H.-D.; Lin, D.-S., ACS Omega 2016, 1, 357-362. [2]. Chen, H.-D.; Chien, K.-H.; Lin, C.-Y.; Chiang, T.-C.; Lin, D.-S. J. Phys. Chem. C 2016, 120, 2698-2702.

O 19.3 Mon 16:30 REC/PHY C213

Direct observation of the conduction bands of single-layer WS$_2$ on Au(111) — •Philipp Eickholt[1], Marcel Holtmann[1], Charlotte Sanders[2], Philip Hofmann[2], and Markus Donath[1] — [1]Physics Institute, University of Münster, Germany — [2]Department of Physics and Astronomy, University of Aarhus, Denmark

In the field of 2D materials, single-layer transition metal dichalogenides, especially MoS$_2$, WS$_2$, MoSe$_2$ and WSe2$_2$, are among the promising materials due to their exceptional optical and electronic properties [1]. The key to understanding these properties is a profound knowledge of the electronic structure. While there have been many studies of the occupied electronic structure, the crucial information about the dispersion and spin structure of the conduction bands is still missing. Spin- and angle-resolved inverse photoemission (SRIPE) [2] is the ideal technique to study dispersion and spin structure of the unoccupied electronic structure. In this talk we present a SRIPE study of the conduction bands of single-layer WS$_2$ grown [3] on Au(111).

[1] D. Xiao *et al.*, Phys. Rev. Lett. **108**, 196802 (2012)

[2] S.D. Stolwijk *et al.*, Rev. Sci. Instrum. **85**, 013306 (2014)

[3] M. Dendzik *et al.*, Phys. Rev. B **92**, 245442 (2015)

O 19.4 Mon 16:45 REC/PHY C213

Study of the anisotropic electronic structure of ReSe$_2$ — •Ph. Eickholt[1], C. Langenkämper[1], K. Miyamoto[2], E.F. Schwier[2], J. Noky[3], M. Drüppel[3], P. Krüger[3], M. Rohlfing[3], and M. Donath[1] — [1]Physics Institute, University of Münster, Germany — [2]Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan — [3]Institute of Solid State Theory, University of Münster, Germany

Transition metal dichalcogenides (TMDCs) are heavily studied due to their fascinating optical and electronic properties and possible technical applications. ReSe$_2$ is a new material of the TMDC family. Unlike the well known MoS$_2$ it grows in a distorted 1T structure. Therefore it has unique anisotropic properties which can be useful in future applications [1]. To develop a fundamental understanding of the optical and electric properties we studied the occupied electronic structure of ReSe$_2$ with the help of angle-resolved photoemission (ARPES) and quasiparticle calculations.

[1] S. Yang *et al.* Nanoscale, **6**, 7226 (2014)

O 19.5 Mon 17:00 REC/PHY C213

Second-harmonic imaging microscopy: a powerful tool for time-resolved investigation of electron dynamics in TMDC heterostructures — •Jonas Zimmermann, Gerson Mette, and Ulrich Höfer — Philipps-Universität Marburg, Germany

Since the discovery of extraordinary luminescence of MoS2 monolayers, 2D transition metal dichalcogenides (TMDC) have been in the spotlight of the materials science community. In particular, heterostructures of different 2D materials attract attention due to their possible application in optoelectronics. As the efficiency of such devices is expected to depend strongly on the relative orientation of the individual layers, experimental techniques to characterize the electron transfer dynamics in dependence on the stacking angle are required.

Here, we present results of our new SHG imaging microscopy setup for time-resolved studies on interfaces of 2D materials. This technique allows us to quantify the crystal structure via polarization dependent measurements and gives us access to the electron dynamics via time-resolved pump-probe experiments. We demonstrate its capabilities with measurements performed on CVD grown WS2 and MoS2 monolayer flakes. The optical excitation tuned to 2.1 eV matches the energies of A- and B-exciton of WS2 and MoS2, respectively. Strong pump-induced features are observed and assigned to exciton generation. The excitonic lifetimes of the two materials correspond to values obtained in linear optical spectroscopy. The results reveal that SHG imaging microscopy is ideally suited to explore the effects of layer stacking on the charge transfer within 2D heterostructures.

O 19.6 Mon 17:15 REC/PHY C213

Electrostatically tuned 2D Heterostructures — •Christian Winkler, Shashank S. Harivyasi, and Egbert Zojer — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

The family of two-dimensional (2D) materials has been growing rapidly since the discovery of graphene. This creates new scientific challenges as well as opportunities because the properties of layered, van der Waals bonded systems are often different from their 3D counterparts, which offers entirely new strategies for band-structure engineering.

In this work, using first principles approaches, we propose a novel strategy for engineering the level alignment in van der Waals heterostructures. In particular, we focus on the inclusion of self-assembling polar molecules (e.g. Titanyl phthalocyanine) into stacks consisting of 2D transition metal dichalcogenides (TMDCs) sheets (MoX$_2$ and WX$_2$, where X = S or Se). For structures of the type TMDC/TiOPc/TMDC we observe a shift in the frontier levels of successive TMDC layers by as much as 0.4 eV. Remarkably, for WSe$_2$/TiOPc/MoS$_2$ this allows switching between type I and type II alignment. Using multiple TiOPc layers even quantum cascades can be realized.

Beyond that, we aim to explore the interplay between strain applied to the individual layers (which is known to induce direct to indirect gap transitions) and the electrostatic design approach.

O 19.7 Mon 17:30 REC/PHY C213

Structure determination of silicene nanoribbons on Ag(110) — •Philipp Espeter[1,2], Christoph Keutner[1,2], Nils Fabian Kleimeier[3], Peter Roese[1,2], Karim Shamout[1,2], Gabi Wenzel[3], Ulf Berges[1,2], Helmut Zacharias[3], and Carsten Westphal[1,2] — [1]Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4, D-44227 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227 Dortmund — [3]Physikalisches Institut - WWU Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster

Since the discovery of graphene much interest came up in graphene analoga from the carbon group. One of the most famous representatives is silicene. Silicene is known to crystallize in different configurations depending on the substrate, such as sheet growth on Ag(111) and nanoribbons on Ag(110). Whereas the structure of silicene sheets is already well known, the structure of silicene nanoribbons remains unclear.

In this study, we demonstrate a structure investigation of silicene nanoribbons on a Ag(110) substrate by means of photoelectron spectroscopy (XPS) and diffraction (XPD). These measurements provide chemical as well as structural information of silicene nanoribbons.

We assess several structure models suggested in literature, ranging from rectangular over pentagonal to hexagonal and from planar over buckled to stacked structures. We will also present a structure model which perfectly fits to the XPD and XPS data.

O 19.8 Mon 17:45 REC/PHY C213

Angle-resolved IPE Study of Silicene Nanoribbons on Ag(110) — •Gabi Wenzel, Nils Fabian Kleimeier, and Helmut Zacharias — Physikalisches Institut - WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Silicene, a two-dimensional buckled honeycomb lattice of silicon atoms, has attracted great interest in the scientific community. To investigate its electronic properties, unoccupied electronic states of silicene nanoribbons grown on Ag(110) were measured by $\vec{k}$-resolved inverse photoemission spectroscopy (KRIPES) in ultra-high vacuum conditions. The IPE setup consisted of a modified Erdmann-Zipf electron gun and an acetone filled Geiger-Müller tube with a CaF$_2$ window acting as a bandpass filter.

The measurements in $\overline{\Gamma \mathrm{X}}$ direction show two main features: one almost linearly dispersing state from 3.2 eV at $\overline{\Gamma}$ to 6.2 eV at $\overline{\mathrm{X}}$, the other depicting a linear continuation of the Dirac cone like feature around the $\overline{\mathrm{X}}$ point from 0 eV to 5.8 eV.

O 19.9 Mon 18:00 REC/PHY C213

SPM study of atomically thin MoS$_2$ grown on HOPG via chemical vapor deposition — •Erik Pollmann and Marika Schleberger — Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

Van der Waals heterostructures are material systems based on combinations of different 2D materials such as graphene, hBN and MoS$_2$ to mix their properties or even create new ones. Monolayers of MoS$_2$ on HOPG could be used as a model system for the MoS$_2$-graphene interface and has been studied e.g. by Koós et al. [1].

The aim of our work is to understand the growth mechanism of MoS_2 on this graphene-like surface in order to exploit this knowledge to grow MoS_2 directly on graphene itself. Therefor MoS_2 flakes are grown by chemical vapor deposition and investigated by different Scanning Probe Microscopy techniques. It will be shown, that MoS_2 is more likely to grow at HOPG edges. These one-dimensional defects act as the growth seeds. This would constitute a serious disadvantage for the direct growth on graphene where no step edges are present. Therefore, we investigated if point defects can act as growth seeds as well. To this end, an HOPG crystal was irradiated by highly charged ions to induce quasi zero-dimensional defects [2] before the chemical vapor deposition of MoS_2. The first results obtained from these experiments will be presented.

[1] A. A. Koós et al. *Carbon* **105**, 408-415 (2016)
[2] J. Hopster et al. *2D Materials* **1**, 1011011 (2014)

O 19.10 Mon 18:15 REC/PHY C213

Probing the Bandstructure of MoS_2 on Au(111) using Scanning Tunneling Spectroscopy — •Nils Krane, Christian Lotze, and Katharina J. Franke — Freie Universtät Berlin, Berlin, Germany

Transition metal dichalcogenides (TMCD) are two-dimensional materials with a natural band gap, making them interesting as sensors, solar cells or LEDs. Single layer molybdenum disulfide is especially interesting, since it provides a direct band gap [1] and a strong spin-splitting of the valence band at the K-point.

Here we grow MoS_2 epitaxially on a Au(111) surface as described in [2] and investigate it with a combined STM/AFM at low temperatures. Since STS measures the projected LDOS without information of the parallel momentum $k_\parallel$ in the Brillouin-Zone, it is not possible to assign a band gap to the K- or Γ-point. To get an insight into the band structure of MoS_2, we measure the decay length κ of the tunneling current, which depends on $k_\parallel$ [3]. We find a strong spatial dependence of κ. We ascribe this to the Moiré reconstruction of MoS_2 on Au(111), which differs between fcp- and hcp-stacking at the hollow sides. Furthermore, we investigate the band structure of quasi freestanding MoS_2.

[1] Mak, *et al.*, PRL 105, 136805 (2010)
[2] Sorensen, *et al.*, ACS Nano 8, 6788-6796 (2014)
[3] Zhang, *et al.*, ACS Nano 15, 6494-6500 (2015)

O 20: Solid-Liquid Interfaces: Reactions and Electrochemistry - Experiment I

Time: Monday 16:30–18:15 Location: WIL B321

O 20.1 Mon 16:30 WIL B321

Novel Quantitative Approach for Characterizing the Buried Metal/Coating Interfacial Kinetics Using Hydrogen Permeation Based Potentiometry — •Dandapani Vijayshankar and Michael Rohwerder — Max-Planck -Institut fur Eisenforschung GmbH

Electrochemical integrity of the buried metal/organic coating interface is crucially governed by the extent to which the cathodic oxygen reduction reaction (ORR) is curtailed. Current electrochemical techniques are unable to quantitatively probe such hidden interfaces due to the restricted ionic transport through the organic coating. Recently, a new non-destructive approach based on using hydrogen permeation as a tool to measure this ORR rate has been introduced. By correlating the dynamic equilibrium potential established between the the oxygen reduction and hydrogen oxidation reactions on the coated exit side with the hydrogen uptake rate on the entry side, a full current-potential curve I(U). Good concurrence between the I(U) curves derived from this permeation based potentiometry approach to that from standard three-electrode setup for the uncoated palladium, proved the correct measurement of the ORR rate. Underneath coatings, owing to interfacial charge transfer processes free of ion mobility, true ORR rate could be measured. Further, interfacial reaction kinetic mechanisms of the electrochemical ORR investigated by prolonged cathodic polarization experiments were found to destroy the interface similar to cathodic delamination process.

O 20.2 Mon 16:45 WIL B321

Photoelectrochemical CO2 reduction at nanostructured gold/copper structures on Si — •Simon Filser[1], Thomas L. Maier[1], Robin Nagel[2], Tianyue Zhang[3], Werner Schindler[1], Josef Zimmermann[1], Qi Li[1], Paolo Lugli[2], and Katharina Krischer[1] — [1]Non-equilibrium chemical physics, TU Munich, Germany — [2]Chair for Nanoelectronics, TU Munich, Germany — [3]Photonics and Optoelectronics Group, LMU Munich, Germany

Due to its unique properties copper is the most promising electrode material for the electrochemical reduction of CO2 to CO, ethylene and methane; their distribution sensitively depends on the electrode surface and the reaction conditions [1].

Our aim is to integrate copper nanostructures into a photoelectrode to directly transform solar energy into chemical fuels. We approach such a system by structuring a silicon substrate with chessboard arrays of gold nanodisks which are electrochemically plated by copper.

In our work we examine how doping, illumination, structure size and copper coverage influence the electrochemical behavior and the product distribution.

Additionally, we show that our structures feature surface plasmon polaritions (SPPs) which are predicted to enhance the electric field close to the metal surface [2], strengthening the adsorption of reactants and to polarizing adsorbates leading to lower overpotentials and a higher selectivity.

[1] Y. Hori, et al., Chem. Lett., 1695-1698 (1985). [2] S. Sun et al., Cat. Comm. 11, 4, 290-293, (2009).

O 20.3 Mon 17:00 WIL B321

Electro-oxidation of CO on model electrodes – Atomic scale level nanostructures and their impact on the catalyst performance — •Jens Klein, Sylvain Brimaud, Valeria Chesnyak und R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

The performance of electrocatalytic reactions, such as the CO oxidation, on monometallic and bimetallic Pt-based electrodes is highly sensitive towards the surface structure and surface composition of the catalyst on the atomic scale level.[1] On Pt an increased activity for the CO oxidation was observed if the amount of monoatomic high Pt step edges increases, while on PtRu electrodes the appearance of adjacent Ru and Pt atoms in the surface were found to enhance the CO oxidation due to a bifunctional mechanism.[1] For a more detailed understanding of the structure-activity relationship on the atomic scale level we studied the CO oxidation on single crystal model electrodes with well-defined nanostructured surfaces. Employing a combined ultrahigh vacuum (UHV) – electrochemical flow cell setup we prepared and structurally characterized by scanning tunneling microscopy (STM) under UHV conditions Pt(111) and Ru(0001), which were structurally modified on the atomic scale, e.g., by varying the Pt step edge density or the number of adjacent PtRu-sites followed by electrochemical characterization. The nature and abundance of specific structure elements was correlated with the CO oxidation activity to obtain information on the nature of different active sites and their relative activity.

[1] N.M. Marković *et al.*, *Surf. Sci. Rep.* **45** (2002) 117.

O 20.4 Mon 17:15 WIL B321

Investigation of the Electrode-Electrolyte Interface in Lithium Ion Batteries Studied by Surface Science Methods — •Thomas Späth, Dirk Becker, Wolfram Jaegermann, and René Hausbrand — Institute of Material Science, Darmstadt University of Technology, Jovanka-Bontschits-Str. 2, 64287 Darmstadt

Reactions and Solid-Electrolyte Interface (SEI) formation between electrodes and electrolytes play a key role for performance and lifetime of batteries. For a better understanding of the reactivity of solvents with Li-ion battery electrode materials, we perform adsorption experiments on model electrodes. In these experiments we use High Resolution Electron Energy Loss Spectroscopy (HREELS) and Photoemission Spectroscopy (PES) to study vibrational modes and chemical composition at the surface. As both techniques offer complementary information, HREELS data can support the PES measurements.

In this contribution we present the results of our investigations of the electrode-electrolyte interface performing a stepwise adsorption of diethyl carbonate and dimetyl carbonate both on sputtered thin films of $LiCoO_2$ and lithiated silicon surfaces. We discuss the assignment of the different features in the pristine sprectra and present HREELS and PES spectra of the electrolyte adsorbed samples. For both techniques several new features can be observed, which are assigned to physically adsorbed species as well as chemisorbed or chemically reacted species. From this data we are able to conclude on the chemical reactions at the interfaces. This information allows us to obtain a deeper understanding of the SEI formation mechanisms in Lithium Ion Batteries.

O 20.5 Mon 17:30 WIL B321

Li-Ion Battery Anodes: Electrochemical Model Studies at the Electrode|Electrolyte Interphase — •Isabella Weber[1], Johannes Schnaidt[2], Carina Bodirsky[1], Thomas Diemant[1], 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-89081 Ulm, Germany

State-of-the-art Lithium-ion batteries (LIBs) consist of Li-intercalating electrode structures and blends of organic solvents mixed with Li-salts. During the charge/discharge process, a protective film forms at the electrode|electrolyte interface which is referred to as the solid-electrolyte interphase (SEI). Due to the complex composition of the electrodes (active material, binder, etc.) and the electrolyte, however, the processes leading to SEI formation are still a matter of discussion. For a more detailed understanding, we systematically studied model systems by varying the anode material (different graphite powders with or without binder) and electrolyte solvents (ethylene carbonate with $LiPF_6$). Cyclic voltammetry was applied to characterize the electrolyte decomposition. Post-mortem XPS allowed the elemental analysis of the reduction products, as well as a depth-profiling of the SEI formed at different scan rates. In-situ infrared spectroscopy, finally, provided additional information on the adsorbed intermediates accumulated during SEI formation. The influence of the different LIB components on the formation, composition and product distribution of the SEI and the implications of our model studies on the understanding of the SEI formation in LIBs will be discussed.

O 20.6 Mon 17:45 WIL B321

Model Studies on the Electrochemical Decomposition of BMP TFSI on Gold and Glassy Carbon Electrodes — •Dorothea Alwast[1], Johannes Schnaidt[2], Kurtus Hancock[1], 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-89081 Ulm, Germany

Ionic liquids (ILs) have shown promise as possible electrolytes for batteries. Therefore, the electrochemical stability of these ILs plays a key role for the use in batteries. In order to better understand the catalytic effect of different electrode materials on the electrochemical decomposition of ILs, we investigated the formation of volatile products of 1-butyl-1-methylpyrrolidinium bis(trifluoromethanesulfonyl)imide (BMP TFSI) formed during linear potential sweeps on polycrystalline Au and GC electrodes. For the online analysis of the volatile decomposition products we used a differential electrochemical mass spectrometry (DEMS) setup specifically designed for studying ILs. On both gold and glassy carbon electrodes decomposition products of the TFSI anion (m/z = 69, CF_3^+; m/z = 64, SO_2^+) are mainly detected at positive potentials, while decomposition products of both ions are formed at negative potentials. The similarities and differences in the products' distribution on the two electrode materials and the implications of these findings on the mechanism of the IL's electrochemical decomposition will be discussed.

O 20.7 Mon 18:00 WIL B321

Live, in situ STM observation of the oxidative roughening of Pt(111) — •Leon Jacobse[1], Yi-Fan Huang[1], Marcel J. Rost[2], and Marc T.M. Koper[1] — [1]Leiden Institute of Chemistry, Leiden University, Leiden, The Netherlands — [2]Huygens-Kamerlingh Onnes Laboratory, Leiden University, Leiden, The Netherlands

Platinum nanoparticles are used in a wide variety of catalytic processes. In many of these applications, e.g. the anodes of fuel cells, the platinum surface is (partly) oxidized. It is known that by oxidizing and reducing platinum electrochemically, its surface structure is altered, which plays a role in the degradation of the catalyst. However, even for well-defined single crystal surfaces, over thirty years of research did not yet yield a conclusive description of this process on the atomic level.

Using our high-speed, electrochemical scanning tunneling microscope (EC-STM) we continuously oxidized and reduced the surface while simultaneously imaging the surface on the atomic level during the full potential sweep. This provides us with unique information, from which we directly can correlate the changes in surface structure to the changes in the cyclic voltammetry. The formation of nanoscale islands, upon oxidizing and reducing the surface, goes hand in hand with an increase in the current related to hydrogen desorption from step edges. Surprisingly, the development of these islands seems to continue on much longer timescales than suggested in literature, where the evolution of the surface structure was studied in great detail by cyclic voltammetry.[1]

[1] e.g. Electrochim. Acta 2012, 82 (0), 558-569.

O 21: Plasmonics and Nanooptics III: Light-Matter Interaction

Time: Monday 17:00–18:30 Location: TRE Ma

O 21.1 Mon 17:00 TRE Ma

Momentum distribution of hot electrons in resonantly excited gold nanorods revealed by time of flight k-resolving photoemission spectromicroscopy — •Martin Lehr[1], Benjamin Foerster[2,3], Katja Krüger[2], Mathias Schmitt[2], Carsten Sönnichsen[2], Gerd Schönhense[1], and Hans Joachim Elmers[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, D-55128 Mainz, Germany — [2]Institut für physikalische Chemie, Johannes Gutenberg-Universität, Duesbergweg 10-14, D-55128 Mainz, Germany — [3]Graduate School for Excellence Materials Science in Mainz, Johannes Gutenberg University Mainz, Staudingerweg 9, D-55128 Mainz, Germany

We investigate plasmon assisted photoemission from individual Au nanorods using a time-of-flight momentum resolving photoemission electron microscope (ToF k-PEEM). The Au nanorods are taylored to obtain a localized plasmon polartion resonance wavelength of 800 nm with a linewidth of just 44 nm. The Au nanorods adhere to a transparent In-Sn oxide substrate enabling illumination from the rear side at normal incidence. The two momentum components parallel to the surface and the kinetic energy of the electrons are measured simultaneously. Both properties depend on laser power and polarization confirming a plasmon assisted emission process mediated by the optical field enhancement at the nanorod's ends. The exponential intensity decrease of emitted electrons with increasing kinetic energy reveals the distribution of hot electrons leading to an additional emission process with a characteristic homogeneous momentum distribution.

O 21.2 Mon 17:15 TRE Ma

Plasmon polaritons in cubic lattices of interacting metallic nanoparticles — •Simon Lamowski[1], Felicitas Hellbach[1], Eros Mariani[2], Guillaume Weick[3], and Fabian Pauly[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Centre for Graphene Science, Department of Physics and Astronomy, University of Exeter, Stocker Rd. EX4 4QL Exeter, UK — [3]Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg, CNRS UMR 7504, F-67034 Strasbourg, France

We investigate theoretically plasmon polaritons in cubic lattices of interacting spherical metallic nanoparticles [1]. Dipolar localized surface plasmons on each nanoparticle couple through the near field dipole-dipole interaction and form collective plasmons, which extend over the whole metamaterial. Coupling these collective plasmons in turn to photons leads to plasmon polaritons. We derive within a quantum model general semi-analytical expressions to evaluate both plasmon and plasmon-polariton dispersions that fully account for nonlocal effects in the dielectric function of the metamaterial. Within this model, we discuss the influence of different lattice symmetries and predict related polaritonic gaps within the near-infrared to the visible range of the spectrum that depend on wavevector direction and polarization.

[1] S. Lamowski, F. Hellbach, E. Mariani, G. Weick, and F. Pauly,

arXiv:1606.04897.

O 21.3 Mon 17:30 TRE Ma

Relaxation of single and collective electron excitations investigated with time- and energy-resolved PEEM — •Michael Hartelt[1], Anna-Katharina Mahro[1], Tobias Eul[1], Benjamin Frisch[1], Philip Thielen[1], Deirdre Kilbane[1,2], Mirko Cinchetti[1,3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]School of Physics, University College Dublin, Ireland — [3]Experimentelle Physik VI, Fakultät Physik, TU Dortmund, Germany

The generation of hot carriers through the internal decay of plasmons in metallic materials has received considerable attention lately, due to its wide range of potential applications [1]. Understanding the differences between photoinduced and plasmon-induced hot electrons is essential for the construction of devices for plasmonic energy conversion. To distinguish between the two processes, it is advantageous to make use of the time-resolved 2-photon-photoemission (TR-2PPE) method that is an established tool for the study of hot electron lifetimes [2] in combination with Photoemission Electron Microscopy (PEEM). This allows us to study hot electron dynamics on the femtosecond and nanometer scale by analyzing the energy distribution and relaxation dynamics of the photoemitted electrons. Here, we present first results of time and energy resolved PEEM (TR-ER-PEEM) measurements of localized and propagating plasmons (LSP and SPP) with focus on the relation between spectral features and local near-field distributions.

[1] Brongersma et al., Nature nanotechnology 10.1 (2015)

[2] M. Bauer et al., Progress in Surface Science 90, 319 (2015)

O 21.4 Mon 17:45 TRE Ma

Parallel mapping of optical near-field interactions by molecular motor-driven quantum dots — Friedrich W. Schwarz[1], Hannah S. Heil[1], Heiko Gross[2], •Jens Ehrig[1], Bert Hecht[2], and Stefan Diez[1] — [1]B CUBE & cfaed, Technische Universität Dresden — [2]Nano-Optics and Biophotonics Group, Universität Würzburg

Absorption and emission rates of photons by quantum emitters strongly depend on the emitters' local environment. This enables the precise control of light–matter interactions, essential for the development of future opto-electronics devices. The design, characterization and optimization of such devices requires high-resolution, yet high-speed and non-invasive tools that allow the nm-precise mapping of the involved optical near-field interactions. Toward this end, we investigate the near-field interaction of optical dipole emitters with nanostructures by recording the fluorescence intensity of quantum dots attached to microtubules being transported across the nanostructure by molecular motors. The power of this parallel approach to near-field imaging is demonstrated by the nm-precise mapping of near-field interactions between individual quantum dots and nanoslits of 110 to 240 nm widths engraved in 25 nm gold layers. The results of these measurements are in excellent agreement with finite-difference time-domain simulations. Thus, by using a minimalistic biomolecular machinery, we are able to perform parallel superresolution mapping of near-field interactions in a virtually artifact-free fashion. We foresee broad applications, such as large-scale multi-probe imaging of meta-surfaces to further the understanding of light-matter interactions.

O 21.5 Mon 18:00 TRE Ma

Adaptive spatial resolution in the finite-difference modal method for the derivation of electromagnetic fields — •Izzatjon Allayarov, Martin Schäferling, Maxim Nesterov, and Thomas Weiss — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Optical devices based on nanostructures have many applications in different fields. For example, it has been shown that photonic crystal slabs can be used to control the polarization state emitted by quantum emitters [1]. One very efficient numerical method to model the optical properties of photonic crystal slabs and periodic arrays of nanoantennas is the Fourier modal method. However, due to the underlying Fourier basis, the Fourier modal method suffers from the Gibbs phenomenon, which results in spurious oscillations of the electromagnetic near fields around interfaces between different materials.

As an alternative to the Fourier basis, we have implemented a finite-difference basis for modal methods based on the approach in [2] and combined it with the coordinate transformation methods that are well-established in the standard Fourier modal method [3]. Thus, we have achieved significantly better convergence of the electromagnetic near fields as compared to the standard Fourier modal method as well as the finite difference modal method without coordinate transformations.

[1] S. V. Lobanov et al., Opt. Letters **40**, 1528 (2015).

[2] I. Semenikhin and M. Zanuccoli, JOSA A **30**, 2531 (2013).

[3] T. Weiss et al., Opt. Express **17**, 8051 (2009).

O 21.6 Mon 18:15 TRE Ma

Strong Coupling of Single Excitons to Curved Optical Nanostructures — •Daniel Hernangómez-Pérez[1,2], Rui-Qi Li[2,3], Francisco José García-Vidal[2,4], and Antonio I. Fernández-Domínguez[2] — [1]Institute of Theoretical Physics, University of Regensburg, D-93050 Regensburg, Germany — [2]Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Key Laboratory of Modern Acoustics, MOE, Institute of Acoustics, Department of Physics, Nanjing University, Nanjing 210093, People's Republic of China — [4]Donostia International Physics Center (DIPC), E-20018 Donostia/San Sebastián, Spain

We systematically analyze plasmon-exciton coupling for a quantum dot situated in-between two nanoparticles. To that purpose, we employ a systematic quasi-analytical approach inspired by transformation optics, which allows us to study the impact of geometry and material configurations in the quantum dynamics. We show that the coupling to multipolar dark modes close to the plasmon resonances allows to enter into a regime wheret the dynamics can be reversible and compare our findings to recent experiments. The findings presented here may serve as a guidance to additional future experiments and for the development of new quantum plasmonic devices. References: PRL 117, 107401 (2016), Nature 535, 127 (2016)

O 22: Organic-Inorganic Hybrid Systems and Organic Films III

Time: Monday 17:00–18:30 Location: WIL A317

O 22.1 Mon 17:00 WIL A317

Focused Electron Beam Induced Processing on Surface-Anchored Metal-Organic Frameworks — •Martin Drost[1], Luisa Berger[1], Fan Tu[1], Christian Preischl[1], Hartmut Gliemann[2], Christof Wöll[2], and Hubertus Marbach[1] — [1]Physik. Chemie II, FAU Erlangen-Nürnberg, GER — [2]Institut f. funktionelle Grenzflächen, KIT, GER

We demonstrate the feasibility of Focused Electron Beam Induced Processing (FEBIP) techniques on Surface-Anchored Metal-Organic frameworks (SURMOFs)1 to lithographically fabricate nanostructures. These are: Electron Beam Induced Deposition (EBID)2, in which adsorbed precursor molecules are locally dissociated by the impact of the electron beam, leaving a deposit on the surface, and Electron Beam Induced Surface Activation (EBISA)3, where the substrate is locally activated by the e-beam in the absence of a precursor, such that a subsequently dosed precursor is catalytically decomposed at these sites and forms a deposit. Both approaches were conducted with Fe(CO)5 and Co(CO)3NO on HKUST-1 and a porphyrin-based SURMOF. We show that Fe(CO)5 is suitable for EBID and EBISA on both SURMOFs, whereas Co(CO)3NO works solely for EBID but is not susceptible to EBISA. We also demonstrate the possibility to fabricate nanostructures with linewidths <10 nm. All deposits were characterized with Scanning Electron Microscopy (SEM) and local Auger Electron Spectroscopy (AES). Supported by the DFG through grant MA 4246/1-2, research unit FOR 1878/funCOS; COST Action CM1301; Excellence Cluster EAM of the FAU Erlangen-Nürnberg.

O 22.2 Mon 17:15 WIL A317

Electronic structure of magnesiumtetraphenylporphyrin on MgO — •Rebecca Pöschel, Gianluca di Filippo, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen

Ultrathin films of magnesium oxide (MgO) covered with magnesium tetraphenylporphyrin (MgTPP) were grown in-situ on a Ag(100) single crystal. The layer thickness of MgTPP was varied as well as the layer thickness of MgO underneath. The influence of the substrate and of the MgTPP layer thickness on the occupied and unoccupied molecular orbitals were investigated using photoelectron spectroscopy. With vacuum ultra-violet photoelectron spectroscopy (photon energy 21.2 eV) the occupied orbitals were studied and for the unoccupied orbitals two-photon photoelectron spectroscopy was used (photon energies of 3.06 eV - 3.16 eV and 4.59 eV - 4.76 eV). We found a HOMO-LUMO gap of around 4 eV similar to previous measurements on Ag(100).

O 22.3 Mon 17:30 WIL A317

Optimization and experimental investigation of hybrid organic-inorganic (plasmon-) nanolaser designs — •Martin Rothe, Günter Kewes, and Oliver Benson — Humboldt-Universität zu Berlin, Department of Physics, Nanooptics Group, Newtonstraße 15, 12489 Berlin, Germany

The understanding of coherent scattering, amplification and lasing in nanoscopic structures is essential for future optical and optoelectronical devices. Due to their nonlinear threshold behaviour, lasing systems could be used as active building blocks or fast modulators in such devices. However this requires a deeper understanding of the interplay between gain medium and resonators. We focus on hybrid nanolaser designs consisting of inorganic resonators and organic gain medium.

In order to optimize those structures we study various nanoresonator geometries and materials. Therefore we investigate both, plasmonic nanowires (to build a spaser) and dielectric resonators (to build a nanolaser). The nanostructures are analyzed in our optical setup, allowing for spatial, spectral and temporal analysis of single systems as well as ensembles, various illumination/excitation geometries, including dark field imaging as well as confocal scanning. In parallel we use numerical simulations to validate our experimental findings and to optimize the designs.

O 22.4 Mon 17:45 WIL A317

Molecular Topology and Surface Chemical Bond: Alternant vs. Non-Alternant Aromatic Molecules — •Benedikt P. Klein[1], Nadine van der Heijden[2], Claudio K. Krug[1], Maik Schöniger[1], Phil Rosenow[1], Martin Schmid[1], Ralf Tonner[1], Ingmar Swart[2], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Debye Institute for Nanomaterial Science, Utrecht University, The Netherlands

The interaction of conjugated organic molecules, in particular aromatic species, with metal surfaces has been a major topic in surface science. So far, the focus has almost exclusively been on molecules with alternant topologies such as pentacene. These molecules have a uniform charge distribution and highly delocalized frontier orbitals. In contrast, non-alternant topologies cause non-uniform charge distributions, and more localized frontier orbitals. We present the first systematic studies of naphthalene and its non-alternant counterpart azulene on the (111) surfaces of Cu and Ag. On the basis of extensive PES, NEXAFS, TPD, nc-AFM and STM studies, we show that the non-alternant topology results in much stronger interaction with metal surfaces, especially in the case of Cu(111), and that the interaction is more localized. Periodic DFT calculations provide insight into the surface chemical bond and charge redistribution between surface and molecule. A major part of the localized interaction is the donation of electron density in the molecular LUMO. This leads to a considerable in-plane and out-of-plane deformation of the adsorbed non-alternant species.

O 22.5 Mon 18:00 WIL A317

Global Structure Search for Organic/Inorganic Interfaces: TCNE on Au(111) — •Veronika Obersteiner, Michael Scherbela, Lukas Hörmann, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

Structure determination at organic/inorganic interfaces is highly challenging. As individual experiments often convey partial or ambiguous information, computational simulations become increasingly important to aid the interpretation. Here, we demonstrate the power of theoretical polymorph prediction on the example of TCNE (tetracyanoethene) on Au(111).

Predicting polymorphs from first principles is far from trivial. The main challenge is the vast configurational space, i.e. the number of different polymorphs raising exponentially with the number of molecules in the unit cell. Here, we present an approach based on a discretization of the potential energy surface (PES), where we first determine the local adsorption geometries and afterwards span the PES as combinations of these. Dispersion corrected density functional theory is then applied for optimization and to obtain their relative energies.

Applying this approach to TCNE/Au(111), we predict the global minimum to be an ordered triangular structure of slightly tilted upright standing molecules with a substrate adatom in the center. The existence of the adatom cannot be inferred from experimental STM alone [1], but we find it crucial to be able to reproduce the experiment. [1] D. Wegner et al. Nano Letters, 8, 131-135, 2008.

O 22.6 Mon 18:15 WIL A317

How a functionalization with cyano groups modifies the adsorption behavior and reactivity of 2H-tetraphenylporphyrin on Cu(111) — Michael Lepper[1], Manuel Meusel[1], Julia Köbl[1], Liang Zhang[1], Michael Stark[1], Abner De Siervo[2], Hans-Peter Steinrück[1], and •Hubertus Marbach[1] — [1]Lehrstuhl für Physikalische Chemie II , Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 — [2]Institute of Physics, Gleb Wataghin, University of Campinas (UNICAMP), Campinas, SP, Brazil

We studied the adsorption behavior of 2H-tetraphenylporphyrin (2HTPP) with 1, 2 and 4 cyano-functionalized phenyl groups on Cu(111) by means of room temperature scanning tunneling microscopy (STM) in ultra-high vacuum. While 2HTPP adsorbs as individual isolated molecule [1], the cyano-functionalized porphyrins form dimers or 1-D molecular chains after mild annealing, depending on the number and geometry of the attached cyano groups. Thereby, the main binding motives are Cu adatoms, which appear to act as linkers between cyano groups of neighboring molecules. In addition, we observe self-metalation [2,3], that is, the metalation of the porphyrin macrocycle with Cu atoms from the substrate. Interestingly, the yield of this reaction is strongly affected by the actual cyano-functionalization, which goes along with the differences in the adsorption behavior of the porphyrin derivatives.

[1] F. Buchner et al., J. Phys. Chem. C, 115 (2011) 24172 [2] K. Diller et al., J. Chem. Phys., 136 (2012) 014705 [3] H. Marbach, Acc. Chem. Res., 48 (2015) 2649

O 23: SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - sulphate- and phosphate-based electrolytes

Time: Monday 17:15–18:00 Location: IFW A

O 23.1 Mon 17:15 IFW A

Aliovalent substitution in garnet type solid-state electrolytes for solid-state lithium-ion batteries — •Anja Paulus[1], Maike Wirtz[1], Sabrina Heuer[1], Peter Jakes[1], Hans Kungl[1], and Rüdiger Albert Eichel[1,2] — [1]Fundamental Electrochemistry (IEK-9), Institute of Energy and Climate Research, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — [2]Institut für Physikalische Chemie (IPC), RWTH Aachen University, D-52074 Aachen, Germany

Conventional lithium-ion batteries consist of an electrolyte containing toxic, flammable organic liquids which lead to several safety issues such as leakage and burning of the battery. In order to overcome these safety issues solid-state electrolytes could be an alternative to obtain powerful lithium-ion batteries. The garnet type electrolyte Li7La3Zr2O12 shows promising properties in terms of high lithium-ion conductivity and a good stability against lithium. There are two modifications known for this material, on the one hand a tetragonal one which is thermodynamically stable at room temperature and on the other hand a cubic high temperature modification. The cubic structure shows a lithium conductivity of two orders of magnitude higher than the conductivity of the tetragonal one. One possibility to stabilize the cubic structure at room temperature or lower temperatures is by aliovalent substitution. Aluminum substitution on the lithium site shows a lithium conductivity of 3.41*10-4 S*cm-1 for Li6.4Al0.2La3Zr2O12 at room temperature [1]. Our focus is to study the influence of aliovalent substitution on the properties of garnet type solid-state electrolytes by various techniques. 1.C.Tsai et al., J. Electroceram., 2015, 35, 25-32.

O 23.2 Mon 17:30 IFW A

Defect chemistry of solid electrolyte $Li_4P_2S_6$ by first-principles calculations — •Marcel Sadowski, Sabrina Sicolo, and Karsten Albe — Institute of Materials Science, Technische Universität Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt, Germany

Glassy, glass-ceramic and crystalline lithium thiophosphates have attracted interest as solid electrolytes for all-solid-state batteries. Despite similar structural motifs, these materials exhibit a wide range of compositions, structures and ionic conductivities. For the glass-ceramic consisting of crystalline $Li_4P_2S_6$ and glassy $Li_4P_2S_7$, for example, contradictory ionic conductivities were reported. In this contribution we present density functional theory (DFT) calculations on the defect thermodynamics and kinetics of crystalline $Li_4P_2S_6$. [1] Despite the existence of low energy diffusion paths, the overall conductivity is inhibited by high defect formation energies. This supports the hypothesis that the conductivity of the $Li_4P_2S_7$/$Li_4P_2S_6$ composite material is determined by the relative amount of glassy and crystalline phases.

Furthermore, thermodynamics predict the instability of $Li_4P_2S_6$ against metallic lithium. Corresponding interface models for different surface terminations of $Li_4P_2S_6$ show the barrierless formation of an interphase reminiscent of Li_2S, which might act as a passivating layer and protect the electrolyte from further decomposition.

[1] C. Dietrich, M. Sadowski, S. Sicolo, D. A. Weber, S. J. Sedlmaier, K. S. Weldert, S. Indris, K. Albe, J. Janek, W. G. Zeier, Chem. Mater. DOI:*10.1021/acs.chemmater.6b04175 (2016).

O 23.3 Mon 17:45 IFW A

Systematic Search for Lithium Ion Conducting Compounds by Screening of Compositions Combined with Atomistic Simulation — •Daniel Mutter[1,2], Daniel Urban[2], and Christian Elsässer[1,2] — [1]Freiburger Materialforschungszentrum (FMF), Albert-Ludwigs-Universität Freiburg, Stefan-Meier-Straße 21, 79104 Freiburg — [2]Fraunhofer Institut für Werkstoffmechanik (IWM), Wöhlerstraße 11, 79108 Freiburg

Solid state electrolytes (SSEs) with high Li conductivity can significantly improve Li ion accumulators in terms of electrochemical efficiency, thermal and mechanical stability, and environmental compatibility, leading to an enhanced range of applications for these high energy density batteries. Compounds crystallizing in the structure of $NaZr_2(PO_4)_3$ (NZP) are regarded as promising SSEs, mainly because of their three-dimensional diffusion network enabling fast transport of Li ions through well defined channels. Starting from $LiTi_2(PO_4)_3$, we analyzed a large variety of NZP compounds by systematically screening the relevant parts of the periodic table, replacing atoms on the Ti and P sublattices by isovalent elements. The influence of these elemental substitutions on structural stability, preferred Li sites, ionic mobility, migration paths and diffusion mechanisms were analyzed by means of a combined approach of multiple computational methods with different levels of accuracy, ranging from static energy landscape and molecular dynamics simulations with ionic bond valence potentials to density functional theory calculations combined with the nudged elastic band method.

O 24: Semiconductor Substrates: Adsorption

Time: Monday 17:30–18:30 Location: WIL C307

O 24.1 Mon 17:30 WIL C307

Conductivity of a two-dimensional hole gas on diamond — •Dennis Oing, Nicolas Wöhrl, Martin Geller, and Axel Lorke — Universität Duisburg-Essen

Diamond is a material with promising properties like robustness, high thermal conductivity and high electric breakdown field. Because of the large band gap of 5.45 eV, diamond shows a low intrinsic charge carrier density at room temperature. However, a two-dimensional hole gas can be established on the surface by hydrogen termination and accumulation of an adsorbate layer.

We have produced a two-dimensional hole gas (2DHG) on chemical vapor deposition (CVD)-grown diamond through a hydrogen plasma treatment with varying parameters. This 2DHG is characterized using current-voltage (I-V) measurements and temperature-dependent Hall experiments. The Hall measurements reveal a p-type conductivity with a charge carrier density of $2 \cdot 10^{13}\,\mathrm{cm}^{-2}$ and a mobility of $60\,\mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$ at room temperature. The temperature is varied in the range from 4.2 K up to 325 K, and we find a maximum of the mobility of $84\,\mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$ at 230 K.

O 24.2 Mon 17:45 WIL C307

Chemoselective adsorption of functionalized cyclooctynes on silicon — Marcel Reutzel[1], Niels Münster[1], Marcus A. Lipponer[1], Christian Länger[2], Ulrich Höfer[1], Ulrich Koert[1], and •Michael Dürr[2] — [1]Philipps-Universität, 35037 Marburg — [2]Justus-Liebig-Universität, 35392 Giessen

The high reactivity of the silicon dangling bonds presents a major hindrance for chemoselective attachment of bifunctional organic molecules on Si surfaces, the first basic reaction step for the controlled organic functionalization of silicon. Due to the high reactivity of the dangling bonds, each functional group of a bifunctional molecule adsorbs with an initial sticking coefficient close to unity and thus the final adsorption product will typically consist of a mixture of molecules adsorbed via different functional groups.

We overcome this problem employing cyclooctyne as the major building block of our strategy [1]. Using XPS and STM, cyclooctyne derivatives with different functional side groups are shown to react on Si(001) selectively via the strained cyclooctyne triple bond while leaving the side groups intact. The achieved selectivity originates from the distinctly different adsorption dynamics of the separate functionalities: A direct adsorption pathway is demonstrated for cyclooctyne as opposed to the vast majority of other organic functional groups. The latter ones react on Si(001) via a metastable intermediate, which makes them effectively unreactive in competition with the direct pathway of cyclooctyne's strained triple bond.

[1] Reutzel et al., J. Phys. Chem. C **120** 26284 (2016).

O 24.3 Mon 18:00 WIL C307

***Ab initio* thermodynamics of adsorbed atomic H at ZnO** $(10\bar{1}0)$ — •Maria E. Stournara[1], Sergey V. Levchenko[1], Santiago Rigamonti[2], Maria Troppenz[2], Oliver Hofmann[3], Patrick Rinke[4], Claudia Draxl[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Faradayweg 4-6 — [3]Technische Universität Graz, Graz, AT — [4]Aalto University, Helsinki, FI

Zinc oxide (ZnO) is a highly multifunctional material with unique properties and a wide range of applications. To understand atomic hydrogen adsorption on the thermodynamically stable $(10\bar{1}0)$ surface at realistic H chemical potentials, we combine a first-principles cluster-expansion model with *ab initio* atomistic thermodynamics. Our study reveals that at coverages below 6%, H atoms adsorb exclusively on surface O. At higher coverages, H adsorbs also on Zn, but there is an excess of O-H over Zn-H at all coverages, except 50% and 100%. Due to an interplay of long- and short-range electrostatic interactions, neighboring O-H/Zn-H pairs form chains along surface -O-Zn- rows, with each chain anchored at the excess O-H, in a wide range of (T, p_{H_2}). Any ordering that could occur due to the long-range repulsion between the excess O-H is destroyed at $T > 60$ K. Our results explain available experimental data and provide detailed microscopic understanding of the ZnO surface properties at realistic (T, p_{H_2}) conditions.—This work was supported by the Hybrid Inorganic/Organic Systems (HIOS) CRC of the DFG.

O 24.4 Mon 18:15 WIL C307

Nanopatterning of Group-V-Elements for Tailoring the Electronic Properties of Semiconductors by Monolayer Doping — •Peter Thissen[1] and Roberto Longo[2] — [1]Karlsruher Institut für Technologie (KIT), Institut für Funktionelle Grenzflächen (IFG), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Department of Materials Science & Engineering, The University of Texas at Dallas, Richardson, Texas 75080, USA

The control of the electronic properties of semiconductors is primarily achieved through doping. Within this context, new techniques such as Monolayer Doping (MLD) represent a substantial improvement towards surface doping with atomic and specific doping dose control at the nanoscale. Here, we address the key questions that will ultimately allow to optimize the scalability of the MLD process. First, we show that dopant coverage control cannot be achieved by simultaneous reactions of several group-V-elements, but stepwise reactions make it possible. Second, using ab initio molecular dynamics, we investigate the thermal decomposition of the molecular precursors, together with the stability of the corresponding binary and ternary dopant oxides, prior to the dopant diffusion into the semiconductor surface. Finally, the effect of the coverage and type of dopant on the electronic properties of the semiconductor is also analyzed. Furthermore, the atomistic characterization of the MLD process raises unexpected questions regarding possible crystal damage effects by dopant exchange with the semiconductor ions, or the final distribution of the doping impurities within the crystal structure.

O 25: Overview Talk: Axel Groß

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

Invited Talk O 25.1 Tue 9:30 TRE Phy

Electrochemistry: A new frontier for a theoretical surface scientist — •Axel Gross — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm/Germany

Despite its relevance in energy conversion and storage, our knowledge about microscopic structures and processes at electrochemical electrode-electrolyte interfaces is still rather limited. The theoretical description of these interfaces from first principles is hampered by at least two factors that are typically not present in surface science. i) In electrochemistry, properties of the electrode-electrolyte interfaces are governed by the electrode potential which adds considerable complexity to the theoretical treatment since charged surfaces have to be considered. ii) The theoretical treatment of processes at solid-liquid interfaces necessitates a proper description of the liquid which in principle requires to perform computationally expensive statistical averages.

I will in particular focus on how, despite these obstacles, the electrochemical environment can be appropriately and efficiently taken into account in theoretical studies. For example, the presence of the electrolyte can be treated in a grand-canonical approach as a reservoir. Thus the equilibrium coverage of metal electrodes with ions present in the solution was derived [1]. In an implicit solvent model, the aqueous electrolyte is treated as a dielectric continuum. Using this approach, we demonstrate the importance of the presence of the electrochemical environment in the methanol electro-oxidation on Pt(111) [2].

[1] F. Gossenberger *et al.*, Electrochim. Acta **216**, 152 (2016).
[2] S. Sakong and A. Groß, ACS Catal. **6**, 5575 (2016).

O 26: SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - NMR studies

Time: Tuesday 10:15–11:30 Location: IFW A

O 26.1 Tue 10:15 IFW A

Investigation of the Li ion conduction behavior in the solid electrolyte Li10GeP2S12 by multidimensional NMR — •Marc Paulus[1], Magnus Graf[1], Peter Notten[1,4], Rüdiger-Albert Eichel[1,3], and Josef Granwehr[1,2] — [1]FZ Jülich, Institut für Energie- und Klimaforschung , D-52425 Jülich, Germany — [2]RWTH Aachen, ITMC, D-52074 Aachen, Germany — [3]RWTH Aachen, IPC, D-52074 Aachen, Germany — [4]Department of Chemical Engineering and Chemistry, TU/e, 5600 MB Eindhoven, The Netherlands

The biggest challenge to overcome in solid electrolytes is the relatively slow and still poorly understood lithium ion migration at solid electrolyte/electrode interfaces as well as at grain boundaries in solid-state electrolytes. Li10GeP2S12 is one of the best Li-ion conductors and therefore an interesting candidate as electrolyte material in Li-ion batteries. To link lithium migration mechanisms with different structural features of LGPS by correlation of spin lattice relaxation and spin alignment echo NMR a pulse sequence with two independently varied evolution times was developed. The obtained data was processed with an algorithm for discrete Laplace inversion. The resulting spin lattice-spin alignment correlation map of LGPS provided several signal components that were assigned to different morphologies and dynamic regions in LGPS. In addition, the experiment facilitated a direct distinction between relaxation-controlled and mobility-induced components in the τc distribution. Further analysis of the spectral NMR dimension in comparison with SEM and XRD measurements yielded a diverse model of lithium motion for the LGPS powder sample.

O 26.2 Tue 10:30 IFW A

Solid-state MAS and in-situ NMR spectroscopy for studying battery systems — Wolfram Münchgesang[1], Viktor Koroteev[2], Tatiana Zakharchenko[3], Daniil M. Itkis[4], Dirk C. Meyer[1], and •Anastasia Vyalikh[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Freiberg, Germany — [2]Nikolaev Institute of Inorganic Chemistry SB RAN, Novosibirsk, Russia — [3]Department of Material Science, Moscow State University, Moscow, Russia — [4]Department of Chemistry, Moscow State University, Moscow, Russia

Current research efforts in the field of energy storage are directed towards improving cost and performance of lithium ion batteries as well as evaluating post lithium ion concepts. Deep understanding of electrochemical processes requires quantitative information on a molecular level, on the one hand, and with temporal resolution, on the other hand. In our studies we apply ex-situ analysis using high-resolution magic angle spinning (MAS) NMR in combination with in-situ NMR, in order to characterize the electrochemical intermediates and reaction products as well as to monitor the formation of solid electrolyte interface (SEI) and surface microstructures in operating cells. The NMR results demonstrate the structural transformations in lithium ion batteries based on vanadia composite and 13C-isotop enriched carbon electrodes.

O 26.3 Tue 10:45 IFW A

^{7}Li NMR studies of lithium ion dynamics in $70Li_2S$-$30P_2S_5$ materials — •Michael Haaks[1], Steve Martin[2], and Michael Vogel[1] — [1]Institut für Festkörperphysik, TU Darmstadt, Germany — [2]Department of Materials Science and Engineering, Iowa State University, Ames, USA

Rising energy demand makes it important to improve the performance of lithium ion batteries. For this purpose it is important to understand the dynamics of lithium ions, in particular, in heterogeneous materials, which are used in modern strategies for material optimization. With combination of ^{7}Li NMR spin-lattice relaxation, diffusion measurements, line-shape, and stimulated-echo analyses it is possible to investigate lithium ionic motion in wide range of time and length scales in $0.5Li_2S$-$0.5(xGeS_2$-$(1-x)GeO_2)$[1] and $70Li_2S$-$30P_2S_5$ glasses[2]. We exploit there capabilities to ascertain the effect of ceramization in $70Li_2S$-$30P_2S_5$. We find that the large variety of lithium environments results in broad distributions of correlation times for the jump motion of the lithium ions. Our results for $70Li_2S$-$30P_2S_5$ allow us to relate the enhancement of electronic conductivity under ceramization[3] to faster lithium ion dynamics on various length scales.

[1] Gabriel et al., Solid State Nuclear Magnetic Resonance 70, 53 (2015)
[2] Haaks et al., work in progress
[3] Mizuno et al., Advanced Materials 17, 918 (2005)

O 26.4 Tue 11:00 IFW A

Combined DFT and solid-state NMR study of ionic mobility in $Li_4Ti_5O_{12}$ — •Simone Köcher[1,2], Andreas Garhammer[2], Hendrik Heenen[2], Magnus Graf[1], Josef Granwehr[1], Rüdiger-A. Eichel[1], Karsten Reuter[2], and Christoph Scheurer[2] —

[1]IEK-9 - Fundamental Electrochemistry, Forschungszentrum Jülich, Jülich, Germany — [2]Chair for Theoretical Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany

Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful tool to gain detailed understanding of the ionic mobility in battery materials. Notwithstanding, experimental spectra of novel high-capacitance electrodes such as the configurationally disordered defect spinel oxide $Li_4Ti_5O_{12}$ (LTO) are highly complex. Support by independent first-principles based calculations is indispensable to achieve an unambigious interpretation. We establish a corresponding framework for ^{7}Li spin-alignment echo NMR studies of LTO by providing first-principles reference values for chemical shielding and quadrupolar coupling from density-functional theory calculations. A detailed comparison of experimental and theoretical data suggests that a local Li ion mobility faster than the experimental time resolution must have a considerable impact on the observed NMR quantities. We present first steps towards accounting for this local dynamics in the simulation of the autocorrelation function of the NMR experiment within a kinetic Monte Carlo model.

O 26.5 Tue 11:15 IFW A

Li-ion batteries cathode materials from extended Hubbard-corrected functionals — •Matteo Cococcioni and Nicola Marzari — Theory and Simulations of Materials (THEOS) and NCCR-MARVEL, EPFL, Lausanne, Switzerland

Predictive modeling of the atomistic structure and electronic properties of transition-metal (TM) compounds is essential for the development of several emerging technologies. This is particularly true for materials explored as electrodes in Li-ion batteries. Unfortunately, most approximate energy functionals fail to capture the localization of electrons on TM ions during the charge/discharge transients, thus compromising the energetics of these systems and the assessment of their performance.

Hubbard-corrected DFT functionals (DFT+U) improve significantly the description of localized valence electrons and have become the standard choice to the modeling of these TM compounds when computational efficiency is required (e.g., for screening large numbers of compounds). This work shows that an extended formulation of DFT+U, including on-site (U) and inter-site (V) interactions, improves the description of mixed valence materials. Focusing on LixMPO4 (M = Fe, Mn, Ni, Co) we discuss their equilibrium structure and electronic properties in dependence of Li content. Contradicting a common practice, we provide theoretical justification to using computed interaction parameters. We also show this is crucial to reliably compare the energy of different phases, to assess the thermodynamic stability of intermediate compositions and to evaluate the voltage of the resulting battery.

O 27: Surface Dynamics: Theory

Time: Tuesday 10:30–12:30 Location: TRE Phy

Invited Talk O 27.1 Tue 10:30 TRE Phy

The role of nonadiabatic friction in chemical dynamics at metal surfaces — •Reinhard Maurer — Department of Chemistry, Yale University, New Haven CT 06520, USA

Despite a large mass discrepancy, hydrogen atoms show inelastic scattering from metal surfaces and, despite vibrational decoupling of intramolecular stretch motion from substrate phonons, adsorbate vibrations are damped efficiently on metals. Both of these effects can be attributed to low-lying electronic excitations or "hot electrons" in the metal substrate that interact with the adsorbate via nonadiabatic coupling. The importance of such effects in elementary processes in surface photophysics, molecular device physics, heterogeneous photocatalysis and ultrafast reaction dynamics motivates the development of efficient first-principles electronic structure methods that account for coupled electron-nuclear dynamics in materials. On examples ranging from hydrogen scattering to vibrational energy dissipation and molecular switching at metal surfaces, I will present our Density-Functional Theory-based approach to describe nonadiabatic effects in two limiting regimes, the surface hopping and the electronic friction regime. In comparison with experiment and current state-of-the-art simulation methods, we find a qualitatively correct description of nonadiabatic effects for a variety of systems. In combining our method with mixed quantum-classical molecular dynamics, I will show how nonadiabatic friction affects the reaction dynamics and contributes to adsorbate-substrate energy transfer.

O 27.2 Tue 11:00 TRE Phy

Non-adiabatic vibrational damping of molecular adsorbates: Beyond electronic friction — •Simon P. Rittmeyer[1], Jörg Meyer[2], and Karsten Reuter[1] — [1]Technische Universität München — [2]Universiteit Leiden

The availability of low-energy electron-hole (*eh*) pair excitations generally questions the validity of the ubiquitous Born-Oppenheimer approximation for adsorbate dynamics on metal surfaces. An in-depth scrutiny thus requires to consider the non-adiabatic coupling of nuclear motion to these *eh*-pair excitations. Unfortunately, an explicit calculation from first principles remains a formidable challenge. Electronic friction theory is very popular to capture the effects of the non-adiabatic energy loss on the nuclear dynamics in a computationally convenient way. This avoids explicit electron dynamics and concomitant ultrafast time scales, but for these reasons also precludes a more fundamental understanding of the underlying *eh*-pair excitations.

In this situation, we advance a perturbative approach rooted in time-dependent density-functional theory which allows to actually evaluate *eh*-pair excitation spectra [1]. Applying this to non-adiabatic vibrational damping of CO on Cu(100) and Pt(111), we find that the non-adiabatic energy loss obtained from our spectra is consistent with experimentally measured lifetimes. Moreover, we discuss intriguing deviations from the linear relationship between non-adiabatic energy loss and kinetic energy predicted by electronic friction theory that might be measurable in new experiments.

[1] J. Meyer and K. Reuter, New. J. Phys. **13**, 085010 (2011).

O 27.3 Tue 11:15 TRE Phy

Quantization of collective excitations in finite systems: An ab initio quasiparticle picture for hot carrier generation in noble metal nano clusters — •Mikael Kuisma[1,2], Tuomas Rossi[3], and Paul Erhart[2] — [1]University of Jyväskylä, Jyväskylä, Finland — [2]Chalmers University of Technology, Gothenburg, Sweden — [3]Aalto University, Helsinki, Finland

Resolving hot electron generation from coherent collective plasmon excitations in nanoparticles is a vital step in understanding a wide variety of physical processes. However, in order to facilitate a quantitative understanding of hot electron generation, a physically sound picture of collective excitations in nanoparticles must be established.

In our time-dependent density functional theory and many body perturbation theory based framework we extract the collective coordinates of plasmons in the electron-hole space. We find that a discrete, topology dependent number of electron-hole pairs is collectively involved in formation of a plasmon. The collective coordinates define the bare plasmons, which are further renormalized due to other electron-hole excitations via the plasmon self energy. The emerging quasiparticle picture is able to explain the plasmon renormalization due to Landau scattering and d-band screening in noble metal nanoparticle with unprecedented simplicity in reasoning and intuition, while maintaining the *ab initio* quantitative nature of the calculation. In order to demonstrate our approach, we analyze hot-electron generation rates in gold clusters.

O 27.4 Tue 11:30 TRE Phy

Insights of the Ultrafast Charge Transfer Process in CdSe Quantum Dot/Organic Molecule System: A Real-Time Time-Dependent Ab Initio Study — •Zhi Wang[1], Jan-Philip Merkl[1], Mona Rafipoor[1], Holger Lange[1], Lin-Wang Wang[2], and Gabriel Bester[1] — [1]Institut für Physikalische Chemie, Universität Hamburg — [2]Material Science Division, Lawrence Berkeley National Laboratory

We report for the first time a real-time time-dependent density function theory (rt-TDDFT) simulation on experimental size CdSe quantum dot/organic molecule system, to analyze its ultrafast (femtosecond to sub-picosecond) photoexcited charge transfer (CT) dynamics.

Non-adiabatic dynamic details, such as the size-dependence of CT process, the carrier separation and cooling, the electron-phonon interaction and Auger-assisted process are presented using our high-efficient rt-TDDFT package. Our results are in excellent agreement with experiment data.

O 27.5 Tue 11:45 TRE Phy

Importance of many-body dispersion and temperature effects on gas-phase gold cluster (meta)stability — •Bryan R. Goldsmith, Philipp Gruene, Jonathan T. Lyon, David M. Rayner, André Fielicke, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

Gold clusters in the gas phase exhibit many structural isomers that are shown to intercovert frequently, even at room temperature. We performed ab initio replica-exchange molecular dynamics (REMD) calculations on gold clusters (of sizes 5-14 atoms) to identify metastable states and their relative populations at finite temperature, as well as to examine the importance of temperature and van der Waals (vdW) on their isomer energetic ordering. Free energies of the gold cluster isomers are optimally estimated using the Multistate Bennett Acceptance Ratio. The distribution of bond coordination numbers and radius of gyration are used to address the challenge of discriminating isomers along their dynamical trajectories. Dispersion effects are important for stabilizing three-dimensional structures relative to planar structures and brings isomer energetic predictions to closer quantitative agreement compared with RPA@PBE calculations. We find that higher temperatures typically stabilize metastable three-dimensional structures relative to planar/quasiplanar structures. Computed IR spectra of low free energy Au9, Au10, and Au12 isomers are in agreement with experimental spectra obtained by far-IR multiple photon dissociation in a molecular beam at 100 K.

O 27.6 Tue 12:00 TRE Phy

Replica-Exchange Grand-Canonical Algorithm for Determining Phase Diagrams of Surfaces in Reactive Atmospheres — •Yuanyuan Zhou, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

A temperature-pressure phase diagram describes the composition and structure of a system at thermal equilibrium and is an essential tool for understanding material properties. The atomistic thermodynamics (AT) approach has been very successful in predicting phase diagrams for surfaces [K. Reuter, M. Scheffler, PRL **90**, 046103 (2003)] and gas-phase clusters [S. Bhattacharya *et al.*, PRL **111**, 135501 (2013)] at realistic T, p conditions. However, its limitation is the lack of an unbiased sampling of the configurational space. Here, we present a novel replica-exchange (RE) grand-canonical (GC) Monte-Carlo (MC) algorithm that allows for the efficient estimate of the partition function of atomistic systems. We specifically target open systems in the GC ensemble, aiming at describing (nano)structured surfaces in a reactive atmosphere (e.g., for heterogeneous catalysis) at realistic T, p. RE allows for an efficient sampling by shuttling configurations from regions of low T or high chemical potential (μ) to regions of high T or low μ. In order to demonstrate the approach, we apply REGC-MC to a two-component Lennard-Jones system with a surface in contact with a gas-phase. In particular, we discuss REGC-MC's viability by comparing our results with calculated ones using AT and find good agreement at low coverage but quite different at relatively high coverage.

O 27.7 Tue 12:15 TRE Phy

Theoretical description of Ge(001) surface reconstruction — •Katharina Noatschk[1,2], Wolfgang Klesse[2], Thomas Schroeder[1,2], and Götz Seibold[1] — [1]Brandenburg Technical University Cottbus-Senftenberg, 03046 Cottbus, Germany — [2]IHP-Innovations for High Performance Microelectronics, 15236 Frankfurt(Oder), Germany

In our work we study the reconstruction of the Ge(001) surface within the Ising model. Due to the reduced bonding of surface atoms adjacent germanium surface atoms tend to form so-called tilted dimers [1]. Experimentally one observes at low temperature the c(4x2) structure which corresponds to an alternating tilt pattern whereas at high temperature the overall tilt vanishes. In addition to the c(4x2) structure experimental and theoretical work also indicates the presence of an intermediate p(2x2) structure with alternating tilts only along one cristallographic axis whereas it is constant along the other. In our investigations we represent the two tilt directions of a dimer by an Ising spin and take the interaction parameters between Ising variables from first principle calculations [2]. We evaluate the phase diagram for the various dimer order parameters within a Metropolis algorithm. Moreover, we obtain from the Monte Carlo simulation domains on the surface which are consistent with the experimental measurements.

[1] D.J. Chadi, Phys. Rev. Lett. 43 (1979) 43

[2] Y. Yoshimoto, et al. Phys. Rev. B 61 (2000) 1965

O 28: Plasmonics and Nanooptics IV: Light-Matter Interaction

Time: Tuesday 10:30–13:00 Location: TRE Ma

O 28.1 Tue 10:30 TRE Ma

Rolled-up active microtubes containing tuneable grating couplers for the excitation of surface plasmon polaritons — •Jan Siebels[1], Hoan Vu[1], Alf Mews[1], Stefan Mendach[2], and Tobias Kipp[1] — [1]Institut für Physikalische Chemie, Universität Hamburg — [2]Institut für Angewandte Physik, Universität Hamburg

Grating structures can be utilized in order to overcome the momentum mismatch between an incident photon and a surface plasmon polaritons (SPPs) at a metal/dielectric interface. We implemented grating structures with gradually varying effective refractive indices into active microtubes containing GaAs quantum wells. The grating consists of triangularly shaped silver bars–varying the filling-factor in the direction perpendicular to the periodicity. This allows for a position-dependent coupling of the quantum well emission to the SPP. To characterize these systems we implemented a photoluminescence mapping technique by means of a streak camera which allows simultaneous recording of spectral distribution and related decay characteristics. The spatially resolved data reveals spectral shifts and changes of the decay lifetime that can be attributed to localized excitation of SPPs due to the embedded gratings. We gratefully acknowledge financial support by the Deutsche Forschungsgemeinschaft (DFG) via ME3600/1.

O 28.2 Tue 10:45 TRE Ma

Tip-Enhanced Raman Spectroscopy of a MoS2 / Au Nanoparticle (2D crystal/Plasmonic) Heterostructure — •Mahfujur Rahaman[1], Raul D Rodriguez[1], Gerd Plechinger[2], Stefan Moras[1], Christian Schüller[2], Tobias Korn[2], and Dietrich RT Zahn[1] — [1]Semiconductor Physics, Technische Universität Chemnitz, Germany — [2]Fakultät für Physik, Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany

Tip-enhanced Raman spectroscopy (TERS) has been rapidly improved over the last decade and opened up opportunities to study phonon properties of materials on a nanometre scale. We report on TERS of a 4-layer MoS2 flake deposited onto a Au nanostructured surface, thus forming a 2D crystal/plasmonic heterostructure. Au nanotriangles are prepared by nanosphere lithography and then MoS2 is mechanically exfoliated on top of it. The TERS spectra are acquired under resonance conditions at 638 nm excitation using a Xplora/AIST-NT TERS system. We obtain a spatial resolution of 10 nm in TERS imaging. We observe the highest enhancement of the Raman intensity of MoS2 on top of Au nanotriangles due to the strong electromagnetic confinement between the tip and single triangle. Our results enable us to determine the local strain in MoS2 induced after the heterostructure formation. The maximum frequency shift of E2g mode is determined to be 3.2 cm-1 which is equivalent to 1% of biaxial strain induced in the film. Our results will help the understanding of the structural and mechanical degrees of freedom to the nanoscale optoelectronic properties of future MoS2/plasmonic based devices.

O 28.3 Tue 11:00 TRE Ma

Strong Exciton-Plasmon Coupling on Core-Shell Nanoparticles — •Wouter Koopman, Felix Stete, and Matias Bargheer — Universität Potsdam, Potsdam, Deutschland

Strong-coupling of molecular excitons to localized plasmons in metal nanoparticles offers a new approach for the investigation and utilization of quantum-effects at room temperature. On the other hand, the fabrication of core-shell molecule-metal nanoparticles is possible by well-established, economic wet-chemical methods. Plasmon-exciton coupling could therefore offer an attractive route for the facile implementation of robust, scalable nanoscale quantum systems. This talk will address the presence of strong exciton-plasmon coupling in two simple nanoparticle geometries: core-shell spheres and rods. We will elaborate on the different possible coupling regimes and discuss the pitfalls when one wants to distinguish these experimentally. In particular we show that relying solely on extinction spectrum to classify the coupling regime, as often encountered in literature, can lead to a wrong identification of the regime. In addition, we will address the pronounced dependence of coupling-strength on the particle size and on the dielectric environment and discuss how to use these factors to tailor the coupling.

O 28.4 Tue 11:15 TRE Ma

SPP-Light Interaction in the Space-Time Domain — •David Janoschka, Pierre Kirschbaum, Pascal Dreher, Michael Horn-von Hoegen, and Frank J. Meyer zu Heringdorf — Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, Germany

Focusing of Surface Plasmon Polaritons (SPPs) with nanooptical elements extends the comprehension of nonlinear phenomena on Au surfaces. We use femtosecond-laser-pulses (<15 fs) to excite SPPs, which can be observed in a direct conceptual visualization in our Photoemission Electron Microscope (PEEM). Focused Ion Beam (FIB) milled structures on Au provide a great control over the shape of the SPP phase fronts. As such, we are able to achieve the formation of a strong SPP-field induced nanofocus with circular shaped excitation structures. This causes highly localized electron emission, exclusively by the SPP-SPP interaction, which was introduced as plasmoemission in previous work.

Here, we investigate the differences between photoemission and plasmoemission. We are in particular interested in the SPP-SPP-interaction in the presence of other nanooptical elements like nanoholes and nanoparticles, especially in the strong field enhancement caused by these nanooptical elements.

O 28.5 Tue 11:30 TRE Ma

Resonant excitation of isolated helical nanostructures in the visible range — Katja Höflich[2], Enno Hansjürgen[1], Heiko Kollmann[1], Silke Christiansen[2], Christoph Lienau[1], and •Martin Silies[1] — [1]AG Ultrafast Nano-Optics, Carl von Ossietzky Universität Oldenburg, Germany — [2]Nanoscale Structures and Microscopic Analysis, Helmholtz-Zentrum Berlin, Germany

Circular dichroism is a phenomenon that describes the extinction difference in chiral objects when excited by left and right-handed circular polarized light. While the circular dichroism of single biomolecules is rather low, the signal can be enhanced by several orders of magnitude using artificial, i.e. plasmonic chiral nanostructures. Thus, the study of these plasmonic structures is a vivid field of research. Here, confocal white-light spectro-microscopy is employed to measure extinction spectra of single silver helices with sub-micrometer dimensions fabricated using electron beam induced deposition for left- and right-handed circular excitation. Circular dichroism spectra of isolated right-handed helices show - besides a near-IR resonance for light at the same handedness - a distinct resonance for left-handed circular polarized light in the visible range around 600 nm. While the resonant behavior for the right-handed circular polarized light is expected [1], the emergence of a pronounced left-handed resonance is surprising. Finite element modeling reliably reproduces the observed spectral features and suggests that a pseudo current at the outer surface of the helices locally switches the polarization state of the incident polarization. [1] Gansel et al. Science 325, 1513 (2009)

O 28.6 Tue 11:45 TRE Ma

The detection of attenuated waveguide modes in $\mathbf{SiO_2}$ on silicon covered with gold-nanoparticles using photo emission electron microscopy — •Alwin Klick[1], René Wagner[1], Malte Grossmann[1], Laith F. Kadem[2], Jost Adam[3], Till Leissner[3], Horst-Günter Rubahn[3], Christine Selhuber-Unkel[2], and Michael Bauer[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — [2]Institut für Materialwissenschaft, Christian-Albrechts-Universität zu Kiel — [3]Mads Clausen Instituttet, Syddansk Universitet

We present a time-resolved photoemission electron microcopy study of propagating electromagnetic modes in the UV spectral regime in SiO_2 covered with self-assembled gold nanospheres on a silicon substrate. Comparison with simulations using the finite element method confirms that guided light modes in the SiO_2 slab are detected. Furthermore, we show that the gold nanospheres play a key role in the observation of guided modes using PEEM due to their high electron density substantially enhancing the detected photoemission yield. Analytic calculations which take into account the size of the nanospheres and their distribution on the surface show that plasmonic interactions have negligible impact on the light mode properties.

O 28.7 Tue 12:00 TRE Ma

Near-field investigation of geometric and material resonances in semiconductor nanowires with doped segments — •Lena Jung[1], Dmitriy S. Boyuk[2], Amar T. Mohabir[2], Michael A. Filler[2], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332, United States

Doped semiconductors (SCs) allow for tunability of plasmon resonances via gating or doping. We investigate Si nanowires (NWs) with doped segments with infrared near-field microscopy (s-SNOM). In s-SNOM, optical near-fields that are excited via laser-illumination of a metalized AFM tip interact with the sample. This enables to determine the samples dielectric properties with a high resolution only limited by the tip radius (∼25 nm). By combining the Drude model for doped SCs with models for the tip-sample interaction, carrier properties of the doped SC can be obtained by spectroscopic imaging in the range of a near-field resonance close to the plasma edge. Additionally, the doped segments in the NWs act as resonators for mid-IR light due to their geometry. Localized surface plasmon (LSP) resonances have been observed in the far-field. Different growth conditions revealed differences in the shape of the spectra, explained by variations in the sharpness of the segment boundaries [1]. Goal of our investigations is to distinguish these different effects and to determine carrier properties, boundary sharpness and map the LSP resonance given by the segment geometry.

[1] Chou et al., ACS Nano **9**, 1250 (2015)

O 28.8 Tue 12:15 TRE Ma

Single-particle spectroscopy of bare and porphyrin-covered silver clusters with multi-photon photoemission electron microscopy — •Klaus Stallberg and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstraße 4, 38678 Clausthal-Zellerfeld, Germany

Coupling of optical excitations in dye molecules with plasmonic excitations in metallic nanostructures holds the potential to provide control over light-matter interaction at a nanoscale level. Plasmonic-excitonic coupling has been reported for dye-coated metallic nanoparticles by application of particle-averaging methods. We apply multi-photon photoemission electron microscopy (nP-PEEM) with tunable-laser excitation to study localized surface plasmon resonances (LSPR) of individual silver clusters, which are grown under UHV conditions on silicon substrates. Simulations elucidate the influence of the supporting substrate on the LSPR, most notably an amplification of LSP modes with a polarization normal to the substrate. For particles covered with porphyrin (ZnTPP) the simulations predict the appearance of a second LSPR near the optical absorption (Soret-) band of the ZnTPP molecules, a consequence of coupling between the plasmonic near-field and and the excitonic polarization inside the ZnTPP layer. Depending on their spectral positions, both LSP modes are predicted to spectrally repel each other as a result of additional coupling between the LSP modes. In our laser spectroscopic nP-PEEM experiments we observe such spectral shifts for silver particles covered with a ZnTPP layer of only four monolayers.

O 28.9 Tue 12:30 TRE Ma

Linear ultra-broadband spectral interferometry for probing coherent surface plasmon polariton propagation in the time domain — Jue-Min Yi[1], •Vladimir Smirnov[1], Dongchao Hou[1], Heiko Kollmann[1], Zsuzsanna Pápa[2], Péter Dombi[2], Sven Stephan[1], Daniel Espeloer[1], Christoph Lienau[1], and Martin Silies[1] — [1]AG Ultrafast Nano-Optics, Carl von Ossietzky Universität Oldenburg, Germany — [2]Wigner Research Centre for Physics, 1121 Budapest, Hungary

Surface Plasmon Polaritons (SPPs) are evanescent coherent wave packets that can both confine the energy of light to metallic nanostructures and transport energy over mesoscopic distances [1]. They can then be used to generate and process information coded as optical signal to realize nanometer-scale all-optical circuitry. The propagation properties of these SPPs are defined by the geometry and composition of nanostructures. Here, we introduce a new ultra-broadband far-field spectral interferometry method to completely characterize coherent SPP propagation in metallic nanostructures, which allows the reconstruction of the plasmonic field in time domain [2]. Group velocity and dispersion of SPPs are determined with high precision in a broad frequency range in the visible and near-infrared regions, and the propagating SPP field at large distance is thus displayed with high time resolution. Our results shed new light on characterizing the interplay between nanostructure geometry and coherent SPP propagation.

[1] M.L.M. Balistreri, et al., Science 294, p.1080 (2001)

[2] J.Yi, et al., submitted to ACS Photonics (2016)

O 28.10 Tue 12:45 TRE Ma

(The Road to) Understanding Localization of Light in Nanosponges — •Felix Schwarz[1], Jan Vogelsang[3], Germann Hergert[3], Dong Wang[2], Heiko Kollmann[3], Petra Gross[3], Erich Runge[1], Christoph Lienau[3], and Peter Schaaf[2] — [1]TU Ilmenau, Institut für Physik und IMN MacroNano, 98693 Ilmenau — [2]TU Ilmenau, Institut für Werkstofftechnik und IMN MacroNano, 98693 Ilmenau — [3]Carl von Ossietzky Universität, Institut für Physik and Center of Interface Science, 26129 Oldenburg

Disorder on the nanometer scale can lead to localization of light and huge electromagnetic field enhancement, which in turn can be used for non-linear optics and for the study and exploitation of quantum optical processes. Most recently, long-lived, highly localized plasmons on the surface of nanoporous gold-nanoparticles (nanosponges) with an unmatched excitation efficiency were reported based on photoemission. Surprisingly, first calculations show that on these sponges localization takes place on the same length scale as the typical pore size. To optimally tailor the disorder for potential applications and increase the understanding of this unusual localization process, we systematically examine the influence of the specific type of disorder. Far-field scattering and near-field properties are calculated for different correlation functions and filling fraction of the sponges. Furthermore, a multiscale approach is presented, where parts of the surface can be simulated with increased resolution while the antenna resonances are evaluated in an effective-medium picture. Very good agreement with experimental data regarding the field enhancement and lifetime is reported.

O 29: Organic-Inorganic Hybrid Systems and Organic Films IV

Time: Tuesday 10:30–13:00 Location: WIL A317

O 29.1 Tue 10:30 WIL A317

Tailoring surface alloys by metal-organic bonds: Adsorption properties of PTCDA on Sn/Ag(111) and Sn/Au(111) surface alloys — •Johannes Seidel[1], Florian Haag[1], Norman Haag[1], Leah Kelly[1], Mahalingam Maniraj[1], Dominik Jungkenn[1], Markus Franke[2], Gerben van Straaten[2], Christian Kumpf[2], Mirko Cinchetti[3], Benjamin Stadtmüller[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

In this work, we extend our new approach [1] of controlling the geometric and electronic interface properties of surface alloys by adsorption of organic molecules. We investigated the PTCDA molecule adsorbed on surface alloys Sn_1Ag_2/Ag(111) and Sn_1Au_2/Au(111) by LEED, NIXSW and momentum photoemission microscopy to reveal changes in the lateral, vertical and electronic structure of the surface alloy caused by the adsorption of PTCDA. In both cases we find a clear vertical relaxation of the Sn atoms upon adsorption of PTCDA, similar to [1], but only in the case of PTCDA on Sn_1Ag_2/Ag(111) a charge transfer into the LUMO is observed. We thus conclude that the driving mechanism for lifting the Sn atoms is not charge transfer rather the formation of local bonds between the oxygen end groups of PTCDA and the Sn atoms. [1] PRL 117, 096805(2016)

O 29.2 Tue 10:45 WIL A317

Adsorbate-Induced Charge Accumulation and Collective Excitations at Metal/Organic Interfaces — •Friedrich Maass, David Gerbert, and Petra Tegeder — Physikalisch-Chemisches Institut; Ruprecht-Karls-Universität Heidelberg, INF 253, 69120 Heidelberg, Germany

The electronic and geometrical structure of organic molecules at metal/organic interfaces have substantial impact on the performance of organic molecule-based devices. We investigated the adsorption geometry and the electronic properties of F_4TCNQ and TCNQ on the Au(111) surface using vibrational and electronic high-resolution electron energy-loss spectroscopy (HREELS), temperature-programmed desorption (TPD), and density functional theory calculations (DFT). With angle-resolved electronic HREELS we characterized a collective excitation of electrons accumulated at the interface[1]. We analyzed the influence of transferred parallel momentum, impinging electron energy, and film thickness. As F_4TCNQ is, in contrast to TCNQ, known to be negativly charged at the Au(111) surface we were also able to investigate the influence of charges in the adsorbate layer on the collective excitation.

[1] Salomon, E., Layet, J. M., and Angot, T. *Phys. Rev. B*, **85**, 125420 (2012).

O 29.3 Tue 11:00 WIL A317

A novel facility for time- and space-resolved molecular dynamics on surfaces — •Bernhard Huber[1], Sebastian Pres[1], Emanuel Wittmann[2], Lysanne Dietrich[1], Julian Lüttig[1], Victor Lisinetskii[1], Matthias Hensen[1], Eberhard Riedle[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Lehrstuhl für BioMolekulare Optik, Ludwig-Maximilians-Universität München, Oettingenstraße 67, 80538 München, Germany

How do energy transport processes between individual molecules or inside large heterogeneous structures like light harvesting complexes occur? Is the transport dominated by step-by-step hopping of excitation or do the individual molecules form a strongly coupled system in which the excitation is delocalized over all constituents? How are these transport phenomena influenced by interactions with the substrate, the environment and external light sources? To investigate these questions the measurement signal of the prepared system has to be retrieved with high temporal (femtosecond regime) and spatial resolution far below the optical diffraction limit (several nanometers). The surface spectroscopy facility presented here combines aberration-corrected photoemission electron microscopy (AC-PEEM) with a widely tunable femtosecond laser system down to the UV range rendered by optical parametric amplification. Thus, the surface dynamics can be explored in a time-interferometric scanning scheme with high spectral addressability of sample specific resonances. Here we demonstrate first results of spectrally selective photoemission microscopy.

O 29.4 Tue 11:15 WIL A317

Electronic and optical properties of Organic/Inorganic Heterostructures from First Principles: PPP@ZnO — •Benjamin Höffling, Dimitri Nabok, Caterina Cocchi, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Zum Großen Windkanal 6, 12489 Berlin, Germany

The electronic properties of poly(*para*-phenylene) (PPP) adsorbed on the non-polar (001) surface of rocksalt (*rs*) ZnO are studied by means of all-electron density functional theory (DFT) and many-body perturbation theory within the G_0W_0 approach. We focus in particular on the question of the electronic band discontinuities at the interface and examine the influence of quantum confinement, molecular polarization, and charge redistribution. For our prototypical system, PPP@ZnO, we find a type-I heterostructure.

The band offsets derived from a G_0W_0 treatment of the interface structure are compared to values derived using simpler mesoscopic methods, like the electron-affinity rule or alignment via the electrostatic potential, revealing that these approaches are insufficient to even qualitatively predict the type of heterostructure of this kind of system.

We also explore the optical excitations of the interface system, compare them to the excitonic properties of the pristine PPP and ZnO, and discuss the methodological implications for the theoretical description of interface electronics.

O 29.5 Tue 11:30 WIL A317

Integer charge transfer induced by insulating layer — •Michael Hollerer[1], Daniel Lüftner[1], Philipp Hurdax[1], Thomas Ules[1], Simon Weiss[2,3], Sergey Soubatch[2,3], Frank Stefan Tautz[2,3], Georg Koller[1], Peter Puschnig[1], Martin Sterrer[1], and Mike Ramsey[1] — [1]Insitute of Physics, University of Graz, NAWI Graz, Universitätsplatz 5, 8010 Graz, Austria — [2]Peter Grünberg Insitut (PGI-3), Forschungszentrum Jülich, 52425, Jülich, Germany — [3]Jülich Achen Research Alliance (JARA), Fundamentals of Future Information Technology, 52425, Jülich, Germany

While it is becoming accepted that charge transfer can occur across thin dielectric films on metal substrates, particularly for organic overlayers, the occupancy of the lowest unoccupied molecular orbital (LUMO), whether fractional or integer, and the distribution of the charged molecules within the layer is under debate. Herein we present a comprehensive analysis of the charge transfer phenomena, facilitated by the strong reduction of the work function, in the model system pentacene on thin MgO(001) on Ag(001). Using scanning tunneling microscopy (STM) and angular resolved photoemission supported by density functional theory we are able to unambiguously deduce integer occupation of all molecules in the monolayer film on MgO(001)/Ag(001) compared to fractional occupation on the bare Ag(100) substrate. Moreover, the energy of the peaks observed in scanning tunneling spectroscopy, above and below the Fermi level, can be directly related to those of the singly occupied and singly unoccupied molecular states.

O 29.6 Tue 11:45 WIL A317

Impact of collective electrostatics on XPS Spectra of organic adsorbate layers — •Thomas C. Taucher, Oliver T. Hofmann, and Egbert Zojer — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

In this contribution we investigate the applicability of slab-type density functional theory-based band structure calculations to quantitatively model XPS core-level shifts at metal-organic interfaces. We compare the performance of the initial state approach (neglecting screening effects) and different variants of the final state approach (inherently considering screening) for the case of self-assembled monolayers of long, upright standing molecules. In particular we here discuss serious artifacts occurring when combining final state approaches with periodic boundary condition based calculations.

Beyond these more technical aspects, we also compare the relative impact of chemical shifts and binding energy shifts caused by collective electrostatic effects. The latter, albeit often overlooked, do play an important role for densely packed adsorbate layers consisting of molecules that bear polar elements.[1] In fact, electrostatic shifts of core-level binding energies pave a way for using XPS as a probe of local changes in the electrostatic energy in a sample.

[1] T. C. Taucher et al., J. Phys. Chem. C., 2016, 120, 6, 3428.

O 29.7 Tue 12:00 WIL A317

Surface-Assisted Diastereoselective Ullmann Coupling of Helicenes — •Christian Wäckerlin[1], Jingyi Li[1], Anaïs Mairena[1], Kévin Martin[2], Narcis Avarvari[2], and Karl-Heinz Ernst[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, 8600 Dübendorf, Switzerland — [2]Laboratoire Moltech Anjou, Université d'Angers, Angers, France

Surfaces functionalized with covalently linked chiral molecules are highly desirable; to name two examples, for stereoselective catalysis or electron spin filtering. However, the way chiral molecules at surfaces interact with each other and assemble is still an open question. Here we report the Ullmann coupling of chiral 2-bromo[4]helicene monomers to helicene dimers on Cu(100). Such dimers can exist as three isomers, the two enantiomers [(P,P) and (M,M)] and the isomer (P,M) which is the diastereomer with respect to the two enantiomers. Using scanning tunneling microscopy (STM), we show that coupling is diastereoselective, i.e. we observe the enantiomers [(P,P) and (M,M)] but not the (P,M)-dimers. Moreover, the (P,P)- and (M,M)-dimers self-assemble and separate into enantiopure domains.

O 29.8 Tue 12:15 WIL A317

NEXAFS study of robust ultrathin Fe(II) spin-crossover films on surfaces — •Sebastian Rohlf[1], Matthias Kalläne[1], Simon Jarausch[1], Benedikt Flöser[2], Felix Tuczek[2], and Kai Rossnagel[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany — [2]Institut für Anorganische Chemie, Universität Kiel, 24098 Kiel, Germany

The spin-state manipulation of Fe(II) coordination complexes by external stimuli is associated with a change in the electronic, magnetic, and structural properties. In particular, the temperature- and light-induced switching mechanisms may be utilized in future spintronic devices. Both of these switching effects were observed even in monolayers adsorbed on the weakly interacting substrate HOPG [1]. Nevertheless, the dissociation of spin-crossover (SCO) molecules in direct contact to a metal surface is still impeding measurements in device-like environments. A novel approach to overcome this limitation is the electronically stabilized SCO system Fe(pyrpy)$_2$(phen), a recently synthesized derivative of the well-studied complex Fe(H$_2$bpz)$_2$(phen). Here, we present near edge X-ray absorption fine structure (NEXAFS) spectroscopy results of Fe(pyrpy)$_2$(phen), adsorbed in thin films on Au(111) and TiTe$_2$, for different temperatures and laser light irradiation conditions. Our results confirm the preservation of the spin-switching ability in thin films of this derivative. Furthermore, the comparison of the measured switching efficiencies on both substrates provides evidence for an intact interface layer in contact to the Au(111) surface. [1] M. Bernien *et al.*, ACS Nano **9**, 8960-8966 (2015).

O 29.9 Tue 12:30 WIL A317

Atomic and Electronic Structure at Metal-Endohedral Fullerene / Metal Interfaces — •Leah Kelly[1], Johannes Seidel[1], Norman Haag[1], Johannes Stöckl[1], Markus Franke[2], Gerben van Straaten[2], Christian Kumpf[2], Benjamin Stadtmüller[1], Mirko Cinchetti[3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

Spin carrying molecules, so called single molecular magnets, are a highly promising class of materials to realize data storage on the nanoscale. Of interest are metal-endohedral fullerenes, with spin centers shielded by a fullerene core.

In this work we studied Sc3:N@C80 on Ag(111). The structural properties were characterized by LEED and NIXSW, the electronic structure by momentum microscopy. In contrast to the gas phase, the N and Sc atoms inside the fullerene cage are vertically displaced due to adsorption of the molecules on the surface. In addition, we find a clear charge redistribution at the metal-organic interface including a transfer into the Sc3:N@C80 LUMO, which has been found to have significant electron density at the metals, yielding a possibility for substrate mediated coupling between spin centers. Our findings provide a basis for studying the cooperative behavior for caged 3 metal spin-systems in contact with a surface.

O 29.10 Tue 12:45 WIL A317

Wavelength sensitivity of the photostationary state of azobenzene-functionalized SAMs — •Wibke Bronsch, Larissa Boie, Cornelius Gahl, and Martin Weinelt — Freie Universität Berlin, Deutschland

Azobenzene is a molecular switch with significantly different static dipole moments in its trans and cis isomer, respectively. Embedded in self-assembled monolayers (SAMs), this property can be used for real-time tuning of the sample work function. A specific work function is hence a measure of a particular photostationary state (PSS) of the SAM. In this contribution we investigate the PSS of azobenzene-functionalized undecane thiol diluted with dodecanethiol on Au(111). Work function variations are monitored by means of two-photon photoelectron spectroscopy. We show that the PSS is very sensitive to the illumination wavelength when tuned across the S$_2$ absorption band of the 2-dimensional molecular aggregate. Due to the interplay of the different absorption cross sections and quantum yields of the two isomers, the PSS changes from mainly trans to mainly cis in the range of 300 to 370 nm.

O 30: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - III

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

Invited Talk O 30.1 Tue 10:30 GER 38

Including spin effects in the strong-coupling limit of DFT — •Paola Gori-Giorgi[1], Juri Grossi[1], Derk Pieter Kooi[1], Klaas Giesbertz[1], Michael Seidl[1], Aron Cohen[2], and Paula Mori-Sanchez[3] — [1]Vrije Universiteit Amsterdam, The Netherlands — [2]University of Cambridge, UK — [3]Universidad Autonoma de Madrid, Spain

The exact strong-coupling limit of density functional theory (DFT) reveals a different mathematical structure with respect to the one of traditional approximations for the exchange-correlation (xc) functional: instead of the local density, local density gradients, or quantities related to the Kohn-Sham orbitals, some integrals of the density appear in this limit. In the recent years, xc functionals directly inspired to this mathematical structure have been constructed and implemented in an efficient way. However, the leading terms (exact or approximate) in the strong-coupling limit of DFT are intrinsically semiclassical and, as such, do not incorporated the spin dependence. In this talk, I will present the first study on the incorporation of the spin-dependence in the exact strong-coupling limit in simple one-dimensional cases. I will then discuss approximations for our findings and routes to the construction of spin-dependent xc functionals for strong coupling. Comparison with exact calculations for the Hohenberg-Kohn functional in the strong-coupling regime confirms the accuracy of our expressions for the leading terms.

O 30.2 Tue 11:00 GER 38

Strong correlation from the Random Phase Approximation and beyond — •Thomas Olsen and Kristian Thygesen — Department of Physics, Technical University of Denmark

We assess the performance of the Random Phase Approximation (RPA) for strongly correlated systems and discuss different routes to venture beyond RPA. It is well-known that RPA reproduces the dissociation curve of molecular H2 correctly and thus accurately captures the strong static correlation inherent in the dissociation limit. It is thus natural to ask whether RPA is able to describe the strongly correlated Mott insulators as well. In particular, the accurate description of anti-ferromagnetic systems is complicated by the fact that the magnetic order often emerges from a detailed interplay between direct exchange and super-exchange couplings, which are respectively exchange and correlation effects. Whereas DFT+U, semi-local and hybrid functionals are often capable of describing either exchange or super-exchange accurately, RPA is shown to give an accurate account of both. We will finally show that RPA can be improved by either including non-local kernel in the framework of TDDFT or including electron-hole interactions in the irreducible response function. Only the latter approach improves the description of strong correlation, whereas the former approach improves atomization energies significantly compared to RPA.

O 30.3 Tue 11:15 GER 38

Surface and adsorption energy calculations within the random phase approximation — •Per Schmidt and Kristian Thygesen — Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The application of density functional theory (DFT) to the calculation of adsorption and surface energies is ever increasing and as a theory, it has the potential to e.g. guide experiments in the search of better catalysts. However, a previous study[1] shows that with standardly used semi-local functionals, DFT is not able to accurately predict surface and adsorption energies simultaneously. By tuning the functional, either the predicted surface or adsorption energies can be improved at the expense of the other. For a few cases however, it has been shown[1] that the many-body approach, the random phase approximation (RPA), yields both excellent surface and adsorption energies.

In this work we expand the use of the RPA method to eight adsorption reactions over 20 transition metal surfaces using the electronic structure code GPAW. We report the difference in surface and adsorption energies compared with the standard DFT functionals: PBE, RPBE and BEEF-vdW. We find that RPA does in general predict less stable surfaces, in better agreement with experiments and the average change in adsorption energies varies between ± 0.5 eV. The RPA values could be used to guide construction of new density-functionals aimed at improving surface science calculations.

[1] L. Schimka, J. Harl, A. Stroppa, A. Grüneis, M. Marsman, F. Mittendorfer, and G. Kresse, Nature Materials 9, 741 (2010).

O 30.4 Tue 11:30 GER 38

Large-scale cubic-scaling RPA correlation energy calculations using a Gaussian basis — •Jan Wilhelm and Jürg Hutter — University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

The random phase approximation (RPA) for computing the electron correlation energy has emerged as an accurate tool for predicting the properties of molecules and condensed phase systems. RPA combines a number of attractive features, most importantly that long-range van der Waals interaction is included, in contrast to semilocal density functionals. The drawback connected with RPA is the computational cost: For canonical implementations of RPA, the numerical effort grows as quickly as $O(N^4)$ with the system size N. We present an algorithm for computing the RPA correlation energy in a Gaussian basis requiring $O(N^3)$ operations and $O(N^2)$ memory. The cubic-scaling RPA method is based on the resolution of the identity (RI) with the overlap metric, a reformulation of RI-RPA in the Gaussian basis and imaginary time as well as the use of sparse linear algebra. We report a massively parallel implementation which is the key for the application to large systems. As first benchmark of the method, we show the RPA correlation energy of thousands of water molecules in a high-quality cc-TZVP basis. For a comparison, the canonical RPA method is restricted to 500 water molecules using the whole Piz Daint supercomputer for two hours. Our RPA algorithm enables the application of RPA to large systems where van der Waals interactions play an important role, e.g. for predicting the adsorption energy of large molecules on surfaces.

O 30.5 Tue 11:45 GER 38

Semi-local exchange functionals showing ultranonlocal response: the hope to replace exact exchange — •Thilo Aschebrock and Stephan Kümmel — Theoretical Physics IV, University of Bayreuth, D-95440 Bayreuth, Germany

The widespread success of Density Functional Theory (DFT) is based on a favorable ratio of accuracy to computional cost, especially with semi-local approximations to the exchange-correlation energy. However, functionals such as the local density approximation (LDA), generalized-gradient approximations (GGA) or meta-generalized-gradient approximations (meta-GGA), typically miss important exact exchange features related to the derivative discontinuity. These are essential for accurately describing long-range charge transfer processes. The electrical response of molecular chains, which is dramatically overestimated by local and semi-local density functionals, is a prime example. The key to its correct description is a term in the Kohn-Sham exchange potential that counteracts the external field and has been named "ultranonlocal". We here present how these field-counteracting properties can be incorporated into semi-local DFT on the meta-GGA level. Thereby we show that by utilizing the kinetic-energy-density, it is possible to model ultranonlocal effects in the Kohn-Sham potential by virtue of a semi-local energy expression.

O 30.6 Tue 12:00 GER 38

(De)stabilizing dispersion interactions via external electric charges — •Andrii Kleshchonok[1] and Alexandre Tkatchenko[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg

Van der Waals (vdW) or dispersion interactions play a central role in the structure, stability, and reaction mechanisms in large variety of molecules and materials. However, in many situations of interest in material science and biophysics, vdW interactions should account for the coupling with external (in)homogeneous electric fields. In this work we address the effect of external static charge field on long-range electron correlations. By using the quantum Drude oscillator model, we derive analytical expressions of the charge induced dipole-quadrupole dispersion energy, that is accounted neither in standard DFT methods, nor in popular vdW correction schemes. Analysing the scaling laws of this dispersion term, we conclude that positive charge stabilizes dispersion interactions, while a negative charge has an opposite effect. Benchmark over S22 molecular dataset estimates the induced dispersion to be in the range of 20-300 % of conventional electrostatic energy. Our findings could have broad potential implications, including exfoliation of 2D materials, chemical reaction rates in charged droplets, and biological membranes.

O 30.7 Tue 12:15 GER 38

An optimisability proof for self-consistent constrained DFT, and its implications for constraint-based self-interaction error correction — Glenn Moynihan[1], Gilberto Teobaldi[2,3], and •David D. O'Regan[1] — [1]School of Physics, CRANN and AMBER, Trinity College Dublin, Ireland. — [2]Stephenson Institute for Renewable Energy and Department of Chemistry, The University of Liverpool, U.K. — [3]Beijing Computational Science Research Center, China.

We develop the connection between constrained DFT energy derivatives and response functions, providing a rigorous assessment of the uniqueness and character of cDFT stationary points while accounting for electronic interactions and screening [1]. In particular, we provide a non-perturbative proof that stable stationary points of linear density constraints occur only at energy maxima with respect to their Lagrange multipliers, generalizing the proof of Ref. [2]. We demonstrate that multiple solutions, hysteresis, and energy discontinuities may occur in cDFT, and we provide necessary conditions for the optimizability of multi-constraint cDFT. We show that the applicability of cDFT in automating symmetry-preserving self-interaction error corrections is limited by a fundamental incompatibility with non-linear constraints. We circumvent this by utilizing separate linear and quadratic correction terms, which may be interpreted either as distinct constraints, each with its own Hubbard U type Lagrange multiplier, or as the components of a generalized, two-parameter DFT+U functional [3]. [1] Phys. Rev. B **94**, 035159 (2016). [2] Phys. Rev. A **72**, 024502 (2005). [3] Phys. Rev. B Rapid Comms., Accepted (2016), arXiv:1608.07320.

O 30.8 Tue 12:30 GER 38

Density-based local hybrid functional for interfaces — •Pedro Borlido[1], Silvana Botti[1], and Miguel Marques[2] — [1]Institu für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743, Jena, Germany — [2]Instiut für Physik, Martin-Luther-Universität Halle Wittenberg, D-06099 Halle, Germany

Hybrid functionals in density functional theory have become the state-of-the-art for the calculation of electronic properties of solids. The key to their performance is how and in which amount a part of Fock exchange is mixed with semi-local exchange-correlation functionals. We propose here a material dependent and local mixing parameter which is a functional of the electron density alone, through an estimator of the local dielectric function inspired by the work done in *Phys. Rev. B* 83, 035119 (2011). This new functional is by construction an approximation of the GW self-energy and it enables therefore calculations of quasiparticle energy levels of comparable quality as GW, but at the reduced cost of a hybrid density functional. In contrast with other recent self-consistent schemes for the mixing parameter, our approach does not require to calculate the dielectric function and leads to a negligible increase of the computation time.

O 30.9 Tue 12:45 GER 38

On the hunt for better functionals in DFT: a new quantum embedding scheme — •Uliana Mordovina[1], Teresa E. Reinhard[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

We propose a new systematic technique to derive functionals for standard density functional theory (DFT) in an ab-initio fashion. This technique origins in the recently developed density-matrix embedding theory (DMET) [1]. DMET is a quantum-in-quantum embedding method, which is based on finding a projection between the high-dimensional wave function of the full system and a lower-dimensional wavefunction living in the active space of the embedded system, which is then solved exactly. In the original DMET scope, the projection is improved via optimization of the reduced one-body density matrix. We replace this optimization by a density inversion, exploiting the one-to-one mapping between electronic density and Kohn-Sham potential.

Not only the DMET scheme is improved by the uniqueness of the density-potential mapping, the proposed density-embedding also allows for finding accurate Kohn-Sham potentials. Moreover, unlike in usual DFT, we can systematically improve the description by increasing the size of the active space.

We show benchmark results of our method for molecules in 1D.

[1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012)

O 31: Oxide and Insulator Surfaces: Structure, Epitaxy and Growth I

Time: Tuesday 10:30–13:00 Location: WIL C107

O 31.1 Tue 10:30 WIL C107

Ultra-thin Germania films on Ru(0001) and Pt(111) studied by Spectromicroscopy — •Alexander Fuhrich[1], Thomas Schmidt[1], Dietrich Menzel[1,2], and Hans-Joachim Freund[1] — [1]Department of Chemical Physics, Fritz-Haber-Institute of the Max-Planck Society, Berlin, Germany — [2]Physik-Department E20, Technische Universität München, Garching, Germany

We studied the growth and structures of ultra-thin GeO_2 films supported on Ru(0001) and Pt(111). Germania is an analogue of Silica and has similar structures. Germanium growths epitaxially on both substrates which allows to determine the thickness of the ultra-thin Germania films. We studied the growth of Germanium in-situ and in real-time by LEEM and LEED. Germanium oxidizes partially already at room temperature on 3O-(2x2)-Ru(0001) and forms small domains. An alternative preparation recipe, where Ge is deposited on the pure (1x1)-Ru(0001) surface at elevated temperatures (540K) and subsequent oxidized in 10^{-6} mbar O_2 at 630K, yield in larger domain size. The morphology and structure of the oxide film will be discussed in dependence of the preparation parameters and the supporting substrate.

O 31.2 Tue 10:45 WIL C107

Ultra-thin films of iron-silicate — •Gina Peschel[1], Alexander Fuhrich[1], Hagen W. Klemm[1], Mauricio Prieto[1], Dietrich Menzel[1,2], Thomas Schmidt[1], and Hans-Joachim Freund[1] — [1]Department of Chemical Physics, Fritz-Haber-Institute of the Max-Planck Society, Berlin, Germany — [2]Physik-Department E20, Technische Universität München, Garching, Germany

Silicates belong to the most widely existing minerals in nature and are thus extensively used in our society. Consisting only of Si and O the system is known as silica. However, some silicon atoms can be substituted by iron in order to prepare a model system for zeolite structures, known for their very high catalytic properties. Preparing ultra-thin films offers the possibility to understand the correlation between structure and reactivity and functionalize these materials even more. This study addresses the growth and structure of ultra-thin iron-silicate films on Ru(0001) using the methods of LEEM, LEED, XPS and XPEEM.

Our studies reveal that on Ru(0001) the formation of iron-silicate is energetically favoured compared to a phase separation of pure iron-oxide and silica domains. XPS results fit well to a model with a silica layer bound to a layer of FeO on top of the Ru(0001) support. Silica orders in form of a ($\sqrt{3}$ x $\sqrt{3}$) R30° regarding the FeO layer, as could be seen in the LEED pattern. Thus silica is well ordered on top of FeO and arranged regarding the Fe atoms.

O 31.3 Tue 11:00 WIL C107

Structure of ultra-thin ZnO films supported on Ag(111) characterized by IR spectroscopy — •Xiaojuan Yu, Alexei Nefedov, Yuemin Wang, and Christof Wöll — Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344, Eggenstein-Leopoldshafen, Germany.

The importance of thin oxide layers on the surface of metals under reaction conditions has already been pointed out in many contexts. The particular interest in ZnO films has recently been reinforced due to the observations of interlayer structural relaxations resulting in depolarized graphitic structures. Here, we report a thorough study of CO absorption on a Zn/Ag alloy single-crystal substrate (Ag/Zn ratio

9:1) subjected to different oxidation procedures using primarily infrared reflection absorption spectroscopy (IRRAS) in conjunction with XPS, LEED and DFT calculations. The evolution of ZnO thin films on Ag(111) is monitored by IRRAS using CO as a probe molecule. The results show a typical CO band at 2160 cm-1 that shifts to 2178 cm-1 with decreasing the coverage. This frequency is slightly lower than those observed for wurtzite ZnO bulk but significantly different from ZnO thin films formed on Cu(111). In the later case, a huge red shift around 70 cm-1 relative to wurtzite ZnO was detected due to strong interactions between ZnO and the supporting metal. Based on the DFT calculations, we propose that the Zn and O atoms are arranged in planar sheets like in the hexagonal boron-nitride prototype structure, in accord to previous results.

O 31.4 Tue 11:15 WIL C107

Well-ordered ultrathin oxides on magnetic substrates: tuning the magnetic properties through atomic scale control of the interface chemistry. — •andrea picone — Dipartimento di Fisica, Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milano, Italy

In the last 20 years, a large body of knowledge has been gained on the preparation and characterization of ultra-thin oxide films on noble and quasi noble metals [1,2]. Oxide/metal inverse model catalysts have been successfully exploited for the study of complex chemical processes occurring on solid surfaces. Despite their extreme importance in the field of spintronics, comparatively much less work has been devoted to the atomic scale investigation of epitaxial oxide films deposited on top of ferromagnetic substrates [3]. Whenever an oxide film is grown on the surface of a ferromagnetic metal, a remarkable structural and chemical modification of the substrate occur. Taking into account these alterations is extremely important, since the magnetic order of the atoms is directly affected by their local chemical environment. By considering the Fe(001) surface as paradigmatic example of ferromagnetic substrate and highly reactive metal, I will show how the chemical composition of the oxide/Fe(001) layered systems can be finely tuned, and how their magnetic properties depend on the interface chemistry.

[1] S. Surnev, A. Fortunelli, F.P. Netzer Chem. Rev. 113, 4314 (2013).

[2] HJ Freund, G. Pacchioni Chem. Soc. Rev. 37, 2224 (2008).

[3] A. Picone et al. Surf. Sci. Rep. 71, 32 (2016).

O 31.5 Tue 11:30 WIL C107

Probing the surface structure of thin TiO$_x$ films on Pt$_3$Ti(111) by IRRAS and XPS — •Ludger Schöttner[1], Marco Moors[2], Fabian Bebensee[1], Xiaojuan Yu[1], Alexei Nefedov[1], Yuemin Wang[1], and Christof Wöll[1] — [1]Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Peter Grünberg Institute, Forschungszentrum Jülich, Wilhelm-Johnen-Straße, 52425 Jülich, Germany

A fundamental understanding of bimetallic catalysts is of great interest because of their important applications in clean energy production. Here we present a thorough study of the structure evolution of TiO$_x$ thin films on Pt$_3$Ti(111) monitored by IRRAS with CO as probing molecule in conjunction with XPS and LEED analysis. The results demonstrate consistently the formation of different oxide phases on Pt$_3$Ti(111) including z'-TiO$_x$, w'-TiO$_x$, z-TiO$_x$ and rect-TiO$_2$, which vary depending on the substrate temperature and the amount of dosed O$_2$. The pure Pt$_3$Ti(111) surface is terminated by Pt atoms as confirmed by the IR band at 2087 cm^{-1} for Pt-bonded on-top CO. During oxidation at elevated temperatures, TiO$_x$ thin film growth was resolved by the observation of an additional CO band at 2100 cm^{-1} in the initial state. For the z'-TiO$_x$ structure, no any CO vibrations are detected, revealing the formation of a closed oxide layer with oxygen termination. The thickness of various TiO$_x$ thin films is estimated by a quantitative XPS analysis. The structure evolution of TiO$_x$ thin films will be discussed in detail based on the elaborate IR and XPS results.

O 31.6 Tue 11:45 WIL C107

Surface Faceting and Reconstruction of Ceria Nanoparticles — •Chengwu Yang[1], Xiaojuan Yu[1], Stefan Heissler[1], Alexei Nefedov[1], Sara Colussi[2], Jordi Llorca[3], Alessandro Trovarelli[2], Yuemin Wang[1], and Christof Wöll[1] — [1]Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany. — [2]Dipartimento Politecnico, Università di Udine, via cotonificio 108 - 33100 Udine, Italy. — [3]Institut de Tècniques Energètiques and Centre for Research in Nanoengineering, Universitat Politècnica de Catalunya, 808028 Barcelona, Spain.

The surface atomic arrangement of metal oxides strongly determines their physical and chemical properties, and the ability to control and optimize structural parameters is of crucial importance for many applications, in particular in heterogeneous catalysis and photocatalysis. While for macroscopic single crystals such structure determinations can be carried out using established methods, for nanoparticles (NPs) this is a challenging task. Here, we report the results of an IR spectroscopic study where CO is used as a probe molecule to determine the structure of surfaces exposed by rod-shaped ceria NPs. After calibrating the CO stretch frequencies using results obtained for different ceria single crystal surfaces we find that the rod-shaped NPs actually restructure and expose {111} nanofacets. This finding has important consequences for understanding the controversial surface chemistry of these catalytically highly active ceria NPs and paves the way for a predictive, rational design of catalytic materials at nanoscale.

O 31.7 Tue 12:00 WIL C107

Surface lattice vibrations of BaO(001) thin film on Pt(001) — •Veronica Goian[1], Florian Schumann[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

In this work, we report the growth of c(2x2) ordered BaO(001) thin films on Pt(001). The thicknesses of the thin films vary from 36 monolayers down to 3 monolayers. The stoichiometry and long range order are analyzed by AES and LEED. According to LEED, BaO thick films start to order near 1075 K. The surface vibrational properties were measured near the surface Brillouin zone center using high-resolution electron energy loss spectroscopy (HREELS). The Fuchs-Kliewer phonon for thick films appears at 390 cm^{-1} and becomes stronger at higher UHV annealing temperatures. A quantitative comparison of the experimental data with the calculated loss function based on dielectric theory reveals an excellent agreement between bulk and BaO thin film phonon properties. Temperature and thickness dependence of HREELS spectra will be discussed.

O 31.8 Tue 12:15 WIL C107

Ordered structures in reduced SrTiO$_3$ on Pd(111) — •Bettina Leibundgut[1], Stefan Förster[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

Ultrathin perovskite films exhibit extraordinary complex structures on Pt(111) in the two-dimensional limit. Upon reduction by UHV annealing, two-dimensional oxide quasicrystal or closely related periodic approximant structures have been reported for BaTiO$_3$ and SrTiO$_3$ on Pt(111) [1-3]. Here we report on the formation of similarly complex structures from SrTiO$_3$ on Pd(111). The films are grown by reactive molecular beam epitaxy from a Nb-doped SrTiO$_3$ single crystal and a Ti rod. For Ti rich growth conditions, a phase separation in TiO$_x$ and SrO occurs upon annealing at 950 K. This is deduced from SPALEED observation of the rectangular phase of reduced TiO$_x$ on Pd(111), which is well-known for Pt(111) [4]. When approaching stoichiometric SrTiO$_3$ films, several large unit cell superstructures are observed, that will be discussed with respect to aperiodic structures. [1] S. Förster K. Meinel, R. Hammer, M. Trautmann, W. Widdra, Nature 502, 215 (2013) [2] S. Förster et al., Phys. Rev. Lett. 117, 095501 (2016) [3] S. Schenk et al., submitted to J. Phys: Condens. Matter [4] F. Sedona et al., J. Phys. Chem. B 7, 697 (2005).

O 31.9 Tue 12:30 WIL C107

DFT study of the stability of thin zirconia films and metastable bulk phases — •Jakub Planer, Wernfried Mayr-Schmölzer, Florian Mittendorfer, and Josef Redinger — Institute of Applied Physics and Center for Computational Materials Science, TU Vienna, Wiedner Hauptstrasse 8-10/134, 1040 Vienna, Austria

Zirconium dioxide (ZrO$_2$) has been intensively studied due to its huge potential in various applications. Bulk ZrO$_2$ and thin films can be used as an electrolyte in solid-oxide fuel cells, an oxygen gas sensor or as a catalyst for methanol synthesis. We used the Vienna Ab-Initio Simulation Package (VASP) to perform DFT calculations comparing the performance of GGA, vdW-DF, hybrid and RPA approaches to investigate the structural stability of the cubic, tetragonal and monoclinic zirconia bulk phases and derived slab configurations. All functionals reproduce the experimentally found order of stability (monoclinic, tetragonal, cubic) and we present two new meta-stable phases. The first one, called meta-monoclinic, is depending on the functional 10-60 meV/f.u. ZrO_2 more stable than the tetragonal phase, but still 50-70 meV less stable than the monoclinic ground state. The second one is structurally similar to anatase titania and is calculated to be 20 meV/f.u. above the monoclinic ground state for GGA and 200 meV/f.u. for vdW-DF functionals. We also present GGA calculations of the stability of thin zirconia films derived from the different bulk phases. We will discuss the dependence of the surface energy and the film stability upon layer thickness.

O 31.10 Tue 12:45 WIL C107

Strain and ordering effects of ultrathin epitaxial ferrite films on $SrTiO_3$(001) — •Jari Rodewald, Tabea Nordmann, Jannis Thien, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück

Ultrathin epitaxial ferrite films as $NiFe_2O_4$ or $CoFe_2O_4$ are in the focus of spintronics since both materials are semiconducting and ferrimagnetic. Thus, they are well-suited to be used as spin filters due to spin dependent tunneling barrier. Here, the homogeneity of the films is essential to form tunneling barriers. Furthermore, the cation ordering on the different sublattices of the inverse spinel structure determines the magnetic properties of the ferrite films which is crucial for the performance as a spin filter. Therefore, the formation of ferrite films has to be carefully controlled if high quality devices are aimed for.

Hence, in this work ultrathin ferrite films of different thicknesses are prepared via reactive molecular beam epitaxy (RMBE) on $SrTiO_3$(001). In order to investigate structural strain and ordering effects in the films, grazing incidence x-ray diffraction (GIXRD) experiments are performed. The chemical composition and structural ordering at the surface are investigated by x-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED), respectively. Magnetic properties are characterized via vibrating sample magnetometry (VSM).

O 32: Focus Session: Charge Transport at Surfaces and Nanostructures with Multi-probe Techniques I

Complex nanostructures on surfaces, e.g graphene nanoribbons, nanorods, atomic wires, or molecules in between junctions, provide a perfect platform to study both fundamental and application driven aspects. Many properties such as a targeted functionality of the nanostructure, instabilities, phase changes, etc. can be addressed and smartly probed by electron transport. 4-tip scanning probe techniques became very popular within the last years and have demonstrated their capability to address important physical and chemical aspects. Compared to conventional, i.e lithographically driven concepts, the 4-tip STM technique can directly contact delicate nanostructures with uttermost precision and variable contact spacings and geometries. Together with the STM, STS, and potentiometry capabilities, an almost complete set of information with respect to the atomic structure, electronic states, and conductivity can be gathered in-situ without the need of elaborative transfers.

Time: Tuesday 10:30–13:00 Location: WIL C307

Invited Talk O 32.1 Tue 10:30 WIL C307

Electrical detection of spin-polarized transport on topological insulator via four-probe spectroscopy — •An-Ping Li[1], Saban Hus[1], Corentin Durand[1], Xiaoguang Zhang[1,2], Giang Nguyen[1], and Yong Chen[3] — [1]Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — [2]University of Florida, Gainesville, FL 32611, USA — [3]Purdue University, West Lafayette, IN 47907, USA

The electrical detection of spin-momentum-locking of topological surface states remains an experimental challenge. The difficulty is twofold. First, there is a lack of a convenient spin-dependent probing technique to measure the spin current. Second, it is hard to separate 2D surface conductivity from often unavoidable and more dominating 3D bulk contributions in transport experiments. Here we present a new method for detection of spin polarized currents in topological insulator, by using a spin-polarized four-probe spectroscopy on the in-situ cleaved Bi2Te2Se surfaces. The variable probe spacing measurements separate the surface 2D and bulk 3D conductions quantitatively, capable of distinguishing the vanishing Ohmic and non-dissipative spin-dependent electrochemical potentials. This method provides an alternative to the transport spectroscopy with lithographically defined contacts and enables us to access the intrinsic spin transport associated with pristine topological surface states. [1] A-P Li et al., Adv. Funct. Mater. 23 (2013), p. 2509. [2] C Durand et al., Nano Lett., 16 (2016), p. 2213. [3] S. Hus et al, to be submitted.

O 32.2 Tue 11:00 WIL C307

Multi-tip STM analysis of freestanding GaAs-NWs in dependence on surface conditioning — •Andreas Nägelein, Matthias Steidl, Peter Kleinschmidt, and Thomas Hannappel — Photovoltaics Group, Institute of Physics, Technische Universität

Nanostructures e.g. III-V nanowires (NW) are promising candidates for optoelectronic applications. The investigated NWs obtain different doping structures and were grown by MOCVD using the VLS (vapor liquid solid) growth mode. In order to investigate these freestanding nanowires electrically, a multi-tip STM (MT-STM) was used. Here, four-point probe measurements are performed non-destructively by contacting three tips at the nanowire and using the substrate as fourth contact. Besides the investigation of doping profiles, a comparison between nanowires prior to, and after, oxidation was carried out. Therefore, after transferring the NW-samples to the MT-STM in UHV, electrical characterization was performed. Subsequently, the samples were stored at ambient atmosphere and resistance profiles were recorded again. The resistance slope in the intrinsic part of the NW increased drastically with oxidation. In contrast to doped NW-parts where the charge carrier transport mainly happens in the center of a NW, a conductive channel does not exist for intrinsic NWs. Besides contamination-induced band bending, the conductivity is also affected by the surface states themselves. Hence, we consider a changed surface conductivity of the intrinsic nanowire segment as a likely explanation of its increased resistance after exposure to ambient atmosphere.

O 32.3 Tue 11:15 WIL C307

Electrical resistance of individual defects at a topological insulator surface — •Felix Lüpke, Markus Eschbach, Tristan Heider, Martin Lanius, Peter Schüffelgen, Daniel Rosenbach, Nils von den Driesch, Vasily Cherepanov, Gregor Mussler, Lukasz Plucinski, Detlev Grützmacher, Claus M. Schneider, and Bert Voigtländer — Peter Grünberg Institute and JARA-FIT, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

We determine the resistance of different kinds of defects at the surface of a $(Bi_{0.53}Sb_{0.47})_2Te_3$ topological insulator thin film by scanning tunneling potentiometry. The largest localized voltage drop we find to be located at domain boundaries in the topological insulator film, with a resistivity about four times higher than that of a step edge. Furthermore, we resolve resistivity dipoles located around voids in the sample surface. The influence of such defects with a typical diameter of 5 nm on the resistance of the topological insulator is analyzed by means of a resistor network model. Here, we show that local changes in the conductivity, e.g. due to the voids in the surface, give rise to a persistent voltage drop across the sample far away from the actual position of the defect.

O 32.4 Tue 11:30 WIL C307

In-situ electro-migration studies on silver(Ag) contacts for nanogap fabrication — •Atasi Chatterjee[1], Ejvind Olsen[1], Frederik Edler[1], Torsten Heidenblut[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Leibniz Universität Hannover,Institut für Festkörperphysik, 30167, Hannover, Germany — [2]Leibniz Universität Hannover, Institut für Werkstoffkunde, 30823, Hannover,Germany

With the aim to create nanometer-spaced silver(Ag) electrodes as testbeds for molecular electronic studies, the process of electro-migration is adopted amongst the different methods available for fabricating atomic contacts. With the help of a 4-tip SEM/STM setup, the lithographically patterned silver (Ag) structures are probed efficiently with an in-situ monitoring of the electro-migration process using the SEM and STM. The step-by-step morphological changes are observed close to the atomic scale, which is an important pre-requisite for the understanding of the phenomena at nanoscale. Temperature dependent and geometry dependent measurements are performed to separate thermal diffusion from electro-migration. All measurements are done using a feedback controlled lab-view program. The well-defined conductance plateaus obtained as a function of time are the characteristic to atomic scale gaps. Tunneling characteristics were analyzed using I-V curves in Fowler-Nordheim representation. In order to better locate these gaps, a focused ion beam (FIB) is used to reduce the cross-section of these wires. With the reduced cross-section, we characterize the gaps of nearly atomic size with an STM and SEM.

Invited Talk O 32.5 Tue 11:45 WIL C307

Probing electron transport with atomic scale precision — •Christian A. Bobisch — Faculty of Physics, Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

To track down the elementary contributions to macroscopic properties such as the electric resistance, nanoscale electron transport measurements are essential. I will discuss that this can be achieved by combining scanning tunneling microscopy (STM) with transport measurements. We use a four probe STM to perform scanning tunneling potentiometry (STP)[1] which gives direct access to the topography and the lateral variations of the electrochemical surface potential μ_{ec} under realistic conditions, i.e. while a lateral current flows along the surface. Thereby, we analyze the spatial variations of μ_{ec} with nm lateral resolution. In particular, we study the interaction of conduction electrons with defect sites, e.g., atomic step edges or grain boundaries.

The two dimensional electron gas system of Si(111)-$\sqrt{3}\times\sqrt{3}$:Ag is a model 2D system, where scattering at step edges and grain boundaries is identified as major contribution to the resistance [2]. Also at the surface of the topological insulator Bi_2Se_3 [3] we find step-like variations of μ_{ec} in the vicinity of defects which is a fingerprint of electron scattering [4]. Here, we evaluate the electric resistivities of individual step edges and grain boundaries.

[1] Appl. Phys. Lett. 48, 514 (1986). [2] Nano Letters 9, 1588 (2009). [3] Rev. Mod. Phys. 82, 3045 (2010). [4] Nature Comm. 7, 11381 (2016).

O 32.6 Tue 12:15 WIL C307

Oxygen adsorption induced tuning of transport in atomic gold chains on vicinal silicion — •Frederik Edler[1], Ilio Miccoli[1], Jan P. Stöckmann[1], Herbert Pfnür[1], Christian Braun[2], Simone Sanna[2], Wolf G. Schmidt[2], and Christoph Tegenkamp[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover — [2]Lehrstuhl für Theoretische Physik, Universität Paderborn, 33098 Paderborn

Adsorption of Au submonolayer on Si(hhk) surfaces results in growth of long-range ordered quasi one dimensional 1D metallic quantum wires. We present a systematic study on the transport properties of these self-assembled chains of gold atoms on vicinal Si(553) and Si(557) surfaces via a multi-tip STM/SEM system in combination with SPALEED. The transport characteristics of these Au/Si(hhk) systems, i.e. conductivity values along and perpendicular to the chains were carefully analyzed during in-situ adsorption of molecular oxygen. In combination with recent DFT calculations, we discuss the transport in terms of the different structural building blocks (Au chains, Si-adatom chain, Si edge) found for the Au/Si(hhk) systems. It will be shown, that the origin for the metallic surface bands along the wires are of different origin. Therefore, while the Si(553)-Au surface turns out to be rather immune against oxidation, the Si(557)-Au surface reveals a strong decrease of the conductance due to complete destruction of the Si-adatom ordering along the chains.

O 32.7 Tue 12:30 WIL C307

Interface Conductivity of Tellurium on Si(111) Investigated by in situ Charge Transport Measurements with a Multi-Tip STM — Felix Lüpke[1], •Sven Just[1], Martin Lanius[1], Gustav Bihlmayer[1], Jiri Dolezal[2], Martina Luysberg[1], Elmar Neumann[1], Vasily Cherepanov[1], Ivan Ostadal[2], Gregor Mussler[1], Detlev Grützmacher[1], and Bert Voigtländer[1] — [1]Peter Grünberg Institut (PGI) and JARA-FIT, Forschungszentrum Jülich — [2]Departement of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University Prague, Czech Republic

A combined experimental and theoretical analysis of the structural and electrical transport properties of a Tellurium layer on Si(111) is presented. The Te forms a Te/Si(111)-(1×1) reconstruction saturating the substrate bonds and forming the template for van der Waals epitaxy, e.g. for the topological insulator Bi_2Te_3 based thin fim growth on Si(111). As DFT calculations propose a high carrier concentration in the Te layer, the interface layer might be highly conductive limiting the applicability of the on-top grown film. For determining the conductivity of the Te interface layer on differently reconstructed Si surfaces directly, in situ distance-dependent four-probe resistance measurements with a multi-tip STM are carried out. In a second part, further four-probe measurements on different material systems are presented, e.g. on semiconductors combined with an N-layer model for describing multiple interface layers arising from an approximation of the space-charge region, and on the weak topological insulator $Bi_{14}Rh_3I_9$ proposed to have one-dimensional edge-channels on the surface.

O 32.8 Tue 12:45 WIL C307

Separating 2D and 3D resistivities using a modified 4-probe method — Snorre Kjeldby, Simon Cooil, and •Justin Wells — Norwegian University of Science and Technology (NTNU), Trondheim, Norway.

4-probe electrical measurements have been in existence for many decades. One of most useful aspects of the 4-probe method is that it is not only possible to find the resistivity of a sample (independently of the contact resistances), but that it is also possible to probe the dimensionality of the sample. In theory, this is straightforward to achieve; by measuring the 4-probe resistance as a function of probe separation. In practice, it is challenging to move all four probes reliable and with sufficient precision over the necessary range. The available instrumentation (usually based on 4 independently driven STM tips) is complex, expensive and often unreliable.

Here, we present an alternative approach. Combining analytical and numerical modelling with scaled experiments, we demonstrate that the dimensionality of the sample resistivity can be directly probed using a modified 4-probe method in which 3 of the probes are kept stationary, and the position of only one probe is changed. This allows 2D and 3D contributions the to resistivity to be easily deconvolved. The required experimental instrumentation is vastly simplified relative to traditional variable spacing 4-probe instruments.

O 33: Nanostructures at Surfaces: Metals, Oxides and Semiconductors I

Time: Tuesday 10:30–13:00 Location: REC/PHY C213

O 33.1 Tue 10:30 REC/PHY C213

Two-color excitation of image potential states and above threshold ionization at gold nanotips — •Thomas Quenzel, Jörg Robin, Jan Vogelsang, Andreas Wöste, Petra Gross, and Christoph Lienau — Institut für Physik, Carl von Ossietzky Universität, 26129 Oldenburg

Metallic nanotapers give access to strong field phenomena at a single solid-state nanostructure [1-3]. Experiments on bulk solid-state systems have established the existence of surface states by two photon photoemission experiments [4]. Here we use femtosecond two-color photoemission from a home-built NOPA to study the excitation and the dynamics of image potential states on a metallic nanotip.

We measure kinetic energy spectra of the photoemitted electrons as a function of delay between the (visible) pump pulse and the (near-infrared) probe pule. Atomic-like above-threshold ionization spectra are observed, which indicate the excitation of long-lived, weakly bound states at the surface of the nanostructure. With the presented work we take a step towards the emission of cold electron pulses as a promising source for ultrafast electron microscopy.

[1]Herink, Nature 483, 190-193 (2012),[2]Krüger, Nature 475, 78 (2011),[3]Piglosiewicz, Nat. Photon. 9, 37 (2014),[4]Höfer, Science 277, 1480 (1997)

O 33.2 Tue 10:45 REC/PHY C213

Effect of Substrate on Plasmonic Signatures of Silver Nanoparticles studied by Photoemission Electron Microscopy — •Kevin Oldenburg, Hannes Hartmann, Karl-Heinz Meiwes-Broer, Sylvia Speller, and Ingo Barke — University of Rostock, Institute of Physics, 18059 Rostock, Germany

The plasmonic response of metal nanostructures not only depends on material, shape and size but also on coupling phenomena to the environment. By optical excitation close to the resonance wavelength, efficient electron emission can be triggered which is accessible using photoemission electron microscopy (PEEM) with spatial, energetic, and angular resolution [1]. Here the electron emission of individual silver nanoparticles in the size range between 5 and 30 nm is measured using fs laser excitation between 355 nm and 460 nm. The data are correlated to geometric properties obtained by atomic force microscopy (AFM). The clusters were produced in the gas phase and soft-landed onto natively oxidized Si(111) and Si(111)-(7x7) to access the role of cluster-surface interaction.

[1] M. Rohmer et al., Phys. Stat. Sol. B 247, 1132 (2010).

O 33.3 Tue 11:00 REC/PHY C213

Multi-photon luminescence of single gold nanoparticles: Exploring the dynamics of plasmons and electron hole pairs — •Frank Wackenhut, Xiao Wang, and Alfred J. Meixner — Eberhard Karls University, Institute of Physical and Theoretical Chemistry, Tübingen, Germany

We utilize non linear excitation to investigate the optical properties of single gold nanoparticles and report on efficient two and three photon luminescence emission based on the excitation of electron hole pairs. Furthermore, we show that the emission of the same gold nanoparticle strongly depends on the excitation conditions and can be controlled by changing the excitation pulse duration from 500 fs to 100 fs. Additionally we are using single gold nanorods with different aspect ratios to investigate the interplay between the particle plasmon and electron hole pairs, which enables us to develop a quantitative model to fully describe the two and three photon luminescence emission of single gold nanoparticles. These findings greatly increase the understanding of the physical processes underlying the luminescence of gold and hence help to increase the usefulness of gold nanoparticles in various application fields, e.g. in material science, bio imaging, microscopy and spectroscopy.

O 33.4 Tue 11:15 REC/PHY C213

Examining small iron clusters by AFM with CO terminated tips — •Sonia Matencio, Ferdinand Huber, Julian Berwanger, Matthias Emmrich, Alfred J. Weymouth, and Franz J. Giessibl — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

Physical properties of metal clusters depend on size and structure. With scanning tunneling microscopy (STM), it is difficult to resolve the adsorption site and number of atoms of a cluster. We use atomic force microscopy (AFM) at low temperature and with a CO terminated tip to study clusters of iron on Cu(111). This technique previously revealed single iron atoms as torii with subatomic features and small clusters (<5 atoms) as connected structures [1]. In this work, we study larger single-layer clusters (10 atoms) and two-layer clusters. Between some atoms of the cluster a repulsive feature is observed. This feature can be laterally manipulated by the tip and provides information about the vertical relaxation of iron atoms [2].

[1] M. Emmrich et al., Science 348, 308 (2015).

[2] S. Polesya, S. Mankovsky and H. Ebert. Unpublished.

O 33.5 Tue 11:30 REC/PHY C213

Ultranarrow Nonlinear Resonances in Hybrid Fiber-Plasmon Cavities — •Qi Ai[1], Domenico Paone[1], Martin Mayer[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCOPE, University of Stuttgart, Germany — [2]Leibniz Institute of Polymer Research Dresden, Department of Physical Chemistry and Polymer Physics, Germany

We demonstrate substantial reduction in the LSPR linewidth of an Au nanorod by depositing it onto the surface of a tapered fiber. When the tapered diameter is reduced to about 1-3 **m, we observe signatures of strong coupling between the LSPR modes and the whispering gallery modes of the tapered fiber. This results in a very narrow hybrid plasmon-fiber resonance of the single Au nanorod, with a much higher quality factor Q (up to 300) when compared with that of an Au nanorod or an uncoated fiber with the same diameter. Meanwhile, the strong coupling leads to a significant enhancement of the peak scattering intensity at plasmon resonance when compared to an uncoupled Au nanorod. Nonlinear optical processes such as second-harmonic generation can therefore be produced from such a simple system with extremely high conversion efficiency, as it should theoretically scale with Q4. Moreover, we observed ultranarrow (linewidth < 10nm) nonlinear resonances in the second harmonic spectrum of this coupled hybrid system.

O 33.6 Tue 11:45 REC/PHY C213

Capability of oxygen related defects in controlling the water wetting properties of metal oxide nanostructure — •Kavita Yadav and J. P. Singh — Department of physics, IIT Delhi, New Delhi-110016, India

The water wetting of metal oxide surfaces is generally governed by the surface topography, surface crystallography and the surface defects. A detailed study suggests that the surface defects are most powerful tool for controlling the water wetting properties on metal oxide nanostructures rapidly and economically. The effect of surface crystallography on water wetting properties of metal oxides was studied using first-principles-based DFT calculations for metal oxide crystallographic planes. On the basis of DFT analysis, we conclude that the water dissociation does not depends on the crystallographic surface planes but depends strongly on the surface stoichiometry. Also, the defects related study further support the DFT results and reveals a truth that the highly oxygen deficient metal oxide nanowires show highly water repellent nature similar to a lotus leaf. By utilizing this idea, we have demonstrated a facile approach for the preparation of metal oxide nanowires with tunable surface wettability. The surface wetting properties can be manipulated reversibly in a controlled manner from a superhydrophilic state to a superhydrophobic state by using hydrogen and oxygen gas annealing treatments. The water resistant properties of the metal oxide nanowires coating is found to be durable and can be applied to a variety of substrates.

O 33.7 Tue 12:00 REC/PHY C213

Ultra small iron nanoparticle superlattice on graphene/iridium(111) — •Konstantin Krausert[1,2], Elin Grånäs[1], Arti Dangwal Pandey[1], Heshmat Noei[1], Dirk Franz[1,2], and Andreas Stierle[1,2] — [1]DESY NanoLab, Notkestraße 85, D-22607 Hamburg — [2]University of Hamburg, D-20355 Hamburg

The physical properties, such as magnetism of ultra small clusters can differ fundamentally from the bulk material and are dominated by their confinement and atomic structure [1, 2]. The arrangement of such nanoparticles in a superlattice not only allows to reach high density and possibly trigger intercluster effects, but it also enables new characterization approaches [2].

Iridium seeded ultra small Fe nanoparticle superlattices were grown on graphene on Ir(111) support [1]. These are studied with various measurement techniques to gain and correlate structural, electronic and magnetic information. The bottom up fabrication is reproducible and gives the oportunity to link different structural characterisation from scanning probe techniques to electron and x-ray diffraction (XRD) measurements. The regular arrangements of the clusters also enables an atomical scale XRD characterisation [2]. Growth on thin film Ir substrates [3] and well defined coverage widens the charaterisation possibilties for ex situ and magnetic measurements. The present findings in the project and an outlook will be given in the talk.

[1] A. T. N'Diaye, et al, New Journal of Physics 11, 103045 (2009) [2] D. Franz, et al, Phys. Rev. B 93, 045426 (2016) [3] A. Dangwal Pandey, et al, J. Appl. Phys. 120, 075304 (2016)

O 33.8 Tue 12:15 REC/PHY C213

Simulation of metal cluster growth on a thin polymer film during sputter deposition — •Jan Willem Abraham[1], Thomas Strunskus[2], Franz Faupel[2], and Michael Bonitz[1] — [1]Institut für Theoretische Physik und Astrophysik, CAU Kiel — [2]Institut für Materialwissenschaft, CAU Kiel

The fabrication of metal-polymer nanocomposites with tailored optoelectronic properties has been a challenge since the early days of nanotechnology. Under typical conditions in plasma-based physical vapor deposition experiments, crucial properties such as composition, size and shape of the nanoparticles evolve in a self-organized process and are hence difficult to obtain in a controlled way. Computer simulations can be helpful to improve the understanding of the relevant processes, but the required length and time scales impose big challenges on all currently available methods. In this work, we present an approach based on Langevin dynamics that allows us to investigate the growth of Au and bi-metallic Ag-Cu clusters on polymer surfaces on experimentally relevant time scales [1]. We show that our results are in good agreement with recent GISAXS experiments that were carried out to study the morphology and optical properties of sputtered gold on a thin polystyrene film in real time [2]. Finally, we demonstrate some approaches to calculate the intensity of scattered X-rays as well as the UV-Vis absorption spectrum for our simulated structures. [1] J. W. Abraham et al., J. Appl. Phys. 119, 185301 (2016). [2] M. Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015).

O 33.9 Tue 12:30 REC/PHY C213

A DFT-based investigation of 3d adatoms and small clusters on Cu(111): magnetism and AFM images — •Svitlana Polesya[1], Sergiy Mankovsky[1], Hubert Ebert[1], and Franz J. Giessibl[2] — [1]LMU München, Dept. Chemie, München, Germany — [2]Inst. Experimentelle Physik, Univ. Regensburg, Germany

Density Functional Theory (DFT) based calculations have been performed in order to investigate the forces on a CO tip in the vicinity of 3d atoms deposited on Cu(111) surface. For this, a full structure relaxation of adatoms and surrounding surface atoms has been taken into account. In the case of an Mn adatom the crucial role of relaxation to stabilize its magnetic state is shown. The effects of local electronic correlations have been investigated via GGA+U calculations. The forces on a CO tip obtained within DFT calculations are discussed in comparison with experimental AFM images. It is found that all magnetic adatoms reveal a three fold symmetry of the lateral AFM-image as observed experimentally for a Fe adatom [1]. The relaxed geometry and magnetic moments distribution have been also calculated for larger Fe clusters (up to 10 atoms). For 10-atom Fe cluster the hexagonal rim shape of the experimental AFM image is obtained. Surprisingly, the force maxima do not fully coincide with the positions of 'hexagon' atoms but are located between these atoms, in full agreement with experiment [2].

[1] M. Emmrich, F. Huber et al., Science **348**, 308 (2015)

[2] S. Matencio, F. Huber, J. Berwanger, M. Emmrich, A. J. Weymouth, F. J. Giessibl. Unpublished.

O 33.10 Tue 12:45 REC/PHY C213

Semiconductor thin films with functionalized crystalline silicon nanoparticles — •Domenikos Chryssikos[1], Francesco Casablanca[1], Willi Aigner[1], Martin Stutzmann[1], Rui N. Pereira[1,2], and Anna Cattani-Scholz[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching bei München, Germany — [2]Department of Physics and Institute for Nanostructures, Nanomodelling and Nanofabrication, University of Aveiro, 3810-193 Aveiro, Portugal

Electronic devices incorporating solution-processable crystalline nanoparticles, in particular thin films of II-VI or IV-VI materials, have been the subject of many studies in recent years. However, up to now, only few works employ elemental semiconductors like silicon nanoparticles (Si-NPs), which are advantageous regarding their abundance and non-toxicity. In this work, we exploit the assembling of thin films of Si-NPs covalently bound to silicon oxide surfaces via alkyldiphosphonic acid molecules. The aim of this investigation is to create a stable immobilization and homogenous distribution of Si-NPs on solid substrates that can also allow for controlling the positioning of the semiconductor nanostructures. The structural and morphological properties of the Si-NP layers have been studied by X-ray photoelectron spectroscopy, contact angle measurements, atomic force microscopy and Raman spectroscopy. Moreover, these novel nanostructures have also been characterized with respect to their electronic properties using electrical conductivity measurements.

O 34: Solid-Liquid Interfaces: Reactions and Electrochemistry - Experiment II

Time: Tuesday 10:30–12:15 Location: HSZ 101

Invited Talk O 34.1 Tue 10:30 HSZ 101

Self-Assembly at the Liquid/Solid Interface: Playing on the Nanoscale and Taming Molecules — •Manfred Buck — University of St Andrews, St Andrews, United Kingdom

The combination of intrinsic atomic precision with structural and functional versatility, and spontaneous assembly on surfaces make organic molecules essential components of a developing toolbox aimed at the routine access to the bottom end of the nanoscale. With options ranging from two-dimensional porous networks of flat lying to densely packed layers of upright standing molecules, thermodynamically and kinetically controlled processes at the liquid-solid interface (including the electrochemical interface) offer a rich playground for surface functionalisation, templating, and patterning on the ultrasmall scale. However, progress on the route to ultimately functional nanostructures will be critically dependent on how well we can control the energy landscape of molecular assemblies. This comprises both static and dynamic aspects and involves the spectrum of intermolecular and molecule-substrate interactions, diffusion processes, and boundary conditions imposed by a highly confined space. Presenting illustrative examples of our work which range from hierarchical assembly based on supramolecular networks to molecular monolayers involving metal-organic coordination, the talk will provide a critical account of achievements and challenges ahead.

O 34.2 Tue 11:00 HSZ 101

Low-frequency conductivity of clay suspensions: Electrokinetic potentials, surface conductance and counterion mobility — •Christian Weber[1], Helge Stanjek[2], and Markus Valtiner[1] — [1]Institut für Physikalische Chemie, TU Freiberg, Leipzigerstrasse 29, 09599 Freiberg — [2]Ton- und Grenzflächenmineralogie, Bunsenstrasse 8, 52072 Aachen

This work presents results on the low-frequency electric conductivity of kaolinite dominated clay suspensions. The theoretical interpretation of conductivity data is guided by the theory of O'Brien & Ward [1] which accounts for the non-spherical particle shape and surface conductance. Essential outcomes of the conductivity experiments are the surface conductance and electrokinetic potential. Alongside with the conductivity experiments the surface charge density of the particles has been measured under similar conditions. A correlation of the surface conductance and the surface charge density allows to estimate tangential counterion mobilities in the Stern layer and a consistency check of the conductivity interpretation.

References

[1] O'Brien R. W. & Ward D. N. (1988) The electrophoresis of a spheroid with a thin double layer. Journal of Colloid and Interface Science, 121(2), 402-413.

O 34.3 Tue 11:15 HSZ 101

Atomic-level electrochemical surface science of TiO_2 rutile (110) — •Matthias Müllner, Jan Balajka, Michael Schmid, Ulrike Diebold, and Stijn Mertens — TU Wien, Institut für Angewandte Physik, Wiedner Hauptstrasse 8-10/134, 1040 Vienna

The rational design of catalysts and other functional materials requires an atomic-level understanding of their structure and of the interface to supporting surfaces.

Here, we present an in situ electrochemical STM study of TiO_2 rutile (110) with atomic resolution. This is achieved using a new wet-chemical cleaning procedure for the substrate and with Pt-Ir tips. If tungsten tips are used, WO_3 is spontaneously formed at the tungsten liquid interface and strongly adsorbs on oxide surfaces below their point of zero charge through an electrostatic mechanism. The tungsten oxide forms 1D oligomers up to a coverage of one monolayer, and can be manipulated and nanopatterned in situ with the scanning probe tip. Under clean conditions, the TiO_2 rutile (110) surface shows a bulk-like, unreconstructed structure, which resembles its appearance in vacuum, even though the surface is probably fully hydroxylated.

O 34.4 Tue 11:30 HSZ 101

Ion Exchange: Reactions of Porphyrins on Oxides and in Liquids — •Ole Lytken[1], Matthias Franke[1], Quratulain Tariq[1], Daniel Wechsler[1], Julia Köbl[1], Norbert Jux[1], Hubertus Marbach[1], Hans-Peter Steinrück[1], Florencia Marchini[2], Federico Williams[2], Tao Wang[3], Cici Wang[3], Qian Xu[3], and Junfa Zhu[3] — [1]Universität Erlangen-Nürnberg — [2]University of Buenos Aires — [3]University of Science and Technology of China

Porphyrins and their analogues are large organic molecules that play significant roles in vivo, e.g. in light harvesting and photosynthesis (chlorophyll) and oxygen transport and storage in the blood cells of mammals (hemoglobin and myoglobin). In recent years the adsorption of porphyrins on metal surfaces has been studied extensively, but, despite the technological importance of oxides, much less work exists on the adsorption of porphyrins on oxide surfaces. Using X-ray photoelectron spectroscopy to study the adsorption and reactions of 5,10,15,20-tetraphenylporphyrin on MgO(100) and TiO2(110) surfaces, the behavior on oxide surfaces is shown to have a lot in common with reactions known from the liquid phase, such as ion exchange and protonation.

O 34.5 Tue 11:45 HSZ 101

Probing surface electrochemical oxidation of gold by non-linear optical vibrational spectroscopy — •Yujin Tong, Felix Gerke, Martin Wolf, and R. Kramer Campen — Fritz-Haber-Institut, Abt. Physikalische Chemie, 14195 Berlin, Germany

Electrochemical water splitting on noble metal surface is an important reaction of both fundamental and application interest. It is well known that the bottleneck of this reaction is the poor kinetics for oxygen generation from water oxidation. In spite of years study, the mechanisms in terms of the roles of the thin oxides film that formed on the metal surface before/during oxygen evolution are still inexplicit. One of the main reasons is the lack of molecular level information about the oxide thin film structures. In this study, we investigated the electrochemical oxidation of gold in solutions with different pH by employing surface specific vibrational sum frequency spectroscopy (VSFS). By analyzing the potential dependent behaviors of different types of adsorbed species, we could gain molecular level information regarding the structures and formation mechanisms of gold-oxides. The results of this study will provide essential data toward understanding the oxygen evolution mechanism and may suggest strategies for developing better water splitting catalysts.

O 34.6 Tue 12:00 HSZ 101

Stability of metallo-porphyrin networks under oxygen reduction and evolution conditions in basic media — •D. Hötger[1], C. Morchutt[1], M. Etzkorn[1], J. Dreiser[2], S. Stepanow[3], D. Grumelli[4], R. Gutzler[1], and K. Kern[1,5] — [1]MPI for Solid State Research, D-70569 Stuttgart — [2]SLS, PSI, CH-5232 Villigen — [3]ETH Zürich, CH-8092 Zürich — [4]CONICET, ARG-1900 La Plata — [5]EPFL, CH-1015 Lausanne

Oxygen reduction and evolution reaction (ORR and OER) are two relevant reactions in important devices like fuel cells, electrolysers and metal-air batteries. The catalytic stability of a catalyst is commonly well explored, but little focus is given to the structural integrity of molecule-based catalysts. We study iron-tetrapyridyl porphyrines (FeTPyP) co-deposited with Co on Au(111). The bimetallic network is bifunctionally active for OER and ORR.[1]

FeTPyP-Co is characterized before and after electrocatalysis by scanning tunneling microscopy (STM) to explore the geometric structure of the molecules on the Au(111) surface. STM shows that the molecules remain intact after ORR but decompose during OER. X-ray absorption spectroscopy (XAS) yields insight into the electronic structure of the metal centers. XAS confirms the integrity of TPyP after ORR. In contrast, after OER XAS reveals the presence of Co and Fe oxide on the surface in absence of TPyP. Thus, OER conditions are more aggressive on organic molecules than ORR. This finding is of great importance for the design of molecule-based electrocatalysts.

[1] B. Wurster, *et al.*; J. Am. Chem. Soc.; **2016**, 138, 3623-3626.

O 35: Solid-Liquid Interfaces: Reactions and Electrochemistry - Theory I

Time: Tuesday 12:15–13:15 Location: HSZ 101

O 35.1 Tue 12:15 HSZ 101

Towards a generally applicable parametrization protocol for first-principles implicit solvation approaches based on the Poisson-Boltzmann method — •Stefan Ringe, Harald Oberhofer, and Karsten Reuter — TU Munich, Garching, Germany

Implicit solvation models are a standard means for efficient first-principles descriptions of solvated systems. Poisson-Boltzmann (PB) methods in particular even provide a mean-field account of ionic effects in electrolytes, which are known to crucially impact chemical stability, geometries or dissociation constants. Although PB methods have been extensively applied, generally applicable parametrization procotols are lacking so far. Recently, we have implemented PB solvation functionality into the full-potential density-functional theory package FHI-aims [1]. Here we argue that experimentally measured Setschenow coefficients, which probe the stability change of solutes with varying ionic strength, offer an intriguing route to determine the ionic parameters entering the PB approach. With a slight modification of the original PB model in terms of a Stern or ion exclusion layer, parameterized as a function of the solute's electron density, we achieve generally good agreement with experimental data for different alkali halide aqueous solutions.

[1] Ringe, S., Oberhofer, H., Hille, C., Matera, S., Reuter, K., *J. Chem. Theory Comput.*, **2016**, *12* (8), pp 4052–4066.

O 35.2 Tue 12:30 HSZ 101

Quantum Chemistry of the Oxygen Evolution Reaction on Transition Metal Oxides — •Craig Plaisance[1], Rutger van Santen[2], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Technische Universiteit Eindhoven, The Netherlands

Density functional theory (DFT) is used to examine the changes in electronic structure that occur during the oxygen evolution reaction (OER) on a model oxide catalyst containing different 3d transition metal cations (Cr, Mn, Fe, Co, Ni). Active sites identified in previous work [1] consisting of both one and two redox-active metal centers were examined. For all sites, the important water addition step was determined to occur by the transfer of two holes from the metal cation(s) to the O-O antibonding orbital of the resulting hydroperoxo. Of the sites examined, Fe was found to have the most efficient single-center site while Co was found to have the most efficient dual-center site. In line with our previous work on Co oxide [2], the activity of an active site is seen to be related to the energy required to localize holes on the oxygen species participating in the reaction, calculated with a constrained-orbital DFT method we have developed. The hole-localization process is further analyzed in terms of screening and changes in metal-oxygen hybridization to identify how the unique electronic structures of Fe and Co lead to their superior performance for the OER.

[1] Plaisance, C.P., van Santen, R.A., J. Am. Chem. Soc. 2015, 137, 14660-72. [2] Plaisance, C.P., Reuter, K., van Santen, R.A.; Faraday Discuss. 2016, 188, 199-226.

O 35.3 Tue 12:45 HSZ 101

Metallic nanoparticles under realistic electrochemical conditions — •Nicolas G. Hörmann, Oliviero Andreussi, and Nicola Marzari — Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), EPFL, CH-1015 Lausanne, Switzerland

We present a study of the stability and equilibrium shape of metallic nanoparticles in electrochemical environments based on periodic density functional theory (DFT) calculations. Metallic surfaces in water are modelled within the self-consistent continuum solvation scheme (SCCS) [2] as recently implemented in the ENVIRON module of Quantum-ESPRESSO [3]. We analyse in detail the effect of the dielectric environment and different adsorbates on surface structure, energetics and potential. The effects of applied potential are treated by studying appropriately charged systems, with explicit countercharge layers in the solution to mimic the effects of the electrical double layer [4]. We will also discuss the difference between this approach and the widely applied “computational hydrogen electrode”[5] with respect to surface termination and adsorbate species. Our results shed light on how to apply ab-initio thermodynamics in electrochemical environments.

[1] A. Jain et al., *APL Materials* **1**, 011002 (2013); [2] O. Andreussi, et al., *J. Chem. Phys.* **136**, 064102 (2012); [3] P. Giannozzi, et al., *J. Phys.: Condens. Matter* **21**, 395502 (2009); [4] N. Bonnet, et al., *Phys. Rev. Lett.* **110** 086104 (2013); [5] J. K. Norskov, et al., *J. Phys. Chem. B* **108** 17886 (2004);

O 35.4 Tue 13:00 HSZ 101

Insights into the mechanism of photocatalytic water splitting on rutile (110) from quantum dynamical calculations — •Thorben Petersen and Thorsten Klüner — Carl von Ossietzky Universität, Oldenburg, Germany

In order to understand the elementary steps involved in photochemical reactions, quantum dynamical calculations are an exceptional tool to acquire a detailed insight into reaction paths on a femtosecond time scale including quantum effects like tunneling as well. Using this approach we want to study the photodissociation mechanism of water on an ideal rutile (110) surface.

Based on previously generated potential energy surfaces [1], the dissociation mechanism will be investigated including the five most relevant degrees of freedom. Regarding the photocatalytic properties of titanium dioxide, a cationic H_2O-adsorbate as a result of a hole attack of the surface has been assumed for the excited state.

By propagating a wave packet representing the adsorbate on the excited state potential energy surface, we obtain dissociation probabilities in dependence of the movement of the resulting OH-group. For a fixed OH-group no complete dissociation occurs [2]. However, by allowing its movement, the potential barrier for a complete dissociation process can be overcome.

[1] J. Mitschker, T. Klüner, Phys. Chem. Chem. Phys. 2015, 17, 268

[2] J. Mitschker, T. Klüner, J. Theor. Comput. Chem. 2016, 15, 1650013

O 36: ELI-ALPS: A New European Light Source for Ultrafast Surface Science

Time: Tuesday 14:00–16:00 Location: TRE Phy

Invited Talk O 36.1 Tue 14:00 TRE Phy

Attosecond control of excited electrons and nuclei in gas- and condensed-phase systems — •Thomas Pfeifer — MPI für Kernphysik, Heidelberg

The physics of (visible) matter is mainly determined by electrons bound to nuclei. Electrons also represent the atomic glue to connect atoms in molecules and clusters and finally form nanoparticles and solids. Dynamics occurs when electrons are, sometimes only for very short times, elevated to excited states, in which they are particularly responsive to small changes in their environment that can influence the product of a chemical reactions or result in a particular phase transition.

Here, we discuss the effect of intense laser fields on the excited states of atoms, molecules, and condensed-phase systems. A universal change of the quantum-mechanical phase evolution (not to be confused with a phase transition) is observed and can be extracted from a broad coherent spectrum of a pulse with a lifetime much shorter than the (atto-, femto-, ..., nanosecond) lifetime of the excited state.

This phenomenon gives rise to a multitude of scientific opportunities, ranging from laser control of few- to many-electron systems, x-ray-frequency combs and (nuclear) precision spectroscopy to observing and understanding the emergence of fundamental quantum processes by time-resolving their spectrum, exemplarily shown here for the buildup of a Fano resonance.

Invited Talk O 36.2 Tue 14:30 TRE Phy

Probing ultrafast electron and spin dynamics in momentum, space, and time - chances and opportunities of a surface science end station at ELI-ALPS — •Stefan Mathias — I. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen

Recent progress in the development of coherent ultrashort laser-based light sources in the extreme ultraviolet regime has paved the way for a completely new generation of real-time photoemission spectroscopy and microscopy techniques. Moreover, when these lightsources are combined with novel spin detectors, ”complete” photoemission experiments can be realized, with full access to the spin-resolved transient band-structure dynamics on the (sub-)femtosecond time scale. In my talk, I will discuss our latest experiments using such novel spin detectors in combination with extreme ultraviolet pulses from high-harmonic generation. From these experiments, it can be extrapolated what might be possible with a dedicated surface science end station at the novel ELI-ALPS facility in coming years.

References:

T. Rohwer et al., Nature 471, 490-493 (2011)

M. Plötzing et al., Rev. Sci. Instrum. 87, 043903 (2016)

S. Mathias et al., Nature Comm. 7, 12902 (2016)

Invited Talk O 36.3 Tue 15:00 TRE Phy

Attosecond electron dynamics on surfaces and layered systems — •Reinhard Kienberger — Fakultät für Physik, TU München, James Franck Straße, 85748 Garching

Attosecond stereaking experiments have been used for a systematic investigation of electron emission times from solids at different excitation photon energies (90 * 145 eV). Different crystal orientations will be disussed. Also, results from time-resolved transport of different types of electrons through defined adlayers on a bulk material on the attosecond timescale will be shown.

Invited Talk O 36.4 Tue 15:30 TRE Phy

Coinicdence ARPES on molecules — •Reinhard Doerner — University Frankfurt

We will show that measuring coincidences between several electrons and ions emitted by photoabsorption is a rich source of information on electron correlation and entanglement. The talk will present experiment on atoms and molecules in the gas phase.

O 37: Plasmonics and Nanooptics V: Light-Matter Interaction

Time: Tuesday 14:00–16:00 Location: TRE Ma

O 37.1 Tue 14:00 TRE Ma

Scanning near-field optical microscopy with inline-homodyne detection — •Jens Brauer, Jinxin Zhan, Petra Gross, and Christoph Lienau — Carl von Ossietzky University, Oldenburg, Germany

Apertureless near-field optical microscopy is a good choice when it comes to optically investigating nanostructures with a size of only a few nanometer and is nowadays widely used in different geometries.

For most of the setups there remains the challenge of distinguishing the desired near-field signal from the very large optical background. To overcome this problem the tip-sample distance often is modulated at some tens of kilohertz and the detection signal is demodulated at higher harmonics. As Knoll & Keilmann [1] have shown theoretically the ratio of near-field to optical background improves with increasing demodulation frequency. However, also the signal amplitude at higher harmonics is decreasing dramatically. Therefore the use of interferometers, either in a homodyne or heterodyne detection scheme, is often used to amplify the near-field signal [2].

As a downside the contrast in the SNOM images critically depends on the stability of the interferometer. Here we present how to disentangle near field from background radiation in the 1st to 4th harmonic signal by measuring approach curves in an inherently stable in-line homodyne detection scheme and we give an outlook to ongoing spectroscopically resolved SNOM measurements.

[1] B. Knoll & F.Keilmann, Optics Communications, 182(4) (2000)

[2] Ocelic et al.,Applied Physics Letters, 89(10) (2006)

O 37.2 Tue 14:15 TRE Ma

Vectorial near-field coupling on the nano scale — •M. Esmann, S.F. Becker, J. Witt, G. Wittstock, R. Vogelgesang, and C. Lienau — Carl von Ossietzky Universität, 26111 Oldenburg, Germany

Dipole-dipole coupling is ubiquitous in nanoscale systems [1,2] leading to optical modes and coherent dynamics which sensitively depend on dipole configuration. To simultaneously study such systems on 5nm length scales and over a wide spectral range, we implemented a novel type of Scanning Near-Field Optical Microscope (SNOM): Grating-coupled Surface Plasmon Polaritions (SPPs) are adiabatically nanofocused [3] at the 10nm sized apex of a metallic nanotaper resulting in a bright, spatially isolated and spectrally broad nano light source, which acts as a probe for background-free near-field spectroscopy.

Here, we apply this technique to a prototypical system formed by dipolar coupling of the nanotaper apex to small 10×40nm gold nanorods. Upon systematic variation of coupling strength we find clear signatures of coupling-induced spectral shifts and broadening of plasmonic resonances with dramatic variations on few-nanometer length scales. We argue that our approach presents a fundamentally new way to interrogate dipole-dipole coupling in nanosystems in the spatial-, spectral- and temporal domain providing full access to coupling energies, mode profiles and the associated coherent dynamics.

[1] Zhang, Y. et al., Nature 531, 623 (2016). [2] Scholes, G.D., et al., Nature Chemistry 3, 763 (2011). [3] Stockman, M.I., PRL 93, 137404 (2004). [4] Esmann, M. et al., BJNANO 4, 603 (2013). [5] Becker, S.F. et al., ACS Photonics 3, 223 (2016).

O 37.3 Tue 14:30 TRE Ma

Modulation of extraordinary optical transmission through nanohole arrays using ultrashort laser pulses — Kellie Pearce[1,2], Benjamin Duschner[1], Robin Dehde[1], Florian Richter[1], and •Ulf Kleineberg[1,2] — [1]Ludwig-Maximilians-Universität München, Am Coulombwall 1, 85748 Garching, Germany — [2]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

We perform pump-probe measurements of the transmission through subwavelength hole arrays in a gold film on ITO using 16-fs laser pulses. By tuning the delay between the pulses, we can modify the contribution from different transmission resonances, and observe plasmon dephasing and decay. Simulations using a 3D FDTD solver show that the modulation of the transmission is due to the change in the intensity and distribution of fields on both interfaces.

O 37.4 Tue 14:45 TRE Ma

Non-linear imaging of individual plasmonic nanostructures using phase-shaped femtosecond laser pulses — •Veit Giegold, Richard Ciesielski, Alexander Biewald, Tobia Mancabelli, Alberto Comin, and Achim Hartschuh — Department Chemie and CeNS, LMU Munich, 81377 Munich

We studied the second harmonic (SH) and near-degenerate four-wave (FWM) mixing response of individual plasmonic nanostructures using a confocal femtosecond pulse shaping setup. We find that the two different signals are maximized for different spectral phases of the laser pulse. We attribute this to different phase terms in the second- and third-order susceptibility of the nanostructures, respectively. We show that by using optimized phase profiles, the contrast of confocal SH and FWM images can be manipulated. This phase-enhanced nonlinear imaging can provide further insight into properties of plasmonic nanostructures.

O 37.5 Tue 15:00 TRE Ma

Modeling of higher harmonic generation with the Fourier modal method using adaptive coordinates — •Josselin Defrance, Martin Schäferling, Maxim L. Nesterov, and Thomas Weiss — 4th Physics Institute and Research Centers SCoPE, University of Stuttgart, Germany

Metallic nano-structures can concentrate light into sub-wavelength volumes resulting in strong nonlinear responses. The influence of the geometry of such nano-systems, however, is not fully understood. Modeling these effects will not only help to optimize the nonlinear response of plasmonic nano-structures, but will also provide a better understanding of these phenomena. Nowadays, different numerical methods to model the interaction of electromagnetic fields with matter exist. The so-called Fourier modal method offers a fast and highly accurate calculation of far-field responses.

It has been shown that the Fourier modal method can be extended in order to calculate the generation of higher harmonics [1]. We have combined this method with adaptive spatial resolution and adaptive coordinates [2], thus providing an efficient and accurate numerical method for the precise analysis of the nonlinear optical responses of complex plasmonic geometries.

[1] T. Paul et al., J. Opt. Soc. B, Vol. 27, Issue. 5, pp. 1118 (2010).

[2] T. Weiss et al., Opt. Express 17, 8051 (2009).

O 37.6 Tue 15:15 TRE Ma

Tracking Plasmon Propagation by Terahertz-Streaking at Metal Nanotips — •Lara Wimmer, Benjamin Schröder, Murat Sivis, Georg Herink, and Claus Ropers — IV. Physical Institute - Solids and Nanostructures, University of Göttingen, Germany

We resolve the propagation time of surface plasmon polaritons (SPP) traveling along the shaft of gold nanotips [1] employing Terahertz (THz) near-field streaking spectroscopy [2, 3]. Surface plasmon polaritons are launched by femtosecond near-infrared (NIR) pulses in a grating coupler at the shaft of the nanostructure, 50 *m from the tip end. At the apex, the nanofocused SPPs induce the (multiphoton) emission of photoelectrons [1], which are streaked in the locally enhanced near-field of a THz transient incident on the tip. Reference spectrograms are obtained by direct NIR-excitation of the apex. The observed temporal shift between both streaking spectrograms provides a direct measure of the group delay [4] in SPP propagation from the grating to the tip apex.

[1] Schröder et al., Phys. Rev. B 92, 085411 (2015).

[2] Wimmer et al., Nature Physics 10, 432-436 (2014).

[3] Herink et al., New Journal of Physics 16, 123005 (2014).

[4] Kravtsov et al., Opt. Lett. 38, 1322-1324 (2013)

O 37.7 Tue 15:30 TRE Ma

Relaxation dynamics of plasmonic hot-carriers in gold nanoparticles — •Emanuele Minutella[1,2], Florian Schulz[1], and Holger Lange[1,2] — [1]Physikalische Chemie, Universität Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, CUI

Using light to drive or control chemical or physical processes is a very interesting field of research. One problem is to guide the light's energy to the specific place where reaction takes place. Due to their plasmonic properties noble metal nanoparticles have the ability to collect very efficiency photons and convert them into hot-electron-hole-pairs. As a result of size and photon energy dependent transient absorption measurements we found a binary kinetic for the relaxation times of the hot electrons. Depending on the photon energy either interband or intraband excitations are possible. We found faster decay rates for the intraband relaxation than for the interband. These results can help to improve possible hot-carrier devices.

O 37.8 Tue 15:45 TRE Ma

Coherent phase-resolved near-field spectroscopy of single gold nanorods enabled by self-interference in an ultrasharp gold taper — Martin Esmann, Simon F. Becker, •Abbas Chimeh, Ralf Vogelgesang, and Christoph Lienau — University of Oldenburg

Plasmonic nanofocusing of light on an ultrasharp gold taper enables spectroscopic analysis of optical near-fields around individual metallic nanoparticles [1]. In order to characterize the ultrafast time-dynamics of these near-fields, the scheme should be extended to include the measurement of phase-resolved spectra. To this end, a stable inline interferometer is implemented in such a taper and plasmonic-nanofocusing spectroscopy is combined with spectral interferometry. In this method, surface plasmon polaritons are launched by a coupler on a pyramidal metallic taper and propagate towards the taper apex where they form a confined nanometer-scale light source [1]. After optical interaction with a sample, a part of the incident field is reflected backwards to the taper and interferes with the incident field on it. The interference signal is then collected from a scatterer on the shaft and spectrally resolved. Here, we implemented this method for the first time and use it to record local broadband optical spectra of single gold nanorod with 10x40 nm dimensions. We demonstrate phase-coherent mapping of optical near-field with sub-10 nanometer spatial resolution and provide a detailed analysis how near-field spectra are generated in this novel and highly sensitive interferometric measurement scheme.

[1] S. Schmidt et al., ACS Nano 6, 6040 (2012).

O 38: Organic-Inorganic Hybrid Systems and Organic Films V

Time: Tuesday 14:00–16:00 Location: WIL A317

Invited Talk O 38.1 Tue 14:00 WIL A317

Tuning excitonic excitations in molecular layers — •Martin Weinelt and Cornelius Gahl — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Excitons constitute the fundamental optical excitations in organic materials. Here intermolecular interactions lead to delocalization and transport of excitons and thereby influence the response of the molecular film. We will discuss two examples where excitonic excitations play an important role.

In azobenzene-alkanethiolate self-assembled monolayers quenching of the optical excitation by the supporting gold substrate is avoided by decoupling the azobenzene chromophore via an alkane linker. However, intermolecular coupling in the SAM strongly shifts and broadens the absorption bands. One strategy to reestablish efficient photoisomerization is to introduce additional molecules as lateral spacers. As a consequence the excitonic coupling of the chromophores can be tuned between single molecules and aggregates, which strongly influences optical switching.

Sexithiophene/gold is a model system for an organic semiconductor/metal - interface. Here we investigated the exciton dynamics by time-resolved two-photon photoemission spectroscopy. We show that resonant excitation and vibrational dissipation of excess energy both lead to exciton population on an ultrafast time scale resulting in a long lived final state. Again the morphology of the organic layer (crystalline vs amorphous) strongly influences the excited state dynamics and energetics relevant for organic electronics.

O 38.2 Tue 14:30 WIL A317

Probing complex adsorbate systems using Angle-Resolved NIXSW — •Gerben van Straaten, Markus Franke, and Christian Kumpf — Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich and Jülich Aachen Research Alliance (JARA) – Fundamentals of Future Information Technology (FIT), 52425 Jülich, Germany

The Normal Incidence X-ray Standing Waves (NIXSW) technique is a popular and very efficient technique for studying adsorbate structures, but unfortunately, it is only of limited use when adsorbate atoms display a range of adsorption heights. In this presentation we show that angle-resolved NIXSW measurements can take advantage of the limited mean-free path of photoelectrons and that more information about the adsorbate distribution can be obtained. This can be used to study vertical disorder in monolayer structures.

O 38.3 Tue 14:45 WIL A317

Multiscale Modeling of Ion-Sensitive Sensor Devices — •Jörg Buchwald, Rafael Gutiérrez Laliga, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials Dresden University of Technology, 01069 Dresden, Germany

An ion-sensitive field effect transistor (ISFET) can be considered as a FET in which the gate is in contact with an ionic solution and covered by a self-assambled monolayer of biomolecules that are able to bind to these specific ions. The number of bound ions is thereby assumed to be a function of ion concentration and determines the gate potential and current of the FET.

We present a continuum model that treats both parts separately. The source-drain current is determined via a drift-diffusion model of the the semiconductor parts under given source-drain voltage and gate potential. Whereas the gate potential can be calculated from a Poisson-Nernst-Planck model of the ionic solution in which the biomolecules are acting as sources/sinks of the mobile ion concentrations.

Additionally one has to consider binding kinetics, conformal changes of the biomolecule and charge transfer from the biomolecule to the surface acting as an aggregated static charge. Both information can be obtained via atomistic/ab-initio methods.

O 38.4 Tue 15:00 WIL A317

Adsorbate-induced restructuring of crystalline and amorphous ZnO surfaces upon formation of phosphonic acid self-assembled monolayers — •Tobias Klöffel[1], Hannah Schlott[1], Alexandra Ostapenko[2], Gregor Witte[2], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Fachbereich Physik, Philipps-Universität Marburg

Among the inorganic oxides, ZnO is of special interest for hybrid organic–inorganic interfaces in molecular electronics due to its high charge carrier mobility. Phenyl phosphonic acids (PPAs) are commonly used linker groups and functional organic units for creating such interfaces. Recent experiments and DFT calculations showed, however, that self-assembled PPA monolayers are only metastable and etch the ZnO substrate [1,2].

DFT calculations were performed to explore systematically the possible PPA monolayer structures on crystalline and amorphous ZnO model surfaces. In addition to regular PPA adsorbate structures on unmodified substrates we find that the PPA molecules can induce strong structural changes in the ZnO surfaces. Configurations with additional Zn and O ions between PPA molecules show a similar thermodynamic stability, which might be the origin of the observed structural instability of the PPA monolayers.

[1] A. Ostapenko, et al., *ACS Appl. Mater. Interfaces* **8**, 13472 (2016).
[2] A. Ostapenko, et al., *Langmuir* **32**, 5029 (2016).

O 38.5 Tue 15:15 WIL A317

Understanding the planarization of shuttle-cock shaped subphthalocyanine molecule on Cu(111) surface — •Shashank S. Harivyasi[1], Oliver T. Hofmann[1], Nahid Ilyas[2], Oliver L.A. Monti[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — [2]University of Arizona, Tucson, Department of Chemistry & Biochemistry, 1306 E. University Blvd., Tucson, AZ 85721, USA

The structure of an organic semiconductor plays a determining role in its adsorption on a metal surface. Large planar molecules like planar phthalocyanines, pentacene and PTCDA typically lie completely flat on most metal surfaces. The situation becomes more complex in case of non-planar molecules. They generally show a tendency to planarize upon adsorption but the extent of this planarization varies from negligible to almost complete for various metal-molecule combinations.

Here, we try to understand the reasons for this planarization by studying an extreme example exhibiting almost complete planarization: adsorption of shuttle-cock shaped Chloroboron subphthalocyanine on Cu (111). Using DFT, we study the steps of the adsorption process by gradually increasing the van der Waals interaction between the adsorbate and the substrate and following the evolution of the molecule's electronic and geometrical structure. We identify the bonding of the molecule as a two-stage process involving Fermi-level pinning followed by a rehybridization of the molecule's frontier orbitals. Especially the observed evolution of charge rearrangements help us to explain why we see an almost complete planarization.

O 38.6 Tue 15:30 WIL A317

Electronic and optical excitations at the pyridine@ZnO hybrid interface — •Olga Turkina, Dmitrii Nabok, Andris Gulans, Caterina Cocchi, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Insight from *ab initio* theory is essential in order to gain an understanding of opto-electronic properties of organic-inorganic hybrid materials, such as the correct level alignment and the creation of hybrid excitons. We investigate a prototypical system composed of a pyridine molecule that is chemisorbed on a non-polar ZnO(10-10) surface. We employ all-electron density-functional theory in combination with many-body perturbation theory (G_0W_0/BSE). The G_0W_0 approximation describing one-particle excitations is used to determine the electronic structure, while the Bethe-Salpeter equation describing two-particle excitations is solved to obtain the absorption spectrum. We reveal the nature of the optical excitations at the interface by analysing the character of the involved transitions and visualizing the exciton wave-function. Thus, we find evidence of excitons exhibiting different character across different spectral regions. The onset of the spectrum is dominated by bright and strongly bound hybrid and ZnO character excitons. In particular, the first strongly bound and most intense exciton at 1.8 eV is of hybrid nature. In the visible region, we find predominantly low intensity hybrid excitons, whereas in the UV region, we find dark excitons exhibiting charge-transfer character, with the corresponding electron and the hole delocalized on either ZnO or pyridine.

O 38.7 Tue 15:45 WIL A317

Interaction of an Ionic Liquid Adlayer with $Li_4Ti_5O_{12}$ and Influence of Pre- and Post-deposited Lithium - A Model Study of the Electrode|Electrolyte Interface — •Jihyun Kim[1], 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-89081 Ulm, Germany

Well-defined spinel lithium-titanium-oxide, $Li_4Ti_5O_{12}$ (111), which is a promising anode material for a lithium-ion batteries, was generated by a solid state reaction (LiOH + TiO_2 (111)) and its crystallinity and stoichiometry were confirmed by X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS), respectively. To mimic the electrode|electrolyte interface (EEI) (crucial for the battery performance), we vapor deposited a monolayer of the battery-relevant ionic liquid (solvent/electrolyte) 1-butyl-1-methyl-pyrrolidinium bis(tri-fluoromethyl-sulfonyl)amide ([BMP][TFSA]) on $Li_4Ti_5O_{12}$ (111) at 300 K. XPS reveals that [BMP][TFSA] is partially decomposed, forming products such as LiF, Li_xS, Li_xSO, SO_x and LiN_3. Post-deposition of 1 ML of Li on a ([BMP][TFSA]) adlayer at 300 K increases the amount of decomposition products in the adlayer. After pre-deposition of 1 ML of Li on pristine $Li_4Ti_5O_{12}$ (111) at 300 K, XP spectra reveal that lithium diffuses (intercalates) into the bulk, most likely forming a Li-rich $Li_xTi_5O_{12}$ ($4<x<7$) phase. Future work will concentrate on the interaction of [BMP][TFSA] with both the Li-poor ($Li_4Ti_5O_{12}$) and the Li-rich ($Li_xTi_5O_{12}$) phases in different temperature ranges.

O 39: Oxide and Insulator Surfaces: Structure, Epitaxy and Growth II

Time: Tuesday 14:00–16:00 Location: WIL C107

O 39.1 Tue 14:00 WIL C107

NEXAFS and EXAFS structure determination within quasicrystalline barium titanate on Pt(111) — •Alireza Bayat[1], Stefan Förster[1], Eva-Maria Zollner[1], Wolf Widdra[1,2], Paula Huth[3], Reinhard Denecke[3], Angelika Chasse[1], and Karl-Michael Schindler[1] — [1]Institut für Physik, Martin-Luther-Universität, Halle-Wittenberg, D-06120 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle, Germany — [3]Wilhelm-Ostwald-Institut, Universität Leipzig, D-04103 Leipzig, Germany

The discovery of an aperiodic barium titanate derived quasicrystalline film on a periodic platinum substrate opened a new field in science and technology [1]. The key point of understanding the physical properties and potential future applications is to determine its geometric structure. EXAFS modulations at the Ti K-edge of the $BaTiO_3$-derived quasicrystal on Pt(111) were recorded and FEFF6 calculations were performed. With respect to the first layer Pt atoms the analysis reveals the Ti in a near 3-fold hollow position with distances in the range of 2.3 - 2.4 Å. The short distances indicate bonding between Ti and Pt and emphasize their relevance for understanding the structure. Furthermore, pre-edge features of the NEXAFS spectrum at the Ti K-edge indicate a coordination of Ti by less than 4 O. In line with this, the chemical shift of Ti $2p$ photoemission lines proves that Ti ions exist only in the 3^+ oxidation state.

[1] S. Förster et al., Nature, **502** (2013) 215-218.

O 39.2 Tue 14:15 WIL C107

Epitaxy of ultrathin nickel ferrite films on MgO(001) — •Tabea Nordmann, Jari Rodewald, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Nickel ferrite ($NiFe_2O_4$) crystallizing in the inverse spinel structure is an interesting material for the use in magnetic devices due to its high magnetic permeability, its high Curie temperature of 865 K and its semiconducting property.

Studies on the growth of nickel ferrite by several deposition techniques have already been performed, but the deposition by reactive molecular beam epitaxy (RMBE) has just been studied rarely.

Hence, in this work ultrathin epitaxial films with different Ni/Fe ratios are deposited on MgO(001) via co-evaporation of nickel and iron in an oxygen atmosphere by using RMBE. The surface structure of the films is characterized by low-energy electron diffraction (LEED), while x-ray photoelectron spectroscopy (XPS) is executed to determine the film composition and the oxidation state of iron. Furthermore, x-ray diffraction (XRD) is performed in order to investigate the crystalline quality and the out-of-plane lattice constant of the films. Last, x-ray reflectivity (XRR) is measured to examine the film thickness.

The surfaces of all films with Ni/(Fe+Ni) contents between 7 % and 60 % are well ordered and the XRD results indicate a single crystalline layer. The XPS results reinforce the formation of nickel ferrite films with Ni contents of about 33 % where iron only exists in the Fe^{3+} oxidation state.

O 39.3 Tue 14:30 WIL C107

Influence of Surface Structure on Solid-State Electrochemistry: Oxygen Exchange on $SrTiO_3(110)$ Surfaces — •Michele Riva[1], Markus Kubicek[2], Xianfeng Hao[3,4], Stefan Gerhold[1], Giada Franceschi[1], Michael Schmid[1], Herbert Hutter[2], Juergen Fleig[2], Cesare Franchini[3], Bilge Yildiz[1,5], and Ulrike Diebold[1] — [1]IAP, TU Wien — [2]CTA, TU Wien, — [3]CMS, Universität Wien — [4]Dep. Chem. Eng., Yanshan Univ., China — [5]Lab for Electrochemical Interfaces, MIT, USA

In solid-state electrochemistry, the efficiency for oxygen incorporation of perovskite oxides is interpreted in terms of the availability of surface oxygen vacancies, or the ease of electron transfer. Intriguingly, none of the standard models considers the role of the surface atomic structure. In the present contribution we show that the latter plays a crucial role in affecting oxygen exchange on $SrTiO_3$. Using a host of surface science techniques (STM, LEED, XPS, etc.) we find that the $SrTiO_3(110)-(n \times 1)$ and $(2 \times m)$ surface structures are remarkably stable under realistic conditions for oxygen-exchange reactions. We use two different ion-based spectroscopy techniques to quantify ^{18}O exchange and find that the reactivity of these two structures differs by a factor of three. From DFT calculations and electron spectroscopic measurements we rule out that this difference is due to oxygen vacancies or differences in work function or surface potential. Instead our results reveal that the structure itself can determine the extent of the interaction with molecular oxygen, governing the surface reactivity to oxygen exchange reactions of perovskite oxides.

O 39.4 Tue 14:45 WIL C107

Scanned probe surface structure analysis of silicas - then and today — •Georg Hermann Simon[1], Burkhard Kell[1], Kristen Burson[1,2], Markus Heyde[1], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Current address: Department of Physics, Hamilton College, 198 College Hill Road, Clinton, NY 13323, USA

Silica and silicate surfaces play an important role in nature and materials applications. They offer a wealth of structures from crystalline quartz [1] via nanoporous zeolite crystals to amorphous silicate glass [2,3]. However, achieving atomic-scale surface science results for these materials has been challenging due to the structural complexity, charging problems common to bulk insulators, and the necessity for well-controlled sample preparations. Ultrathin silica films enable atomic-scale structural characterization and aid the study of bulk quartz and glass surfaces. Such silica films have been shown to exist in crystalline and amorphous modifications [4] which are stable in ultrahigh vacuum, air, and water [5]. Here we present an atomic scale study of ultrathin silica films and bulk silica samples in vacuum and liquid performed using scanning probe microscopy.

[1] F. Bart et al.; Surf. Sci. 311 (1994) L671.
[2] Raberg et al.; J. Non-Cryst. Solids 351 (2005) 1089.
[3] J.-F. Poggemann et al.; J. Non-Cryst. Solids 326-327 (2003) 15.
[4] Lichtenstein et al.; Angew. Chem. Int. Ed. 51 (2012) 404.
[5] Burson et al.; Appl. Phys. Lett. 108 (2016) 201602.

O 39.5 Tue 15:00 WIL C107

The (O12) surfaces of hematite and their interactions with water - a DFT study — •Magdalena Bichler[1], Florian Kraushofer[2], Zdenek Jakub[2], Gareth Parkinson[2], and Peter Blaha[1] — [1]Institute of Materials Chemistry, TU Wien — [2]Institute of Applied Physics, TU Wien

Hematite (α-Fe_2O_3) is a promising material for electrochemical water splitting with a suitable bandgap (2.2 eV) and valence band edge position. Moreover, the material is cheap, stable in water and harmless in terms of ecology. Nevertheless, it shows poor electrochemical performance, which might be improved by morphology and surface modifications.

We focus on the (012) surface of hematite (R-cut). Two different types are known. On the one hand, the (1x1) bulk terminated, stoichiometric surface exists, but at low O2 pressure, a (2x1) reconstruction with missing oxygen atoms is formed. [1]

We carried out ab initio calculations by using the WIEN2k code. [2] In addition, STM, AFM and LEED experiments were done. Based on our DFT calculations, we present a new model of the (2x1) reconstruction, which is energetically more stable than the one that has been proposed so far [3] and agrees with experiment. Furthermore, the surfaces' interactions with water were investigated in both experiment and theory.

[1] M. A. Henderson et al., Surf. Sci. 1998, 417, 66-81
[2] http://www.wien2k.at
[3] M. A. Henderson, Surf. Sci. 2010, 604, 1197-1201

O 39.6 Tue 15:15 WIL C107

Morphology, structure, topological defects, and electronic effects of epitaxial SnTe topological crystalline insulator films — Omur E. Dagdeviren[1], Chao Zhou[1], Ke Zou[1], •Georg H. Simon[1,2], Stephen D. Albright[1], Mayra D. Morales-Acosta[1], Xiaodong Zhu[1], Frederick J. Walker[1], Charles H. Ahn[1], Udo D. Schwarz[1], and Eric I. Altman[1] — [1]Center for Research on Interface Structures and Phenomena (CRISP), Yale University, New Haven, CT 06520, USA — [2]Current Address: Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany

SnTe has been researched in the past as an ingredient in phase change materials and in the context of infrared detection and thermoelectrics [1]. Moreover, it gained renewed attention for properties of a topological crystalline insulator (TCI), which have been predicted [2,3] and experimentally confirmed for SnTe(100) and (111) surfaces [4]. However, its enormous lattice constant should lead to large misfit epitaxy on most substrates. The resulting defects may or may not be detrimental or even beneficial for TCI properties and their applications. Here we present a surface science characterization of thick, ex situ grown, SnTe(001) films on insulating SrTiO3(001) [5]. STM and electron diffraction data show morphology and surface structure in detail. Furthermore the growth and post-processing related defect structure as well as surface standing waves are revealed. [1] Zhang et al.: PNAS 110 (2013) 13261. [2] Fu: PRL 106 (2011) 106802. [3] Hsieh et al.: Nat. Comm. 3 (2012) 982. [4] Tanaka et al.: Nat. Phys. 8 (2012) 800. [5] Dagdeviren et al.; Adv. Mater. Interfaces, in press.

O 39.7 Tue 15:30 WIL C107

Plasma-assisted growth of VO_2 on TiO_2(110) and study of its chemical and structural properties — •Simon Fischer, Jon-Olaf Krisponeit, Jan Ingo Flege, and Jens Falta — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

With VO_2 exhibiting a temperature-induced metal-insulator transition, thin film growth of this material is of interest for various applications such as switching devices and sensors. The transition is accompanied by a structural change from a monoclinic insulating phase, in which vanadium atoms are dimerized, to a rutile metallic phase. Since a multitude of different vanadium oxides can form, VO_2 growth by molecular beam epitaxy poses challenges in selecting a viable oxidation source and adjusting growth temperature as well as metal-oxygen ratio.

In this study, we have deposited vanadium on TiO_2(110) samples continuously and subjected the sample cyclically to different doses of atomic oxygen from a plasma source. Between growth cycles film thickness as well as vanadium oxidation state was determined from x-ray photoelectron spectroscopy analysis. While atomic oxygen is critical in ensuring VO_2 stoichiometry, apparently high doses of atomic oxygen lead to the formation of a V_2O_5 capping. This observation is supported by ex-situ transport measurements. Furthermore, we discuss different surface reconstructions revealed by low-energy electron diffraction in terms of surface oxygen concentration.

O 39.8 Tue 15:45 WIL C107

Transport along grain boundaries through alumina investigated by atom probe tomography — •Torben Boll[1,2], Kinga A. Unocic[3], Bruce A. Pint[3], and Krystyna Stiller[2] — [1]Institut für Angewandte Materialien, Karlsruhe Institut für Technologie, 76344 Eggenstein Leopoldshafen — [2]Department of Physics, Chalmers University of Technology, SE-412 96 Göteborg, Sweden — [3]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak, Ridge TN, 37831, USA

It is generally agreed upon that transport through growing alumina scales occurs predominantly due to inward oxygen diffusion along grain boundaries (GBs). However, it is also accepted that there exists some amount of concurrent outward aluminum diffusion along the GBs. Moreover, the effect of alloying elements on oxidation behavior and how they affect diffusional fluxes still remains uncertain.

For this study different Ni-Al alloys with additions of Hf, Y and Zr were investigated. The materials were subjected to an initial exposure in O_2 at 1100°C. The initial exposure was continued again at 1100°C for 5h after a smoothing of the surface. After this double exposure SEM a growth of ridges above the GBs, as an indication foroutward diffusion were observed. Scanning transmission electron tomoggraphy energy dispersive X-Ray spectroscopy investigations were complemented with atom probe tomography, which gave quantitative information about the concentration of the different elements at the GBs. This helped to calculate the Gibbsian excesses and to discuss the influence of different dopants.

O 40: Focus Session: Charge Transport at Surfaces and Nanostructures with Multi-probe Techniques II

Time: Tuesday 14:00–15:15 Location: WIL C307

Invited Talk O 40.1 Tue 14:00 WIL C307

Performances of the new low temperature ultrahigh vacuum 4 scanning tunneling microscopes — •christian Joachim[1,2], Delphine Sordes[1], Corentin Durand[1], We-Hyo Soe[1], and Marek Kolmer[3] — [1]CEMES-CNRS, 29 rue J. Marvig, 31055 Toulouse Cedex, France — [2]MANA-NIMS, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan — [3]NANOSAM, Jagiellonian University, Lojasiewicza 11, 30-348 Krakow, Poland

The performances of our new ScientaOmicron LT-UHV 4-STM are presented by a series of single tip experiments on the Au(111) surface [1]. Each of the 4 STM have performances equivalent to a single tip state-of-art LT-UHV-STM. We have also started to explore passivated Si(100)H surfaces with this instrument with 1 cm lateral size surfaces prepared from a 200 mm wafer [2] essential for the fabrication of atomic scale circuits [3]. Atomic resolution imaging confirms the position of the surface dimers relative to the surface atomic structure [4]. A gentle mechanical jump to contact was observed on a single H atom with very low G/Go contact conductance. Our LT-UHV 4-STM was transformed for the first international molecule car race in Toulouse, spring 2017 [5]. This competition will be shortly described with registered teams from Germany, France, Japan, Switzerland, Austria and US. A poster per team is presented in the poster session. [1] J. Yang et al. Eur. Phys. J. AP, 73, 10702 (2016) [2] M. Kolmer et al. Appl. Surf. Sci., 288, 83 (2014) [3] M. Kolmer et al., Nanoscale, 7, 12325 (2015). [4] T. L. Yap et al. Surf. Sci., 632, L13 (2015) [5] F. Eisenhut et al., Eur. Phys. J. AP, 76, 10001 (2016).

O 40.2 Tue 14:30 WIL C307

New Perspectives in Scanning Tunneling Potentiometry — Philip Willke[1], Thomas Kotzott[1], Jan Voigt[1], Rainer G. Ulbrich[1], M. Alexander Schneider[3], Thomas Pruschke[2], and •Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Universität Göttingen, Göttingen, Germany — [2]Institut für Theoretische Physik, Universität Göttingen, Göttingen, Germany — [3]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Erlangen, Germany

We present a new STP setup with a home-built low-temperature STM operating at 6 K and applicable magnetic field of up to 6 T. First, we study high-resolution STP of scattering centers on a sub-nanometer scale, especially the spatial evolution of the electrochemical potential for 1D defects in graphene.[1] We show that the voltage drop at a monolayer-bilayer boundary in graphene clearly extends spatially up to a few nanometers into the bilayer and hence is not located strictly at the structural defect. We explain this behaviour by the weak coupling between the two bilayer sheets extending the voltage drop at the interface due to the required current transfer. Second, we perform magnetotransport STP measurements mapping the local electrochemical potential as a function of the applied magnetic field.[2] Thus, we are able to extract graphene's charge carrier concentration locally by the emerging Hall field. Additionally, we show that the defect resistance of local defects such as steps, wrinkles and ML/BL-junctions remains constant for all magnetic fields. This work was supported by SPP 1459 'Graphene'. [1] P. Willke et al. Nature Commun. 6399 (2015) [2] P. Willke et al., under consideration (2016)

O 40.3 Tue 14:45 WIL C307

Kelvin probe force microscopy as a tool to measure local transport properties in graphene on SiO2 — Philip Willke[1], •Anna Sinterhauf[1], Christian Möhle[1], Thomas Kotzott[1], Hak Ki Yu[2,3,4], Alec Wodtke[2,3], and Martin Wenderoth[1] — [1]IV. Physical Institute, University of Göttingen, 37077, Göttingen, Germany — [2]Institute for Physical Chemistry, University of Göttingen, 37077, Göttingen, Germany — [3]Max Planck Institute for Biophysical Chemistry, 37077, Göttingen, Germany — [4]Department of Materials Science & Engineering, Ajou University, Suwon, 443-749, South Korea

We combine the AFM-based method of Kelvin probe force microscopy (KPFM) with an additionally applied electric field across the sample to map the electrostatic potential on a nanometer scale. Thus we investigate the local voltage drop in graphene on SiO2 under ambient conditions and room temperature [1]. We can quantify the variation of the local sheet resistance and resolve a localized voltage drop at folded wrinkles for the first time. Furthermore, we map local resistances as a function of temperature by using Joule heating. These measurements show that the local monolayer sheet resistance reflects the macroscopic increase in resistance with temperature while the defect resistance for folded wrinkles is best described by a temperature-independent model which we attribute to interlayer tunneling. This work was supported by SPP 1459 'Graphene'.

[1] Willke et al., Carbon 102, 470-476 (2016)

O 40.4 Tue 15:00 WIL C307

Two-probe measurements on the atomic scale wires: ballistic transport through surface states of Ge(001) — •Marek Kolmer[1], Piotr Olszowski[1], Rafal Zuzak[1], Szymon Godlewski[1], Christian Joachim[2,3], and Marek Szymonski[1] — [1]Centre for Nanometer-Scale Science and Advanced Materials, NANOSAM, Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, Lojasiewicza 11, 30-348 Krakow, Poland — [2]Nanoscience Group & MANA Satellite, CEMES/CNRS, 29 rue Marvig, BP 94347, 31055 Toulouse, France — [3]International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

We will present our recent results obtained on the new Scienta-Omicron low temperature ultra-high vacuum 4-probe STM (LT-Nanoprobe). Firstly, we will show our methodology for fine relative positioning of two STM probes on Ge(001) and Ge(001):H surfaces with unprecedented atomic precision and with a lateral exact probe to probe distance below 50 nm. Moreover, we will discuss our design of the 2-probe experiment, which allows a direct testing of the electronic transport through atomic-scale structures in a fully planar geometry. That will be shown on an example of a model system: bare Ge dimer wire supported on Ge(001) and Ge(001):H surface. In this case we determine ballistic transport regimes in the atomic wire by systematic 2-probe experiments on the probe to probe distances below 50 nm.

O 41: Nanostructures at Surfaces: Metals, Oxides and Semiconductors II

Time: Tuesday 14:00–16:00 Location: REC/PHY C213

O 41.1 Tue 14:00 REC/PHY C213

Lattice dynamics of laser-excited Au nanoclusters observed by femtosecond electron diffraction — •Thomas Vasileiadis[1], Dawn Wells[2], Lutz Waldecker[1], Alessandra Da Silva[2], Roman Bertoni[1], Richard Palmer[2], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]Nanoscale Physics Research Laboratory, School of Physics and Astronomy, University of Birmingham, Birmingham B15 2TT, UK

Metallic nanoclusters (NCs) have dominated the field of light-harvesting technologies and photo-catalysis [1]. For all these applications it is important to know how heat flows in the nanoscale and if the crystalline order is affected. We address this question using femtosecond electron diffraction [2] to study size-selected Au NCs on various substrates [3]. We resolve lattice-heating, expansion and surface disordering using the height, scattering vector and width of diffraction peaks respectively. In addition, we show that for NCs on 2D crystals a pre-existing crystallographic texture can reveal morphological changes. Finally, we present a model of heat flow in low-dimensional heterostructures to estimate electronic and vibrational coupling to the substrate.

[1]M.L. Brongersma et al., Nat. Nanotech. 10, 25-34 (2015).

[2]L. Waldecker et al., J. Appl. Phys. 117, 044903 (2015).

[3]S. R. Plant, L. Cao, and R.E. Palmer, J. Am. Chem. Soc., 136, 7559-7562 (2014).

O 41.2 Tue 14:15 REC/PHY C213

3d-metal nanoparticles on tungsten, tungsten-oxide and tungsten-carbide — •Hendrik Bettermann, Knuth Scheiff, Jens Schubert, and Mathias Getzlaff — Institute of Applied Physics, Heinrich-Heine-Universität Düsseldorf

Supported clusters and nanoparticles are rather interesting objects not only from a fundamental point of view but also for technological applications due to their electronic and magnetic properties. These properties typically show a strong size dependence. Interaction with the substrate during and after deposition significantly influences the particles' properties.

Our contribution is focused on size-selected nanoparticles made from Fe, Co, and Ni and their binary alloys. These particles are deposited on W(110) as well as the corresponding tungsten-oxide and -carbide superstructures. Two UHV-compatible nanoparticle sources, an Arc Cluster Ion Source (ACIS) and a magnetron sputter source (Haberland-type), can produce a wide range of particle sizes (4 to 15 nm).

Size and structural properties are investigated by STM (scanning tunneling microscopy) and LEED (low energy electron diffraction) under UHV conditions. Samples are tempered to determine the melting behaviour of the nanoparticles.

O 41.3 Tue 14:30 REC/PHY C213

A monolayer of hexagonal boron nitride on Ir(111) as a template for cluster growth — •Moritz Will[1], Philipp Valerius[1], Charlotte Herbig[1], Vasile Caciuc[2], Nicolae Atodiresei[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Peter Grünberg Institut (PGI) and Institute for Advanced Simulation (IAS), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Chemical vapor deposition of $B_3N_3H_6$ molecules on Ir(111) results in a well aligned monolayer of hexagonal boron nitride (h-BN). The center of each unit cell provides a chemisorbed valley area, where h-BN is hybridized with the Ir substrate. Through a scanning tunneling microscopy study we provide evidence that the valley regions are reactive and pin deposited atoms. In consequence, highly regular cluster arrays with a periodicity of 2.9 nm can be formed. For the case of Ir clusters, the size distribution is narrow. The average size can be tuned between a few to about 200 atoms for room temperature deposition. The thermal stability of the clusters is extraordinary, with a decay of the cluster lattice setting only at around 850 K, primarily through intercalation of the cluster material. Regularly positioned C clusters on h-BN are even observed after annealing to 1500 K. Compared to cluster arrays using graphene on Ir(111) as a template, the better order and the higher thermal stability make the arrays on h-BN/Ir(111) superior in terms of potential applications for nano-catalysis. We elucidated the cluster binding mechanism of Ir clusters to h-BN/Ir(111) with the help of density functional theory calculations.

O 41.4 Tue 14:45 REC/PHY C213

Aggregation behaviour of silver clusters in room temperature ionic liquids — •Stefanie Roese, Alexander Kononov, Florian Lippert, and Heinz Hövel — Fakultät Physik / DELTA, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany

Room temperature ionic liquids (RTIL) are well-known stabilizers for nanoparticles [1]. For now only a few studies of the stability of nanoparticles in RTILs are available [2], nevertheless the nanoparticle stability is of critical importance in controlling aggregation processes.

2 nm silver nanoparticles with a well-characterized size distribution (± 0.6 nm) are preformed in a supersonic nozzle expansion [3] and deposited afterwards into the ionic liquid. The cluster plasmon is investigated in-situ by UV/Vis absorption spectroscopy during cluster deposition as well as in temperature dependent measurements after deposition [4]. We observed that the storage temperature as well as the choice of anion and cation influences the cluster stability on timescales of several days. An activation energy for different aggregation states was calculated.

The geometric cluster structure is determined in first EXAFS measurements performed at beamline P64, DESY, where the effect of aggregation can be seen in a change in the resulting lattice constant.

[1] J. Dupont, J. D. Scholten, Chem. Soc. Rev. 39, 1780 (2010). [2] K. Richter, A. Birkner and A. Mudring, Phys. Chem. Chem. Phys. 13, 7136 (2011). [3] H. Hövel, S. Fritz, A. Hilger, U. Kreibig and M. Vollmer, Phys. Rev. B 48, 18178 (1993). [4] D. Engemann, S. Roese and H. Hövel, J. Phys. Chem. C, 120, 6239 (2016).

O 41.5 Tue 15:00 REC/PHY C213

Size dependent changes in the electronic structure of manganese oxide nanoparticles and clusters probed by soft X-ray absorption and emission spectroscopy — •Marc F. Tesch[1], Maryam N. Shaker[1,2], Daniela Schön[1,2], Niklas Cibura[3], Emad F. Aziz[1,2], and Jennifer Strunk[3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, 12489 Berlin — [2]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin — [3]MPI für chemische Energiekonversion, 45413 MÜLHEIM an der Ruhr

Nanoscale objects are of tremendous interest for novel applications since they can exhibit significant changes in their material properties compared to the bulk material. This is interesting for catalytic applications because the quantum size effect, causing a bandgap widening, can facilitate photocatalytic reactions. We present a study on MnOx nanoparticles, which are promising candidates to act as environmental friendly water oxidation catalysts. Nanoparticles of different sizes were obtained by pulsed laser ablation and nanoclusters were produced in a self-arrangement process from solution with grafting and impregnation techniques on mesoporous silica. The samples are studied by means of soft X-ray absorption spectroscopy and resonant inelastic X-ray scattering at the Mn L-edges. The combination of these techniques allows tracking changes in the electronic structure of the unoccupied as well as of the occupied 3d valence states. The two sample systems are compared with respected to each other and to spectra of bulk references and an overview of the particle size dependence on the catalytic activity and the electronic structure will be given.

O 41.6 Tue 15:15 REC/PHY C213

The diffuse scattering pattern from nanostructured surfaces — •Victor Soltwisch[1], Analia Fernandez Herrero[1], Mika Pflüger[1], Jürgen Probst[2], Anton Haase[1], and Frank Scholze[1] — [1]Physikalisch-Technische Bundesanstalt — [2]Helmholtz-Zentrum Berlin

Laterally periodic nanostructures were investigated with grazing incidence small angle X-ray scattering. To support an improved reconstruction of nanostructured surface geometries, we investigated the origin of the contributions to the diffuse scattering pattern which is correlated to the surface roughness. Resonant diffuse scattering leads to a palm-like structure of intensity sheets. Dynamic scattering generates the so-called Yoneda band caused by a resonant scatter enhancement at the critical angle of total reflection and higher-order Yoneda bands originating from a subsequent diffraction of the Yoneda enhanced scattering at the grating. Our explanations are supported by modelling using a solver for the time-harmonic Maxwell's equations based on the finite-element method.

O 41.7 Tue 15:30 REC/PHY C213

Flux- and Fluence-dependent Nanocone-formation on InP under ion-irradiation — •Detlef Kramczynski[1,2] and Hubert Gnaser[1] — [1]AG Grenzflächen/Nanomaterialien/Biophysik, Uni Kaiserslautern — [2]Nanoparticle Process Technology, Uni Duisburg-Essen

Samples of InP-wafers have been irradiated with 2.1 keV Ar-ions at various combinations of flux (0.9 to $1.6 \cdot 10^{14} ions/(cm^2 s)$) and fluence (0.4 to $2.4 \cdot 10^{18} ions/(cm^2)$), at vertical incidence and at room temperature.

The result is a rich phase-diagram wherein the size-distribution of the Nanocones, their global-scale surface-coverage and their local-scale tendency to agglomerate as islands very delicately depend on the proper combination of flux and fluence.

The suggested explanation is a multi-species adatom-diffusion-process, with thermally-enhanced adatom-diffusion being responsible for the global-scale phenomena and the energy-deposition of the ions being responsible for the local-scale phenomena.

O 41.8 Tue 15:45 REC/PHY C213

Topological States and nearly flat Electron Band in engineered atomic Lattices — •Robert Drost[1,2], Teemu Ohjanen[1], Ari Harju[1], and Peter Liljeroth[1] — [1]Aalto University Department of Applied Physics, Puumiehenkuja 2, 02150 Espoo, Finland — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

Topological materials exhibit protected edge or boundary modes that have been proposed for applications in spintronics and quantum computation. The essential physics of several topological systems are captured in two-dimensional tight binding models which can be implemented in artificial lattices. This approach makes it possible to test theoretical proposals in systems with precise control over the models parameters or design quantum materials with tailored properties. We use low-temperature scanning tunnelling microscopy to fabricate such lattices with atomic precision and probe the resulting density of states. We implemented two Hamiltonians of fundamental importance using vacancy defects in a chlorine layer on Cu(100): The Su-Schrieffer-Heeger dimer chain with topological domain walls and the Lieb lattice with a nearly flat electron band.

O 42: Solid-Liquid Interfaces: Reactions and Electrochemistry - Theory II

Time: Tuesday 14:00–16:00 Location: WIL B321

O 42.1 Tue 14:00 WIL B321

First-principles free-energy barriers for photo-electrochemical surface reactions: Proton abstraction at TiO_2(110) — •Thomas Stecher, Karsten Reuter, and Harald Oberhofer — Technische Universität München, Garching, Deutschland

First-principles modelling of electrocatalytic surface reactions is still largely defined by the computational hydrogen approach. This approach evaluates free energy differences between consecutive reaction steps and thereby accounts only for thermodynamic barriers. In order to access additional kinetic barriers in the photocatalytic oxidation of water, we present an approach based on *ab initio* molecular dynamics (AIMD) simulations and umbrella sampling. [1] We showcase the method by explicitly calculating the free-energy barrier for the initial proton abstraction in the water splitting reaction at rutile TiO_2(110), which was previously studied within the computational hydrogen electrode approach. [2] Combining electrostatic QM/MM embedding, an energy based reaction coordinate and state-of-the-art free-energy reconstruction techniques renders the calculation tractable at the hybrid density-functional theory level, which is required for a realistic description particularly of the transition state. The obtained free-energy barrier of approximately 0.2 eV, depending slightly on the orientation of the first acceptor water-molecule, suggests a hindered reaction on the pristine rutile surface.

[1] T. Stecher, K. Reuter and H. Oberhofer, *Phys. Rev. Lett.*, accepted for publication (2016).

[2] H. Oberhofer and K. Reuter, *J. Chem. Phys.* **139**, 044710 (2013).

O 42.2 Tue 14:15 WIL B321

Thermodynamic sampling of the electrode potential on a Pt(111) electrode from first principles — •Sung Sakong and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

The potential of zero charge (pzc) is an important electrochemical quantity that is determined by the work function of a metal covered by an ion-free water film. Recently we derived the pzc from large scale ab initio molecular dynamics simulations by statistically averaging the work function [1] and reproduced the experimentally observed value. However, hydronium and hydroxyl ions can be present in the water film at metal electrodes created by the self-ionization of water. We have studied the consequences of the creation of these ions on the water properties separately. They modify the charge distribution at the water-metal interface. Consequently, the local dipole field and thus also the work function are influenced by the ions. Furthermore, we will establish a connection to computationally less demanding methods for the description of electrochemical water metal interfaces [2].

[1] S. Sakong, K. Forster-Tonigold, and A. Groß J. Chem. Phys. **144**, 194701 (2016)

[2] S. Sakong and A. Gross, ACS Catal. **6**, 5575 (2016).

O 42.3 Tue 14:30 WIL B321

Computational hydrogen electrode modelling of water electrolysis at IrO_2 nanoparticles — •Daniel Opalka and Karsten Reuter — Technische Universität München, Germany

IrO_2 is the primary active anode component of proton-exchange membrane cells for water electrolysis in acidic operating conditions. Its superior performance has generally been rationalized through the optimized binding of relevant reaction intermediates at IrO_2(110) as assessed within the computational hydrogen electrode (CHE) approach based on density-functional theory (DFT) calculations. At present, it is unclear though whether this level of theory is sufficient to guide ongoing activities that aim at improving the anode activity and stability through nanostructuring and doping. To this end we revisit critical practical components of the CHE approach, such as the employed DFT functional or the degree of hydroxylation under operating conditions. Extending the calculations to other low-index facets allows to attempt a first description of IrO_2 nanoparticles through an *ab initio* thermodynamics based Wulff-construction.

O 42.4 Tue 14:45 WIL B321

Coadsorption of anions and cations on platinum — •Florian Gossenberger and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

The relevant reaction steps in electrochemistry occur in the region were ion-conduction of the electrolyte merges electron-conduction of the electrode. This area is crucially influenced by the presence or absence of both anions and cations, which are - dependent on the electrode potential - specifically adsorbed on the electrode.

To understand the structure and stability of the adsorbate layer, we have investigated the simultaneous adsorption of different anions (Cl^-, Br^-, I^-, SO_4^{2-}/HSO_4^-) and protons/hydronium on platinum, using density functional theory [1]. The dependence of the adsorption structures on the ionic concentrations in the electrolyte and on electrode potential have been derived using the concept of the computational hydrogen electrode, allowing to derive phase diagrams and Pourbaix diagrams. Thus we have been able to reproduce the experimental finding of the competitive adsorption of hydrogen and halides on Pt(111). With respect to sulphate adsorption our results suggest the need to revisit previously suggest structural models.

[1] F. Gossenberger, T. Roman, A. Groß, Electrochim. Acta **216**, 152-159 (2016).

O 42.5 Tue 15:00 WIL B321

Experimental and theoretical investigation of Prussian blue type catalysts for photoelectrochemical water-splitting —

•Franziska Hegner, Núria López, and José-Ramón Galán-Mascarós — Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain

The development of an efficient, cheap and robust water-oxidaton catalyst remains the bottleneck step to realizing artificial photosynthesis. Materials based on Prussian blue (iron hexacyanoferrate), which fulfill all those criteria, have shown high catalytic activities with exceeding long-term stabilities.

In combining experimental methods with theoretical calculations we aim to elucidate the underlying photo-physical mechanisms and its determining factors. Catalytic systems were prepared by modifying the well-known photo-catalytic material BiVO4, with cobalt iron analogues of Prussian blue (CoFe-PB), which largely increases the photocurrent and significantly lowers the onset potential of light-induced water oxidation.

It was found that common density functional theory (DFT) methods are insufficient to accurately describe the complex electronic and magnetic structure of Prussian blues and functionals of higher degree of complexity are needed. We developed a robust computational scheme to evaluate electronic structure relationships of the combined semiconductor system, which might be crucial to its photo-catalytic applications.

O 42.6 Tue 15:15 WIL B321

Driving Forces for Aggregation and Dissociation of Water on Zinc Oxide — •P. Ulrich Biedermann[1] and Stephane Kenmoe[1,2] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]current address Department of Theoretical Chemistry, University of Duisburg-Essen, Essen, Germany

The interactions of water with zinc oxide play an important role in the fields of catalysis, corrosion protection and biomedical applications. The properties of water adsorbed at the interface of oxides are significantly different from bulk water. In particular, the high degree of water dissociation observed in the contact layer indicates O-H bond activation. This facilitates proton transfers, an important step in many catalytic processes. We present a comprehensive DFT study of water adsorbed on the non-polar ZnO $(10\bar{1}0)$ and $(11\bar{2}0)$ surfaces using PBE. In view of the band-gap problem of GGA-DFT, the results are benchmarked against hybrid DFT results. Several new interface structures have been discovered in the coverage regime of 0-3 ML. Water aggregation on ZnO is controlled by a subtle interplay of direct water-water interactions including H-bonds and dipole-dipole interactions versus surface- or adsorption-mediated interactions including enhanced water-surface interactions and reduced relaxation energies required to optimize the geometry of the water molecules and ZnO surface for adsorption. While water dissociation also depends on aggregation and the geometrical arrangement of the molecules on the surface, direct water-water interactions do not contribute to this process. Water dissociation is driven by enhanced water-surface interactions.

O 42.7 Tue 15:30 WIL B321

Proton dynamics and structure of confined sulfuric acid liquid between graphene sheets from ab-initio molecular dynamics — •Steffen Seiler and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

The wet-chemical exfoliation of graphite via Hummers' method [1,2] is a promising route for large-scale graphene production. The first relevant reaction intermediate, the stage-1 sulfuric acid graphite intercalation compound, is an interesting model system of a confined liquid. To unravel the proton dynamics and the structural properties of the confined liquid in this compound, extensive Car-Parrinello molecular dynamics simulations were performed. We show that the stability of the hydrogen-bond network in the sulfuric acid film is affected neither by the extreme confinement (mono-molecular layer) nor by graphite oxidation. Also the proton-transfer reaction barrier is not increased upon confinement. In contrast, oxidation of graphite reduces the barrier, which provides an explanation for the fast and efficient intercalation of graphite with sulfuric acid in the presence of oxidizing agents.

[1] W.S. Hummers, *J. Am. Chem. Soc.* **80**, 1339 (1958).
[2] D.C. Marcano, et al., *ACS Nano* **4**, 4806 (2010).

O 42.8 Tue 15:45 WIL B321

Functionalization of Oxide Surfaces: Chemical Reactions at the Solid/Liquid Interface — •Paul Schwarz and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Using ab-initio molecular dynamics we have studied the anchoring of methylsilanetriol (MST) linker units to aluminum oxide surfaces via condensation reactions in the presence of residual water and liquid isopropanol at standard temperature and pressure. While in vacuum MST molecules spontaneously attach to the surface Al ions via one of their oxygen atoms, adding the residual water molecules and the liquid isopropanol suppresses the direct approach of MST to the surface and solvent molecules have to be displaced. To accelerate this process and to study the mechanism of the subsequent condensation reaction, the metadynamics technique is applied. The simulations show a variety of reaction pathways which differ in how MST deprotonates and how the OH group at the same Al site is converted to water and desorbs. In addition, several competing processes are observed: 1) reprotonation of MST with a subsequent detachment of the molecule and diffusion into the liquid; 2) detachment of MST and spontaneous reaction with a neighboring surface Al atom; 3) binding of a second OH group of MST to the same Al site. Free energy profiles of these paths will be compared and the stability of reaction intermediates will be compared by static DFT calculations.

O 43: Gaede Prize Talk

Time: Tuesday 15:30–16:00 Location: WIL C307

Invited Talk O 43.1 Tue 15:30 WIL C307

STM-induced light emission: from molecular LED to subnanometric optical microscopy. — •Guillaume Schull — Institut de Physique et Chimie des Materiaux de Strasbourg, UMR 7504 (CNRS - Universite de Strasbourg), Strasbourg, France

The electric current traversing the junction of a scanning tunneling microscope (STM) may generate a local emission of light. During the last years, we have used this method to study the intrinsic luminescence properties of individual molecules. This work has progressed in two directions. On one side we have used the ability of the STM to manipulate matter with atomic-scale precision to form single-molecule light emitting devices. Composed by individual molecular wires suspended between the tip and the sample of the STM, these devices generate an emission of light whose color, intensity and bandwidth can be controlled with high precision. On the other side, we used the intrinsic resolution of the STM to performed sub-molecularly resolved vibronic spectroscopy of molecules separated from a metallic surfaces by a thin insulating layers. These results constitute an important step towards photonic measurements with atoms-scale resolution.

O 44: Metal Substrates: Structure, Epitaxy and Growth

Time: Tuesday 18:30–20:30 Location: P1A

O 44.1 Tue 18:30 P1A

On the Thin Film Growth of Two Isomers of Dibenzopentacene on Ag(111) — •Tobias Huempfner, Lennart Vorbrink, Felix Otto, Maximilian Schaal, Bernd Schroeter, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

We report on the thin film growth of two isomers of the molecule dibenzopentacene (DBPen) deposited on a Ag(111) surface. The different molecular configurations, namely 1,2:8,9-DBPen (trans) and 1,2:10,11-DBPen (cis), differ only in the position of one of the additional benzene rings relative to the pentacene backbone. The optical properties during the growth were measured via differential reflectance spectroscopy (DRS) and interpreted by comparing to calculated excitation spectra obtained from time-dependent density functional theory (TD-DFT) of the isolated molecule. Furthermore, the films were characterized structurally via low-energy electron diffraction (LEED) and low-temperature scanning tunneling microscopy (STM) for different film thicknesses. While the optical properties of the two isomers hardly differ in the visible region, the structural properties vary significantly. The first monolayer of the trans-isomer grows in a highly ordered structure. In contrast, for the monolayer of cis-DBPen no well-defined adlayer exhibiting translational order was observed, although first-order LEED-spots occur owing to the preferential molecular alignment with the substrate.

O 44.2 Tue 18:30 P1A

Surface Chemistry and Growth of $SnCl_2Pc$ on Ag(111) — •Christian Zwick, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Tin(IV) phthalocyanine dichloride ($SnCl_2Pc$) is an n-type semiconductor already used in organic field-effect transistors [1], but still very little is known about the actual interface formation when $SnCl_2Pc$ is deposited onto a substrate. This molecule is not planar owing to its two protruding Cl atoms. These are known to act as spacers in bulk crystal formation, and thereby significantly influence the intermolecular orbital overlap. On the other hand, Cl is known to be highly reactive in contact with certain metals, for example Ag. Hence, these two opposing effects draw attention towards the adsorption behavior of $SnCl_2Pc$ on a silver substrate. Here we report on the observed surface chemistry, the partial dechlorination of $SnCl_2Pc$ on Ag(111), and its role concerning the interface formation on Ag(111). Using in situ differential reflectance spectroscopy (DRS), low-energy electron diffraction (LEED) and low-temperature scanning tunneling microscopy (STM), we investigate the optical and structural properties of $SnCl_2Pc$/Ag(111) for effective layer thicknesses up to 2 monolayers.
[1] SK. Md. Obaidulla *et al.*, Appl. Phys. Lett. **104**, 213302 (2014).

O 44.3 Tue 18:30 P1A

X-ray spectroscopy of thin film free-base corroles on Ag(111) — Hazem Aldahhak[1], Mateusz Paszkiewicz[2], Francesco Allegretti[2], Stefano Tebi[3], •Wolf Gero Schmidt[1], Stefan Müllegger[3], Florian Klappenberger[2], Eva rauls[1], and Uwe Gerstmann[1] — [1]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany — [2]Physik-Department E20, Technische Universität München, James-Franck-Str. 1, D-85748 Garching, Germany — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University, Linz, Austria.

Corroles are structurally closely related to the well-known porphyrins that possess aromatic tetrapyrrole macrocycles. Compared to the corresponding porphyrins, they have a lower symmetry and a smaller, congested cavity. The latter property and the resulting changes in the electronic structure promote the stabilization of metal ions in exceptionally high oxidation states. X-ray spectroscopy is a powerful tool for the investigation of functional interfaces. For corrolic species, however, the required reference data are missing. The X-ray fingerprints are simulated using the continued-fraction approach within density functional theory (DFT) for extended, (quasi-)periodic molecular structures. The excellent agreement between experimental and theoretical spectra enables a thorough interpretation of the detailed spectral features and proves an accurate description of the free-base corrole electronic structure within the present DFT approach. The present study provides an ideal starting point for the comprehensive understanding of the complex chemistry of corroles in the adsorbed state.

O 44.4 Tue 18:30 P1A

Comparison of tin(II)- and lead(II)-phthalocyanine layers adsorbed on 1 ML PTCDA/Ag(111) — •Philipp Mueller, Marco Gruenewald, J. Peuker, F. Sojka, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

We investigate the growth of ultrathin, highly ordered layers of the shuttlecock-shaped molecules tin(II)-phthalocyanines (SnPc) and lead(II)-phthalocyanines (PbPc) on top of one monolayer 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on Ag(111). The films have been characterized structurally by means of low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) as well as optically using differential reflectance spectroscopy (DRS). We find that neither their lateral structures formed nor their fingerprints in optical absorption allow distinguishing between both molecules when they are adsorbed on 1 ML PTCDA/Ag(111). In fact, the condensed phases of both systems yield the same commensurate registries with respect to PTCDA. Even the structures formed for higher film thicknesses are rather similar. Also their fingerprints in optical absorption are almost identical. Here we report a possibility of distinguishing both molecules in the respective monolayer phases by means of their different STM-tip-induced switching behavior: SnPc can easily be switched from Sn-down to Sn-up configuration and vice versa by applying tip voltage pulses, whereas PbPc did not respond to our switching attempts. This provides one method of chemical identification on the molecular scale.

O 44.5 Tue 18:30 P1A

On the adsorption behavior of cyano-functionalized 2H-tetraphenylporphyrin derivatives on Cu(111): a scanning tunneling microscopy study — •Manuel Meusel, Michael Lepper, Julia Köbl, Michael Stark, Hans-Peter Steinrück, and Hubertus Marbach — Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

One important objective within surface science is the bottom-up fabrication of functional nanostructures via self-assembly of molecular building blocks. In this context, we study porphyrins as prototype functional molecules on surfaces and target the controlled modification to tweak their adsorption behavior. One method to tailor the properties of porphyrins is the attachment of functional groups. In this study, we compare the adsorption behavior of differently cyano-functionalized 2H-tetraphenylporphyrin (2H-TPP) derivatives on Cu(111) under ultra-high vacuum conditions by scanning tunneling microscopy. We observe a variety of binding motives ranging from isolated individual molecules over dimer formation to one-dimensional molecular chains. The corresponding adsorption behaviors can be correlated with the number and symmetry of the cyano groups. The results show that the functionalization of supramolecular building blocks is a well-suited method to influence the adsorption behavior. Latest results will be presented and discussed. This work was funded through DFG FOR 1878 (funCOS) under grant MA 4246/2 -1.

O 44.6 Tue 18:30 P1A

Silver segregation near oxygen chain structures on a gold-silver alloy surface: A cluster expansion study combined with ab initio MD simulations — •Sandra Hoppe[1], Yong Li[2], Lyudmila V. Moskaleva[2], and Stefan Müller[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Applied and Physical Chemistry and Center for Environmental Research, University of Bremen, Bremen, Germany

The high catalytic activity of nanoporous gold has been attributed to its residual silver content originating from the parent Ag-Au alloy. Therefore, the knowledge about the thermodynamically stable positions of silver atoms on the surface of nanoporous gold is crucial for understanding elementary stages of various catalytic processes, in particular, the chemical nature and adsorption properties of active oxygen species. In this study, we investigate the surface segregation of silver in the presence of atomic-oxygen adsorbates arranged in chains on the stepped and kinked Au(321) surface. Remarkably, we find that up to very high silver surface concentrations, the silver atoms do not occupy positions within the oxide chain, but prefer locations next to it. We identify two effects responsible for this behavior. First, gold is stabilized within the chain by partially covalent bonds with oxygen. Second, silver located in the vicinity of the chain binds stronger to oxygen than gold at the same position does. Ab initio molecular dynamics simulations support our conclusions and reveal that not only silver atoms but also the entire oxide chains may diffuse on the surface to maximize the binding contacts between adjacent silver and oxygen atoms.

O 44.7 Tue 18:30 P1A

Low temperature bias assisted RF-sputtering process for heteroepitaxial growth of iridium on various oxide substrates — •Frank Meyer[1], Eduard Reisacher[1], Johannes Preussner[1], Andreas Graff[2], Alexander Fromm[1], Lukas Gröner[1], and Frank Burmeister[1] — [1]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg i. Br., Germany — [2]Fraunhofer-Institut für Mikrostruktur von Werkstoffen und Systemen IMWS, Halle, Germany

By using the so called bias enhanced nucleation process followed by a growth process in an ellipsoidal reactor, artificial CVD-diamond can be grown on many refractory metal surfaces. The fabrication of single crystal diamond, however requires well-oriented (mostly [100]) substrates with lattice constants close to diamond and high chemical and thermal stability. A suitable candidate is iridium, deposited e.g. on A-plane sapphire [1], yttrium stabilized zirconia (YSZ) (100) [2] or lanthanum aluminate (LaAlO3) (100). In related works, we've already established a low-temperature deposition process for the hetereroepitaxial growth of iridium (100) on A-plane sapphire. In this study we investigated the influence of different oxidic substrate surfaces on the iridium film characteristics with respect to surface morphology and growth behavior by characterizing the surface morphology, crystallinity, and growth defects of iridium on LaAlO3 and YSZ with X-ray diffraction, electron backscattering diffraction, and high resolution transmission electron microscopy. [1] Z. Dai et al., Appl. Phys. Lett., 82, 3847 (2003), [2] S. Gsell et al., Appl. Phys. Lett., 84, 4541 (2004)

O 44.8 Tue 18:30 P1A

Simulation of TiN crystal growth - a combined ReaxFF+ and Monto-Carlo study. — •Stephan Pfadenhauer[1] and Roman Leitsmann[1,2,3] — [1]AQcomputare Gmbh, Annaberger Straße 240, 09125 Chemnitz Germany — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz Germany — [3]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01069 Dresden, Germany

In order to simulate the crystal growth process of TiN on metal substrates one has to treat simultaneously chemical process at very short time scales on the one hand and slow deposition rates on the other hand. To achieve this goal we have combined the reactive force field method ReaxFF+ with a Monte-Carlo approach to simulate the growth of TiN on different metal substrates.

A reliable ReaxFF+ parameter set for titanium und nitrogen has been obtained using the scheme described in [1]. For the investigated metal substrates different growth patterns - namely Frank-van-der-Merwe and Volmer-Weber - could be observed. The obtained results are consistent with [2]. Furthermore, a direct comparison of our theoretical predictions with experimental results [3] could be achieved by calculating a XRD spectra of the obtained structures.

[1] Oliver Böhm et al, The Journal of Physical Chemistry C 2016 120 (20), 10849-10856 [2] Titannitrid- und Titan-Schichten für die Nano-Elektromechanik, Marcus Pritschow, Dissertation 2007 [3] H. Z. Wu et al, Thin Solid Films, 191(1990)

O 45: Organic-Inorganic Hybrid Systems and Organic Films

Time: Tuesday 18:30–20:30 Location: P1A

O 45.1 Tue 18:30 P1A

Preparation of well-defined metal films on top of self-assembled monolayers — •Michael Zharnikov — Applied Physical Chemistry, Heidelberg University, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

Self-assembled monolayers (SAMs) can be potentially used as ultrathin insulating dielectric layers or intermediate films in future electronic and spintronic devices. Whereas the bottom electrode in such devices is provided by the metal substrate, the top electrode should be prepared in controlled fashion at the SAM-ambient interface. Regretfully, this is a non-trivial task, since the metal atoms deposited onto the SAM-ambient interface do not stay there, but penetrate into the monolayer and diffuse to the metal substrate. Here I discuss three new approaches to suppress the above penetration and diffusion, taken nickel, as a test adsorbate. The first approach relies on irradiation-induced cross-linking of a thiol-substituted aromatic SAM. Whereas 2D-polymerization of such a SAM prevents penetration of the metal atoms into the monolayer, the thiol groups at the SAM-ambient interface serve as nucleation centers for the growing "top" metal film. The second approach, relying on SAMs of perfluoroterphenyl-substituted alkanethiols, utilizes a chemical reaction between the SAM constituents and adsorbate atoms. Finally, the penetration of deposited metal atoms into a SAM can be nearly completely inhibited by preliminary formation of palladium-chloride seeding layer at the SAM-ambient interface. The Pd atoms in the seeding layer serve as nucleation centers for the growing metal film while the Cl atoms perform as surfactants.

O 45.2 Tue 18:30 P1A

Assembly of metal-organic complexes on solid support: design, properties, and applications — •Michael Zharnikov — Applied Physical Chemistry, Heidelberg University, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

Transition metal complexes allow a high degree of molecular design flexibility through symmetry considerations and ligand architecture, which can be explored for the fabrication of ordered molecular and oligomer assemblies through bottom-up approach. Here I describe the preparation of such assemblies, viz. monocomponent and multicomponent coordination-based monomolecular, dimer, trimer, and oligomer films on siloxane-based templates by wet-chemical layer-by-layer deposition process. In these films optically-rich metal polypyridyl complexes having pendant pyridine groups (so called metallo-ligands) were combined with a coinage metal (copper or silver) that acted as a linker between the polypyridyl complex moieties. The properties of the above assemblies were studied in detail by suitable combination of several complementary experimental techniques. Examples of potential applications are given, including volatile memory devices, logical gates, high-selectivity sensors, systems for photoinduced DNA cleavage, and catalytically active surfaces.

O 45.3 Tue 18:30 P1A

Transition from fractional to integer charge transfer at the inorganic-organic interface via alloying — •Elisabeth Wruss, Egbert Zojer, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

When investigating interfaces consisting of an organic layer on an inorganic substrate, two different types of charge transfer toward the adsorbate can arise. Either all molecules get fractionally charged or the charge localizes on individual molecules. While fractional charge transfer appears mostly in case of pristine metals, coexistence of charged and uncharged molecules occurs on more unreactive surfaces. In this work we address the transition between these two situations via DFT simulations. Starting with an acceptor molecule on a metallic substrate, we continuously decrease the density of states at the Fermi edge via alloying of the substrate until an integer charge transfer situation is established. By investigating the system at different alloying concentrations we analyze the properties of this transition. As a model system we have chosen the acceptor molecule TCNE on copper, which can be converted into the semiconducting cupric oxide Cu2O. To adequately model the charge transfer within DFT, large unit cells containing a sufficient number of molecules and hybrid functionals are needed. Therefore these simulations are computationally very demanding. This is one of the main reasons why the possibility of integer charge transfer has often been neglected in computational studies, although its consideration can be of uttermost importance for the understanding of the electronic properties of many inorganic-organic interfaces.

O 45.4 Tue 18:30 P1A

A monolithic setup for preparation of thin films and time-resolved multidimensional spectroscopy at the nanoscale — •Sebastian Pres[1], Bernhard Huber[1], Emanuel Wittmann[2], Lysanne Dietrich[1], Julian Lüttig[1], Victor Lisinetskii[1], Matthias Hensen[1], Eberhard Riedle[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Lehrstuhl für BioMolekulare Optik, Ludwig-Maximilians-Universität, Oettingenstraße 67, 80538 München, Germany

We present a versatile experimental setup for preparing thin organic and inorganic films which can be characterized by low energy electrons (LEEM, LEED). To investigate the nature of energy transport processes between individual molecules or inside large heterogeneous structures, we want to combine the femtosecond time resolution of coherent 2D spectroscopy with nanoscale selectivity: Instead of measuring optical diffraction-limited light fields, we detect photoemitted electrons with spatial resolution <10 nm using aberration-corrected photoemission electron microscopy (AC-PEEM). The sub-30 fs optical excitation is generated by a two-branch noncollinear optical parametric amplifier (NOPA) featuring wide spectral tunability from the NIR to the UV range at repetition rate up to 1 MHz. Here we demonstrate the tunability of the laser system from 230 nm - 900 nm at simultaneously high pulse compressibility down to 20 fs. Using collinear four-pulse sequences we want to explore well-defined organic-inorganic hybrid systems by time-resolved multidimensional spectroscopy.

O 45.5 Tue 18:30 P1A

How K-doping affects the properties of DBP monolayers on Ag(111) — •Tino Kirchhuebel, Felix Otto, Marco Gruenewald, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Doping is a suitable tool to tune the electronic properties and the absorption of organic semiconductors for the purpose of specific technical applications. Recently, tetraphenyldibenzoperiflanthene (DBP), which is applicable as a donor or acceptor for other molecules,[1] was used as a component of optoelectronic devices. Here, we investigate how doping affects DBP itself, by studying the interplay between the optical and electronic properties, as well as the structure of potassium doped epitaxial DBP thin films on Ag(111). For DBP sub-monolayers several different laterally ordered structures depending on the local K:DBP stoichiometry are observed using low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). As concluded from ultraviolet photoelectron spectroscopy (UPS) experiments, an electron transfer from potassium to DBP is achieved. Our differential reflectance spectroscopy (DRS) measurements show that this lowest unoccupied molecular orbital (LUMO) filling leads to tremendous alterations of the molecular absorption and even reduces the molecule-substrate interactions significantly. The optical fingerprints of DBP anions with reduced hybridization to the silver surface and dianions, which are rather effectively decoupled from the substrate, are identified by comparison to optical spectra of K-doped DBP films on inert mica.

[1] A. N. Bartynski *et al.*, *J. Phys. Chem. C*, **2016**, *120* , 19027.

O 45.6 Tue 18:30 P1A

Ordered superstructures of a molecular electron donor on Au(111) — •Alexander Mehler[1], Tino Kirchhübel[2], Nicolas Néel[1], Roman Forker[2], Torsten Fritz[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [2]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, D-07743 Jena, Germany

The molecular donor tetraphenyldibenzoperianthene (DBP) exhibits coverage-dependent superstructures on Au(111). At submonolayer coverages the molecules align parallel to each other. They arrange in row-like structures, which exhibit a nearly rectangular primitive unit cell. The closed molecular monolayer is characterized by a herringbone-type DBP arrangement spanned by an almost square unit cell containing two molecules. Both superstuctures simultaneously occur in a narrow coverage range close to completion of the molecular monolayer. Structural properties were consistently probed in real and reciprocal space by scanning tunnelling microscopy and low-energy electron diffraction, respectively.

O 45.7 Tue 18:30 P1A

Manipulation of H_2Pc tautomerization by multi-atom structures — •Markus Leisegang[1], Jens Kügel[1], Andreas Krönlein[1], Markus Böhme[1], and Matthias Bode[1,2] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Wilhelm Conrad Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Recent scanning tunneling microscopy (STM) studies showed that the switching behavior of hydrogen protons between different molecular sites, a so-called tautomerization, can be influenced by a molecule–substrate symmetry mismatch [1] or by the proximity of a single atom [2]. Here, we will show how the controlled switching behavior of a single H_2Pc molecule and its dehydrogenated form can be modified by nanostructures assembled in an atom-by-atom process. Towards this goal we developed an experimental procedure that allows for the highly controllable release of single atoms from silver STM tips onto a Ag(111) surface. Manipulating these adatoms facilitates the creation of various molecular environments that reduce or amplify the tautomerization processes.

[1] J. Kügel *et. al.*, ACS Nano (DOI: 10.1021/acsnano.6b05924).

[2] T. Kumagai *et. al.*, Nat. Chem., **6**, 41-46 (2014).

O 45.8 Tue 18:30 P1A

Adsorption and desorption of water on oligo(ethylene glycol) substituted alkanethiolate monolayers — •Mustafa Sayin[1], Alexei Nefedov[2], and Michael Zharnikov[1] — [1]Applied Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — [2]Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

We studied kinetics and thermodynamics of the water adsorption and desorption as well as wetting and nucleation behaviors of water on a series of model organic surfaces, formed by oligo(ethylene glycol) substituted alkanethiolate (OEG-AT) self-assembled monolayers. The ultimate goal of the study was to get a better understanding of the mechanism behind the inertness of poly(ethylene glycol) and OEG-based organic surfaces with respect to protein adsorption and biofouling. The kinetic and thermodynamic parameters were studied by thermal desorption spectroscopy. Two adsorbate phases with different parameters and behavior were observed, viz. the interfacial and hydration phase. The bonding character of the hydration phase as well as the structure and morphology of the interfacial phase were investigated by high resolution X-ray photoelectron spectroscopy and near edge X-ray absorption fine structure spectroscopy.

O 45.9 Tue 18:30 P1A

Computational Phase Diagram Prediction for Organic Monolayers on Metal Substrates — •Lukas Hörmann, Michael Scherbela, Veronika Obersteiner, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

Monolayers of organic molecules on inorganic substrates often show rich polymorphism with diverse structures in differently shaped unit cells. Determining the different commensurate structures and their epitaxy matrices from first principles is far from trivial due to the large number of possible polymorphs.

We pursue a novel approach based on coarse-graining the potential energy surface and applying machine learning to efficiently determine the energetically most stable structures. First the adsorption geometries of isolated molecules as well as all possible unique super cells of the substrate are determined. Then all configurations are generated by combining each adsorption geometry with every super cell. For a subset of configurations adsorption energies are determined using dispersion-corrected DFT. This subset serves as training data for a machine learning algorithm, that allows us to predict the adsorption energies for all configurations. Configurations with an adsorption energy below a predefined energy threshold are then probed using DFT.

We demonstrate the capability of our approach for TCNE (tetracyanoethene) on Cu(100) and Naphtalene on Cu(111). We determine the adsorption energies for a large number of polymorphs and compare the results to the experimentally obtained phase diagram.

O 45.10 Tue 18:30 P1A

Investigating the stability of thiolates and selenolates on Au(111) using density functional theory — •Giulia Nascimbeni, Elisabeth Verwüster, and Egbert Zojer — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8020 Graz, Austria

Considering that chemical and physical properties of sulfur and selenium are very similar, self-assembled monolayers (SAMs) of selenoles

are frequently used as an alternative to the thiole ones, often achieving superior film properties. In this work we study the stability of thiole and selenole based SAMs on Au(111) using dispersion-corrected density functional theory. As test systems we consider both aromatic and aliphatic SAMs, which have been experimentally intensively characterized [1, 2]. Our main goal is to gain fundamental insight into the relative stabilities of the bonds between the metal and the docking groups and between the docking groups and the SAM backbones. In order to account for the contributions of zero point energy and thermally activated vibrations, we also calculated the vibrational properties of the extended metal-SAM interfaces and of the individual components of the system of interest.
[1] Ossowski et al., *ACS Nano*, 2015, **9**, 4508.
[2] Ossowski et al., *Angew. Chem. Int. Ed.*, 2015, **54**, 1336.

O 45.11 Tue 18:30 P1A

Topology Dependent Molecule-Substrate Interactions: Azulene vs. Naphthalene in Temperature-Programmed Desorption — •Stefan Renato Kachel, Maik Schöniger, Martin Schmid, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

Understanding the interaction of π-conjugated organic molecules with metal surfaces is crucial for the development of modern organic electronic devices. To uncover how the topology of the π-system influences the surface chemical bond, the structural isomers azulene and naphthalene on Ag(111) and Cu(111) were investigated by temperature-programmed desorption. While naphthalene has a benzoid, alternant topology, azulene is a prototypical example for a π-system with a non-alternant topology. On Cu(111), azulene has a much higher desorption temperature (520 K) than naphthalene (340 K) in the limit of low coverage, while the difference is less pronounced on Ag(111). With increasing submonolayer coverage, all systems show substantial peak broadening towards lower temperatures, which is typical for intermolecular repulsion. The effect is most pronounced for azulene/Cu(111), where the monolayer signals spread over almost 300 K. Refined analysis on the basis of heating-rate variation studies provides desorption energies of 165 kJ/mol for azulene and 100 kJ/mol for naphthalene, both on Cu(111). The large energy difference indicates that the topology of the molecular π-system has enormous influence on the molecule-substrate interaction.

O 45.12 Tue 18:30 P1A

Topologically Different Aromatic Isomers on Metal Surfaces: A Molecular Model System for 5-7 Defects in Graphene — •Katharina K. Greulich[1], Benedikt P. Klein[1], Nadine van der Heijden[1], Claudio K. Krug[2], Stefan R. Kachel[1], Maik Schöniger[1], Phil Rosenow[1], Martin Schmid[1], Ralf Tonner[1], Ingmar Swart[2], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Debye Institute for Nanomaterial Science, Utrecht University, The Netherlands

While conjugated systems with alternant topologies and their interaction with metal surfaces have been subject to intensive investigation, much less is known about their non-alternant isomers. A conjugated system with non-alternant topology occurs in the 5-7 defects of graphene. As a molecular model system for these defects, we investigated azulene and compared it to naphthalene as a model for the regular 6-6 motif. Both molecules were studied on Cu(111) and Ag(111) surfaces with PES, NEXAFS, TPD, nc-AFM, STM and periodic DFT calculations. The non-alternant topology causes non-uniform charge distribution and more localized frontier orbitals, resulting in a much stronger and more localized interaction with both metal surfaces. Manifestations of the stronger interaction of the non-alternant molecule with the surface include interfacial charge transfer and substantial inplane and out-of-plane deformations. The latter result from the donation of electron density into the LUMO of the non-alternant molecule.

O 45.13 Tue 18:30 P1A

Effects of Surface Modification by Silane Based Self-Assembled Monolayers — •Franziska Maercks, Julia Rittich, Sebastian Jung, Carolin C. Jacobi, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

The performance of organic devices such as Organic Light Emitting Diodes (OLED) or Organic Thin Film Transistors (OTFT) depends on the interfaces between the different layers. Hence, the optoelectronic device properties can be strongly altered by the choice of electrode material. Therefore, it is important to investigate the organic-inorganic interface with respect to electronic structure changes driven by electrode surface functionalization.

A unique class of modifications is provided by Self-Assembled Monolayers (SAMs). This type of modification is able to tailor the work function of the electrode. Furthermore, the growth of a subsequently deposited organic layer can be influenced. In this study silicon (001) substrates were modified by silane based SAMs. The work function change and the electronic structure at the interface is investigated with photoelectron spectroscopy measurements (XPS, UPS, IPES) allowing us to investigate the interaction of the organic layer and the SAM modified electrode surface.

O 45.14 Tue 18:30 P1A

The initial stages and local configurations of ultrathin TiOPc layers on Ag(111) — •Sebastian Thussing, Laura Fernandez, Alexander Mänz, Gregor Witte, and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany

The evolution of titanyl-phthalocyanine (TiOPc) thin films grown on Ag(111) has been investigated using IRAS, SPA-LEED, TDS and STM. In the (sub)monolayer regime a 2D-gas, a commensurate (c) and a point-on-line (POL) phase can be observed, thereby the non-planar TiOPc molecule is adsorbed in an oxygen-up configuration with the molecular backbone oriented parallel to the surface. The c-phase contains two molecules at inequivalent adsorption sites within the unit cell displaying different azimuthal orientations with respect to the Ag(111) substrate. Approaching full saturation (POL-phase) Pauli repulsion leads to a further azimuthal reorientation that enables a higher packing density. By monitoring the prominent Ti=O stretching mode in IRAS and identifying local molecular packing configurations in STM, a microscopic model for the growth of TiOPc bilayers on Ag(111) is suggested and defect structures within these bilayers are identified. The TiOPc bilayer displays a high thermal stability up to 500 K, which is attributed to hydrogen bonds between oxygen of the titanyl unit and the hydrogen rim of phthalocyanines in the second layer, in addition to contributions arising from the oppositely oriented axial dipole moments and the ubiquitous van der Waals interactions.

O 45.15 Tue 18:30 P1A

Morphology and Electronic Structure of Tris-HCl crystals on pure and alloyed gold surfaces — •Seyma Nayir and Oğuzhan Gürlü — Istanbul Technical University, Department of Physics, Maslak, 34469, Istanbul, Turkey

Tris-HCl is one of the components of widely used buffer solution Tris-EDTA for the storage of DNA and RNA. Apart from the biological studies and medicine, tris also finds use in solar cell systems as an organic thermal energy storage material. When drop casted from the solution, Tris-HCl crystallizes on gold coated pure mica and gold coated chromium on mica surfaces differently. In this work we investigated the reasons for differences in such crystallization behavior of Tris-HCl. The surface topography and crystalline structure of Tris-HCl deposits were investigated by atomic force microscopy. Additionally we performed Kelvin Probe Force Microscopy measurements in order to measure the local contact potential difference of Tris-HCl crystallites and films on gold surfaces, and calculated the local work function changes. Our results indicate a strong dependence of the crystallization behavior of the Tris-HCl on the electro-static landscape of the host surfaces rather than their morphology.

O 45.16 Tue 18:30 P1A

Light-induced spin-state switching in Fe(II) spin-crossover thin films on $TiTe_2$ studied with NEXAFS and ARPES — •Simon Jarausch[1], Sebastian Rohlf[1], Matthias Kalläne[1], Benedikt Flöser[2], Felix Tuczek[2], and Kai Rossnagel[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany — [2]Institut für Anorganische Chemie, Universität Kiel, 24098 Kiel, Germany

Coordinative Fe(II) complexes are model systems for organic molecules whose electronic, magnetic, and structural properties can be manipulated by external stimuli. Moreover, the temperature- and light-driven spin transitions observed in a number of these materials may provide a suitable testbed for the development of future spintronic devices. The temperature- and light-induced spin-state switching of the spin-crossover complex (SCO) $Fe(H_2bpz)_2(phen)$ adsorbed on Au(111) is well established, but not preserved for molecules in direct contact to the surface due to molecular dissociation. To avoid this effect, one can either increase the stability of the SCO complex or reduce the substrate-mediated interactions. For the latter approach, the layered transition-metal dichalcogenide $TiTe_2$ may be a promising alternative due to its weak van-der-Waals-like interaction with adsorbates. Here, we present a combined near edge X-ray absorption fine structure (NEXAFS) spectroscopy and angle-resolved photoemission spectroscopy (ARPES) study of the spin-state switching of a stabilized Fe(H$_2$bpz)$_2$(phen) derivative adsorbed on TiTe$_2$.

O 45.17 Tue 18:30 P1A

On-Surface Synthesis of Naphthalocyanine and Corrole Complexes — •Malte Zugermeier[1], Min Chen[1], Lukas Heuplick[1], Martin Liebold[1], Nicolas Bock[1], Falk Niefind[1], Lukas Ruppenthal[1], Martin Schmid[1], Peter Schweyen[2], Martin Bröring[2], Jörg Sundermeyer[1], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Institut für Anorganische und Analytische Chemie, Technische Universität Braunschweig, Germany

Tetrapyrrole macrocycles are important examples of biomimetic systems that found the way into real-life applications. Porphyrins possess interesting catalytic and optoelectronic properties. The usage of their metal complexes for surface functionalization can benefit from oxidation state tuning of the metal center to control its chemical and electronic properties. This is possible with axial ligands or modifications of the equatorial tetrapyrrole ligand. In contrast to porphyrins, adsorbed corroles can oxidize metal atoms to their +III oxidation state. For detailed insight into this surface coordination reaction, we studied mono- and multilayers of an octa-alkyl corrole and their reaction with transition metals by XPS, UPS, NEXAFS and STM. Furthermore, we report the on-surface synthesis of the closely to porphyrins and corroles related, artificial naphthalocyanines on Ag(111) by tetramerization of dicarbonitriles in the presence of iron. STM and XPS studies reveal that pre-reaction dicarbonitrile forms organometallic structures with the Fe atoms, whereas the post-reaction layer consists of iron naphthalocyanine complexes.

O 45.18 Tue 18:30 P1A

Surface crystallography of large organic molecules on metal and insulator surfaces by LEED-IV using Fourier coefficients — •Ina Krieger[1,3], Georg Held[2], Christian Kumpf[3], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn, 53115 Bonn, Germany — [2]Department of Chemistry, University of Reading and Diamond Light Source, UK — [3]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52428 Jülich, Germany

We will report on LEED-IV analysis of the large organic molecules PTCDA and NTCDA on the metal and insulator surfaces Ag(100), Ag(111), and KCl(100). Using data from different angles of electron incidence and optimizing the LEED-IV program code we were able to extend the experimental data set and shorten the calculation times required for the complex and large unit cells. Furthermore, the distortion of the PTCDA molecule and the buckling of the Ag surface were described by Fourier coefficients taking into account the symmetry of the system [1]. The idea of this procedure is to suppress unphysical vertical displacements of atoms on a short-wave-length scale by restriction to lower order coefficients.

By this, we obtain good Pendry R-factors, for PTCDA/Ag100 of about 0.23. We were able to derive the vertical distortions of the oxygen atoms in the functional group and the buckling of the Ag surface in rather good agreement with earlier results from DFT and NIXSW studies.

[1] W. Moritz et al, Phys. Rev. Lett. 104, 136102 (2010).

O 45.19 Tue 18:30 P1A

Theoretical Insights into Highly Selective Organic-Inorganic hybrid NO$_2$ Gas Sensors — •Giulio Cocco[1], Leonhard Mayrhofer[1], Alaaeldin Gad[2], Olga Casals[3], Nicolai Markiewicz[2], Juan Prades[3], Andreas Waag[2], and Michael Moseler[1] — [1]Freiburg Materials Research Center, University of Freiburg, D-79104 Freiburg, Germany — [2]Institute for Semiconductor Technology, Braunschweig University of Technology, Hans-Sommer-Straße 66, D-38106 Braunschweig, Germany — [3]MIND-IN[2]UB, Department of Electronics, University of Barcelona, C/Martí i Franquès 1, E-08028 Barcelona, Spain

The low selectivity of inorganic gas sensors is among the issues hindering their applications in environmental monitoring. Semiconductor nanowires (NWs) functionalized by self-assembled monolayers (SAMs) of organic molecules are a promising class of materials offering selectivity and sensitivity towards single gas species [1][2][3]. DFT simulations will be used to give insights on this new approach of highly selective NO$_2$ gas sensors. However, moisture is a critical factor influencing stability and responses towards gas. A novel concept of mixed SAMs is introduced to improve such issues. Here, by means of DFT, we analyze the different responses of NWs functionalized with silanes toward NO$_2$ at different relative humidity. We show that water can modify the response although no direct electronic interaction between water and functionalized NWs is observed.

[1]Adv. Funct. Mater. **2014**,24, 595 [2]Adv. Mater.**2014**, 26, 8017 [3]ACS Sensors **2016**, acssensors.6b00508

O 45.20 Tue 18:30 P1A

Deposition of tetracene on Si(111)-(7x7) — •Christian Völkner, Bahaaeddin Irziqat, Kevin Oldenburg, Ingo Barke, and Sylvia Speller — University of Rostock, Institute of Physics, 18059 Rostock, Germany

Organic electronics and their individual components are becoming increasingly smaller nowadays. To precisely control the deposition of small amounts of organic molecules on a substrate a dedicated evaporator chamber was built and attached to a commercial Low Temperature Scanning Tunneling Microscope system. The performance of the evaporator is evaluated depositing tetracene molecules on Si(111)-(7x7). The structure of the tetracene layers is investigated.

O 45.21 Tue 18:30 P1A

Vibrational properties of organic thin films on graphene/Ru(0001) — •Sebastian Flade and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany

Ultrathin films of fullerene (C_{60}) and pentacene (PEN) have been prepared on graphene/Ru(0001) and their vibrational properties, as well as thermal evolution investigated by using Fourier-transform infrared spectroscopy. Monolayer species are found to display distinctly different vibrational signatures as compared to higher layers which indicates a weak chemical interaction. From the variation of relative intensities of vibrational modes structural changes within the organic films are derived. In particular, the thermal stability of grown layers, as well as their layered structure in case of C_{60} - PEN heterolayers on g/Ru(0001) has been monitored. Comparison to layers deposited directly on the Ru(0001) surface illustrates the effect of graphene acting as a passivation layer between the transition metal substrate and the molecular film.

O 45.22 Tue 18:30 P1A

Polarization-Dependent Excitation of Porphyrin Nanostructures investigated by PEEM — Hannes Hartmann, Karl-Heinz Meiwes-Broer, •Ingo Barke, and Sylvia Speller — University of Rostock, Institute of Physics, 18059 Rostock

In photoemission the dependence on light polarization can help to access the internal structure of molecule aggregates. Recently we selectively mapped excited states in copper tetraundecylporphyrin (CuTUP) nanostructures on graphite (HOPG) using two-photon photoemission electron microscopy (2PPE-PEEM) [1]. Here we present polarization-dependent and spatially resolved electron yields of the same system using varying excitation wavelengths. We observe a Davydov-like splitting of the Soret band which shows a systematic dependence on the specific location. By varying the light polarization this spatial effect is correlated with the direction of the transition dipole moments. These results are discussed in view of orientation and internal structure of the CuTUP assemblies. In addition we observe characteristic variations of the photoelectron intensity which is found to be connected to the local height as determined by correlative atomic force microscopy measurements. This behavior is analyzed in the framework of vertical optical standing waves within the CuTUP structures.

[1] H. Hartmann et al., J. Phys. Chem. C **120**, 16977 (2016)

O 45.23 Tue 18:30 P1A

The Ionic Liquid|Graphite(0001) and Ionic Liquid|Li$_4$Ti$_5$O$_{12}$ (111) Interface as a Model for the Electrode|Electrolyte interface in Li-ion Batteries — •Jihyun Kim[1], Florian Buchner[2], Christiane Adler[1], Maral Bozorgchenani[1], Joachim Bansmann[1], 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, Helmholtzstr. 11, D-89081 Ulm, Germany

In this ultrahigh vacuum model study, we explore two anode processes which are highly important for the function of Li-ion batteries: (1) the reversible inter- and deintercalation of lithium (Li) and (2) the formation of the so-called electrode|electrolyte interface (EEI). Employing X-ray and UV photoelectron spectroscopy (XPS / UPS) and using well-defined anode surfaces such as graphite (0001) and $Li_4Ti_5O_{12}$ (111) (LTO) we found that vapor deposition of metallic Li on graphite (0001) at 80 K results in partially charged $Li^{\delta+}$ atoms, while for deposition at 300 K Li intercalates, forming Li_xC_6. Using $Li_4Ti_5O_{12}$ as substrate, Li diffuses into the bulk for deposition at 300 K as well, while for deposition at 80 K XPS reveals the formation of very small amounts of Ti^{3+}. Evidently, under these conditions some of the Li remains near the surface, generating the Li-rich $Li_7Ti_5O_{12}$ phase, while the majority dissolves into the bulk. Finally, to mimic the EEI, we studied the temperature-dependent interaction of (sub-)monolayers of the ionic liquid [BMP][TFSA] with both graphite/lithiated graphite and the Li-poor/Li-rich LTO.

O 45.24 Tue 18:30 P1A

Spectroscopy from 1,3-Diphenylisobenzofuran films on Cu(111) and Au(100) — •Janek Rieger, Angelika Demling, David Nobis, Daniel Niesner, Feifei Xiang, M. Alexander Schneider, and Thomas Fauster — Lehrstuhl für Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Thin films of 1,3-Diphenylisobenzofuran (DPIBF) show singlet fission, a mechanism for multi-exciton generation that might be used to enhance the efficiency of organic photovoltaics [1]. The yield of singlet fission depends strongly on the structural polymorph of the film [2]. Mixtures of several polymorphs were shown to form on oxide substrates. We use optical and photoelectron spectroscopies, scanning tunneling microscopy and thermal desorption spectroscopy to investigate DPIBF deposited on Cu(111) and Au(100) by thermal evaporation. Results are presented for various growth temperatures and for film thicknesses from one monolayer to 40 nm. While growth on Au(100) results in coexisting structures at all tested conditions, phase-pure films are prepared on Cu(111). The first layer adsorbs in an ordered structure at room temperature, with a molecular arrangement similar to the one in crystals. For thicker films, single series of photoluminescence peaks are found. The singlet transition blueshifts with increasing preparation temperature for DPIBF on both substrates. The maximum singlet energy is close to 2.8 eV, sufficient to support singlet fission [2].

[1] J. C. Johnson et al., J. Am. Chem. Soc. **132** (2010) 16302
[2] J. L. Ryerson et al., J. Phys. Chem. C **118** (2014) 12121

O 45.25 Tue 18:30 P1A

Dielectric properties of carbon nanomembranes prepared from aromatic self-assembled monolayers investigated by impedance spectroscopy — Paul Penner, Emanuel Marschewski, •Xianghui Zhang, and Armin Gölzhäuser — Faculty of Physics, University of Bielefeld, 33615 Bielefeld

Carbon nanomembranes (CNMs) are two-dimensional materials that are made by cross-linking self-assembled monolayers (SAMs) of aromatic molecules via low energy electron irradiation. Here we investigate the dielectric properties of pristine SAMs and CNMs with an EGaIn top electrode by impedance spectroscopy. Analysis and comparison of the tunneling resistance and capacitance density of pristine and cross-linked SAMs revealed a thickness dependent capacitance associated with the monolayer as well as a thickness independent capacitance. The latter could be attributed to the appearance of a new interface due to the decoupling of molecules from the underlying gold surface upon electron irradiation. We adopted an equivalent circuit to take into account the interfacial capacitance as well as the oxide layer of the EGaIn top electrode. An interfacial capacitance of about 5 $fF/\mu m^2$ was obtained for CNM-based molecular junctions. The tunneling decay constant β remains unaffected after electron irradiation, which exhibits a value of about 0.5 $Å^{-1}$ for both systems. Determination of dielectric constants of SAMs and CNMs from the impedance spectra will also be analyzed and discussed.

O 45.26 Tue 18:30 P1A

Investigating the orientation of halogenated benzene molecules on Cu(111) surfaces using IR spectroscopy — •Christina Pentzek and Karina Morgenstern — Ruhr-Universität Bochum, Chair of Physical Chemistry I, Germany

Adsorption of organic molecules on metal surfaces is important to understand the mechanisms in heterogeneous catalysis. In this study, vibrational spectra of chlorobenzene and bromobenzene molecules adsorbed on a Cu(111) surface are investigated by reflection-absorption infrared spectroscopy (RAIRS). While it is well established that unsubstituted benzene molecules adsorb with their molecular plane in parallel to the surface, it is not known how halogen molecules influence the adsorption orientation. Because of the selection rules of RAIRS we are able to identify the orientation of halogenated benzene molecules on Cu(111) surfaces. However, the vibration modes depend on the layer thickness of molecules at the surface. In this presentation we want to discuss different orientations of halogenated benzenes at different coverages at low temperatures.

O 46: Electronic Structure of Surfaces: Spectroscopy, Surface States

Time: Tuesday 18:30–20:30 Location: P1A

O 46.1 Tue 18:30 P1A

Influence of the Surface Structure on Photoelectron Momentum Maps Measured for Coronene Monolayers on Ag(111) — •Christian Udhardt[1], Felix Otto[1], Tino Kirchhübel[1], Falko Sojka[1], Tobias Hümpfner[1], Matthias Meissner[1], Christian Kern[2], Daniel Lüftner[2], Peter Puschnig[2], Bernd Schröter[1], Roman Forker[1], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Institute of Physics, University of Graz, 8010 Graz, Austria

Photoelectron momentum maps (PMMs) can be helpful to investigate molecular states near the Fermi edge, even though their discussion may be complicated by substrate- and film-induced effects. Here, we present PMMs of 1 ML coronene thin films on Ag(111) and compare them to simulations of a free coronene molecule, the 4 × 4 film structure observed with low-energy electron diffraction (LEED), and angle-resolved ultraviolet photoemission spectroscopy (ARUPS). While the substructure observed in the PMM of the highest occupied molecular orbital (HOMO) is shown to coincide with the structure of the coronene film, the features in the PMM taken at the Fermi edge are conform with a film-induced back-folding of substrate bands without the influence of a molecular state.

O 46.2 Tue 18:30 P1A

STM-Investigations of κ-(BEDT-TTF)$_2$X-Charge Transfer Salts — •Torge Mashoff, Johannes Regel, and Hans-Joachim Elmers — Institut für Physik, Johannes Gutenberg-Universität, Mainz

Organic charge-transfer salts of the κ-(BEDT-TTF)$_2$X family offer exciting many-body physics manifesting in an interesting phase diagram with a neighboring superconducting and Mott insulating phase. This results in a strong deviation of the superconducting properties from BCS theory and has been attributed to their two-dimensional structure leading to electronic correlation effects. We investigated small crystals of the two charge-transfer salts κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br and κ-(BEDT-TTF)$_2$Cu(NCS)$_2$ using a low temperature scanning tunneling microscope and obtained good topographic resolution of the crystallographic structure. Both crystals show similar crystallographic order but due to the higher chemical pressure of κ-(BEDT-TTF)$_2$Cu(NCS)$_2$, they have different positions in the phase diagram. We used scanning tunneling spectroscopy to investigate the electronic properties and the influence of the proximity to the Mott phase.

O 46.3 Tue 18:30 P1A

Time-resolved momentum microscopy with fs-XUV light — •Christina Schott[1], Markus Rollinger[1], Sebastian Emmerich[1], Johannes Seidel[1], Florian Haag[1], Norman Haag[1], Steffen Eich[1], Mirko Cinchetti[2], Benjamin Stadtmüller[1], and Martin Aeschlimann[1] — [1]University of Kaiserslautern and Research Center OPTIMAS, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

Time resolved photoemission spectroscopy with a fs-XUV light source is a powerful technique to investigate ultrafast optically induced electron dynamics in solid state systems [1,2]. The combination of this technique with momentum microscopy, a novel tool for angle resolved photoemission, allows us to capture transient snapshots of the ultrafast dynamics for both parallel momentum components for one fixed binding energy. Together with the large photon energy of our fs-XUV light source, we can access the electron dynamics throughout the entire first Brillouin zone of typical sample systems. Here, we will show the capability of our new setup for time-resolved optical-pump, fs-XUV probe momentum microscopy. We will discuss experimental challenges such as space charge effects and long-term stability using dedicated sample systems. Moreover, we will present our first results of the transient band structure dynamics of metallic surfaces using time-resolved momentum microscopy.

[1] Rohwer et al, Nature (2011) [2] Eich et al, J el. Spec (2014)

O 46.4 Tue 18:30 P1A

Spin-polarized surface states of Pb monolayers on Si(111) — Christian Brand[1], Herbert Pfnür[1], Jan-Hugo Dil[2,3], Stefan Muff[2,3], Michael C. Tringides[4], and •Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Germany — [2]Swiss Light Source, Villigen, Switzerland — [3]École Polytechnique Fédérale de Lausanne, Switzerland — [4]Ames Laboratory & Iowa State University, Ames, USA

Atomic monolayers (ML) of Pb/Si(111) have recently been found to be superconducting below $T_\mathrm{C} \approx 1.8\,\mathrm{K}$, but the mechanism behind the evolution of these 2d states is not understood yet. In the range from 6/5 ML to 4/3 ML supercells consisting of linear combinations of $(\sqrt{7}\times\sqrt{3})$ and $(\sqrt{3}\times\sqrt{3})$ unit cells are formed (so-called Devil's staircase regime). This allows us to tune the spin-orbit interaction (SOI), the electronic and atomic structure via adsorption of minute amounts of Pb. In this study we present STM and (SR)-ARPES measurements at low T ($> T_\mathrm{C}$) to evaluate the influence of the SOI on the Pb surface states. As it turns out the local adsorption geometry and symmetry of the atomic structure plays an important role for the understanding of the measured spin-polarization by SR-ARPES showing strongly spin-polarized metallic surface states. The experimental results are in very good agreement with DFT calculations and reveal beside a complex spin-texture at E_F large Rashba- and Zeeman-type spin-splittings of the Pb surface states.

O 46.5 Tue 18:30 P1A

2D Dirac cones at the Fermi level in ZrSiTe — •Shweta Sheoran[1], Andreas Topp[1], Judith M. Lippmann[1,2], Andrei Varykhalov[3], Viola Duppel[1], Bettina V. Lotsch[1,2,4], Christian R. Ast[1], and Leslie M. Schoop[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Department of Chemistry, Ludwig-Maximilians-Universität, D-81377 München — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, D-12489 Berlin — [4]Nanosystems Initiative Munich (NIM) & Center for Nanoscience, D-80799 München

A new class of materials exhibiting non-symmorphic symmetry has generated great interest, due to the associated rich physics such as ultra high mobility, giant magneto-resistance and also it's essential role in the discovery of new quasi particles beyond the usual Dirac, Weyl and Majorana fermions. Experimental analysis shows that the material ZrSiS, exhibits Dirac cones protected by non-symmorphic symmetry below the Fermi level [1]. A major requirement for pinning these non-symmorphic crossings at the Fermi level is a half filled band, which is quite difficult to achieve. A possible workaround could be the application of uniaxial tensile strain. In ZrSiS, this would be equivalent to substitution of S by Te, leading to the isostructural and isoelectronic compound ZrSiTe. Here we present the DFT bandstructure calculations and ARPES measurements performed on ZrSiTe, showing that it exhibits a Dirac line node on the Fermi level.

[1] Schoop, L.M. *et al.*, Nat.Commun. 7, 11696 (2016).

O 46.6 Tue 18:30 P1A

Multi-electron photon-emission from a tunnel junction — •Philip Kapitza, Ebru Ekici, Kira Kolpatzeck, Rolf Möller, and Christian A. Bobisch — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Inelastic tunneling processes in the tip/sample junction of a scanning tunneling microscope (STM) can excite tip induced plasmon modes (TIP), which can decay radiatively. The emitted light carries information about the underlying inelastic processes. We observe light emission between the visible and the near infrared range from the junction between a silver covered STM tip and a Ag(111) surface. The applied voltage V_{Bias}, limits the maximum energy $\mathrm{E}_{max} = \mathrm{eV}_{Bias}$ of the tunneling electrons. Normalized Emission spectra show emission tails exceeding E_{max}, supposedly caused by natural linewidth broadening. A comparison with calculated tunneling probabilities for inelastic transitions results in electron-lifetimes of the excited states in the range of 30 fs to 80 fs. If the tunneling current I_T is unusual high (nA to μA), two or more electrons may interact and exchange energy and non-linear processes may be triggered [1], [2]. In this case, photons with an energy $\mathrm{E}_{max} < \mathrm{E}_{photon} < 2\mathrm{E}_{max}$ can be observed. For these cases, spectra of emitted light are discussed as a function of the tunneling parameters. However, the emission spectra reveal the same spectral features, indicating that the same TIP modes are excited.

[1] G. Hoffmann et al., Phys. Rev. Lett. 90, 046803-1 (2003).

[2] G. Schull et al., Phys. Rev. Lett, 102, 057401 (2009).

O 46.7 Tue 18:30 P1A

Investigation of charge puddles at the surface of the compensated topological insulator BiSbTeSe$_2$ — •Timo Knispel, Wouter Jolie, Nick Borgwardt, Zhiwei Wang, Jonathan Lux, Achim Rosch, Yoichi Ando, Markus Grüninger, and Thomas Michely — II. Physikalisches Institut, Universität zu Köln, Germany

BiSbTeSe$_2$ is a three dimensional topological insulator which is characterized by an insulating bulk state and a gapless Dirac cone at the Γ-point, with the chemical potential near the Dirac point [1]. Large fluctuations in the Coulomb potential of the dopants cause self-organized charge puddles in the bulk, which in turn cause substantial rigid shifts of the local bulk band structure. Surprisingly, these charge puddles evaporate around 50 K [2]. Here we investigate by STM and STS charge puddles at the surface of BiSbTeSe$_2$ and how they are linked to the bulk ones.

In atomic resolution STM and STS measured over a broad energy range we identify (i) a short length scale due to variations in chemical composition, (ii) a medium energy-dependent length scale due to quasi-particle scattering, and (iii) a large length scale which we attribute to surface charge puddles. By point spectroscopy we measure Dirac point fluctuations of $\Delta E = 25$ meV around an average of +30 meV. Through temperature dependent experiments we analyze the coupling of the surface charge puddles to their bulk counterparts.

[1] T. Arkane et al., Nat. Comm. 3, 636 (2012)

[2] N. Borgwardt et al., Phys. Rev. B 93, 245149 (2016)

O 46.8 Tue 18:30 P1A

Studying the type-II Weyl semimetal *Td*-WTe$_2$ with two-photon photoemission — •Petra Hein[1], Stephan Jauernik[1], Yulin Chen[2], Lexian Yang[2], Binghai Yan[3], Claudia Felser[3], and Michael Bauer[1] — [1]Institute of Experimental and Applied Physics, University of Kiel, Germany — [2]Physics Department, Tsinghua University, Beijing, China — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

With their first experimental observation in 2015, topological Weyl semimetals have attracted enormous attention: In these materials, the long sought-after Weyl fermions are realized as quasi-particle excitations in condensed matter [1]. Weyl semimetals feature an unusual electronic structure with touching points in the bulk band structure – the so-called Weyl points - that are connected by unique topological surface Fermi arcs. The key technique to gain access to these signatures is angle-resolved photoelectron spectroscopy (ARPES) [2,3].

Here, we present a combined photoemission and two-photon photoemission (2PPE) study of the type-II Weyl semimetal *Td*-WTe$_2$. Using a widely tunable femtosecond laser system with photon energies between 1.3 eV and 5.0 eV, we are able to access a variety of both occupied and unoccupied electronic states. The results are discussed under consideration of band structure calculations and current ARPES studies of *Td*-WTe$_2$.

[1] A. Vishwanath, Physics **8**, 84 (2015).

[2] S.-Y. Xu *et al.*, Science **349**, 6248 (2015).

[3] Y. Wu *et al.*, Phys. Rev. B **94**, 121113(R) (2016).

O 46.9 Tue 18:30 P1A

Thickness-dependent photoelectron spectroscopy study of 1,2;8,9-dibenzopentacene on Au(111) — •Maximilian Schaal, Felix Otto, Christian Udhardt, Bernd Schröter, Roman

Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Alkali-metal-doped polycyclic aromatic hydrocarbons received broad attention as potential organic superconductors during the last years. A representative of this class is potassium-doped 1,2;8,9-dibenzopentacene (DBPen) which has a reported transition temperature of 33 K in bulk powder samples [1]. Here we investigate thin films of DBPen on Au(111) by means of thickness-dependent x-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS). The XPS results show a thickness-independent line shape and an energy shift by the formation of an interface dipole. The UPS results show an asymmetric broadening of the highest occupied molecular orbital (HOMO) in the monolayer which is attributed to the occurrence of vibronic states. The HOMO splitting in the bilayer indicates the formation of a dimer structure via π-stacking. Furthermore, we explore the thickness-dependent modification of the binding energy and effective mass of the Shockley surface state of Au(111) by angle-resolved UPS (ARUPS).

[1] M. Xue *et al.*, Sci. Rep. **2**, 389 (2012).

O 46.10 Tue 18:30 P1A

Electronic Properties of Coronene on (111)-Surfaces of the Coinage Metals. — •Christian Simon Kern[1], Daniel Lüftner[1], Christian Udhardt[2], Felix Otto[2], Roman Forker[2], Torsten Fritz[2], and Peter Puschnig[1] — [1]University of Graz, Institute of Physics, NAWI Graz - Universitätsplatz 5, A-8010 Graz, Austria — [2]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743 Jena, Germany

Mono-layers of the polycyclic aromatic hydrocarbon coronene adsorbed on (111)-surfaces of the metals copper, silver and gold are investigated by density functional theory.

First, we have determined the most favorable adsorption sites and molecular orientations based on the experimentally known over-layer structures. Particularly, for Ag(111) we find a flat adsorption geometry with an azimuthal orientation in good agreement with the experimental orientation. In a second step, we have simulated angle-resolved photoemission spectroscopy (ARPES) experiments for coronene on the three coinage metal (111)-surfaces, focusing on the emission from the HOMO. Simulated photoelectron angular distributions (PADs) for the coronene/metal interface show pronounced differences to PADs of the two-fold degenerate HOMO of the isolated molecule. We conclude that the observed symmetry-breaking results from the molecule-substrate-interaction and intermolecular band dispersion. The observed sub-structure of the major emission features in the PADs compares well to the experimental findings.

O 46.11 Tue 18:30 P1A

Charge-ordered state in the low-temperature phase of Pb/Si(111) — •Florian Adler[1], Manuel Laubach[2], Stephan Rachel[2], Jörg Schäfer[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, Germany

Two-dimensional triangular lattices of Group IV adatoms on diamond lattice substrates provide a rich playground for experimental studies and many-body calculation techniques. For the system investigated in this work, 1/3 monolayer of Pb on Si(111), preceeding studies have noted a phase transition from $\sqrt{3} \times \sqrt{3}$ to 3×3 at 86 K. In our high-resolution scanning tunneling microscopy and spectroscopy measurements in the low-temperature phase, we have unveiled the formation of a charge-ordered state by carefully mapping the local density of states. Furthermore, we find a structural rearrangement with a 2-up/1-down configuration. These results are supported by state-of-the-art many body calculations using the Variational Cluster Approach (VCA), which is sensitive to both spin- and charge-densitiy wave instabilities. I will present a comparison of our measurements and the latest results from VCA calculations.

O 46.12 Tue 18:30 P1A

A new dual analyzer system for surface analysis of liquids under UHV conditions — •Francesco Greco, Inga Niedermaier, Claudia Kolbeck, Hans-Peter Steinrück, and Florian Maier — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

In the last decade, ionic liquid (IL) systems have emerged for UHV studies of liquid surfaces and interfaces due to the extremely low IL vapor pressure. It has been demonstrated that particularly angle-resolved X-ray Photoelectron Spectroscopy (ARXPS) allows for investigating phenomena that occur at gas-liquid and liquid-solid interfaces on the molecular level. In all of these ARXPS studies, the sample holder had to be tilted in order to change the polar detection angle of the emitted photoelectrons, which restricted the investigations to very thin and high-viscous IL films only. We here report on a new and unique laboratory "Dual Analyzer System for Surface Analysis (DASSA)" which enables fast ARXPS, UV photoelectron spectroscopy, imaging XPS, and low-energy ion scattering of macroscopically thick non-volatile liquid samples.[1] As core element, it comprises a UHV analysis chamber equipped with two electron analyzers mounted for simultaneous measurements in 0° and 80° emission relative to the surface normal for horizontally mounted IL samples.

F.G. and H.P.S. thank the ERC for financial support through an Advanced Investigator Grant to H.P.S.!

[1] I. Niedermaier, C. Kolbeck, H.-P. Steinrück, F. Maier, Rev. Sci. Instrum. 87 (2016) 045105

O 46.13 Tue 18:30 P1A

Quasiparticle interferences in highly doped bilayer graphene — •Wouter Jolie[1], Jonathan Lux[2], Mathias Pörtner[1], Tobias Hartl[1], Timo Knispel[1], Sabina Simon[1,3], Charlotte Herbig[1], Thomas Michely[1], and Carsten Busse[1,4] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Theoretische Physik, Universität zu Köln — [3]Fachbereich Physik, Universität Konstanz — [4]Institut für Materialphysik, Universität Münster

When two graphene layers are Bernal stacked as in graphite, the two low-energy bands can be described by massive Dirac fermions and it has been demonstrated that doping such a graphene bilayer not only shifts its chemical potential, but also opens up a band gap [1]. We dope bilayer graphene to populate the second conduction band and measure quasiparticle interferences (QPI) with scanning tunneling microscopy and spectroscopy.

We grow bilayer graphene on Ir(111) with a combination of chemical vapor deposition (creating a monolayer of high perfection) and physical vapor deposition (forming a second graphene layer at the interface). Subsequently, Cs is intercalated between the bilayer and the metal underneath.

We observe complex standing waves patterns at various energies and obtain the scattering vectors responsible for QPI using a Fourier transform analysis. We compare our results with simulations based on the T-matrix theory as well as tight-binding calculations and explore the origin of the suppression of certain scattering processes.

[1] E. V. Castro et al., Phys. Rev. Lett. 99, 216802 (2007)

O 46.14 Tue 18:30 P1A

Systematics of 3d transition metal–doped Sb$_2$Te$_3$ — •Johannes Jung, Thomas Bathon, Paolo Sessi, and Matthias Bode — Universität Würzburg; Physikalisches Institut; Experimentelle Physik II, Würzburg, Germany

Time-reversal symmetry plays a crucial role in topological insulators (TIs). Once broken, topological surface states become gapped and unconventional states of matter such as the quantum anomalous Hall effect can be realized.

Here, we present a systematic investigation of the prototypical TI Sb$_2$Te$_3$ where different magnetic perturbations are introduced by bulk-doping with 3d transition elements (V, Cr, Mn, Fe). The dopants adsorption sites are localized and classified by atomically resolved scanning tunneling microscopy, while scanning tunneling spectroscopy allows to visualize their influence on the local electronic environment of the host material.

[1] P. Sessi *et. al.*, Nature Communications, **7**, 12027 (2016).

O 46.15 Tue 18:30 P1A

New insights into the LaB6 (001)-surface obtained by Scanning Tunneling Microscopy — •Philipp Buchsteiner[1], Martin Wenderoth[1], and Geetha Balakrishnan[2] — [1]IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Department of Physics, University of Warwick, United Kingdom

Lanthanum Hexaboride (LaB6) has attracted much attention due to its surface properties, such as an unusually low work function [1]. However, up to now only few investigations of the (001)-surface of single crystalline LaB6 using Scanning Tunneling Microscopy (STM) have been performed [2]. Our STM findings of that surface have led to striking differences for the surface structure: firstly, we have not observed any vacancies at the surface, which we relate to our different sample preparation by cleavage. Secondly, we have observed a long range height modulation within atomically resolved constant current topographies. We are hypothizing that the modulation is caused by single interstitial and vacant boron atoms within the hexaboride lattice. Such imperfections are probably generated during crystal growth, since the B/La ratio deviates slightly in the bulk material for most crystals from 6.00 [3]. [1] M. Trenary, Sci. Technol. Adv. Mater. 13 (2012), [2] J.S. Ozcomert, M. Trenary, Surf. Sci., 265 (1992), [3] T. Tanaka, S. Otani, Prog. Cryst. Growth Charact. Mater. 16 (1988)

O 46.16 Tue 18:30 P1A

Preparation and Characterization of Sub-Monolayer Ge on Cu — •Thomas Kotzott, Wei Li, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

Semiconductor growth on metals is of interest for designing and producing devices in semiconductor-based electronics. In this study, we have prepared different copper-germanium surface structures. Clean Cu single crystal surfaces are fabricated by sputtering and annealing and characterized by LEED and AES. Sub-monolayer Ge is deposited at 100K using electron beam evaporators in-situ under UHV conditions at a base pressure of $p < 10^{-10}$ mbar. The Ge/Cu surfaces are investigated by low temperature (6K) scanning tunneling microscopy. We present topography data and the corresponding electronic structure obtained by scanning tunneling spectroscopy as well as thermovoltage measurements. The scattering processes at the Cu surface are examined, finally aiming for the scattering properties of a single semiconductor impurity within the bulk metal using dilute alloys.

O 46.17 Tue 18:30 P1A

Polarization-dependent two-photon photoemission from p-doped topological insulators $\mathbf{SnBi_xSb_{2-x}Te4}$ and $\mathbf{GeSb_2Te_4}$ — •Sebastian Otto, Jonas Rietsch, Philipp Rosenzweig, Daniel Niesner, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany

Polarization-dependent, time- and angle-resolved two-photon photoemission is used to study the electronic structure of septuple-layered antimony telluride crystals of different p-dopings. All surfaces show a linearly dispersing surface state bridging the band gap with a Dirac point at $E_F + 0.42 \pm 0.05$ eV for $GeSb_2Te_4$ and $E_F + 0.31 \pm 0.02$ eV for the $SnBi_xSb_{2-x}Te_4$ crystals. The Bi-doping of the $SnBi_xSb_{2-x}Te_4$ (with $x = 0, 0.1, 0.2$) causes no shift of the energetic position of the Dirac point, but a decrease in group velocity which is reflected in the dynamics of the systems. The lifetimes of the topological surface states range from 10 ± 5 fs to 120 ± 20 fs and time constants of the conduction band minimum are found between 180 ± 10 fs and 300 ± 20 fs. Measurements with circularly polarized probe pulses verify the topological nature of the surface states. The excitation of the topological surface state shows no dependence on the polarization of the pump pulse.

O 46.18 Tue 18:30 P1A

Characterisation of Beryllides with XPS — •Nicola Helfer, Petra Hansen, Hans Rudolf Koslowski, and Christian Linsmeier — Forschungszentrum Jülich GmbH, Institut für Energie und Klimaforschung – Plasmaphysik, 52425 Jülich

Future fusion reactors need to produce their tritium fuel. A self-sustained fuel cycle requires a neutron multiplier material, e.g. Be, within the breeding blanket. Beryllides are promising materials since their chemical reactivity with structural material is lower than for pure Beryllium [Y. Mishima et al., J. Nucl. Mat. 367–370, 1382 (2007)]. Beside the production process, the thermal stability and phase transitions are of great interest.

Be-metal alloy samples, produced by Wright Air Development Center already in 1959 were available for experimental investigation. The characterisation of the thermal stability of $Be_{12}Ta$ and $Be_{12}Ti$ with x-ray photoelectron spectroscopy (XPS) is presented here. X-ray diffraction measurements are utilised to confirm the crystalline phase of the samples.

Binding energy shifts of the Be 1*s* states have been observed and are compared to recent Density Functional Theory (DFT) simulations with an all-electron code (FLEUR) [J. Bröder, master thesis, RWTH Aachen 2015].

O 46.19 Tue 18:30 P1A

Polarization-dependent ARPES investigation for organic molecules on Ag(110) and Cu(110) — •Xiaosheng Yang[1], Daniel Lüftner[2], Georg Koller[2], Peter Puschnig[2], Michael Ramsey[2], Matteo Jugovac[3], Giovanni Zamborlini[3], Vitaliy Feyer[3], Serguei Soubatch[1], and Stefan Tautz[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Physik, Karl-Franzens-Universität Graz, 8010 Graz, Austria — [3]Elettra-Sincrotrone Trieste, 34149 Basovizza, Trieste, Italy

The angle-resolved photoemission spectroscopy (ARPES) is often used to study electronic properties of molecule/metal interfaces. In particular, for planar π-conjugated molecules, utilizing a plane wave approximation for the photoelectron final states, it is possible to completely reconstruct the spatial distribution of the molecular orbitals [1,2]. However, recently it has been shown that the plane wave approximation fails to describe correctly the angular distribution of photoemission induced by the s-polarized light [3] and a better final states approximation is needed to predict experimentally observed photoemission patterns. In this contribution, we revisit this issue and report on ARPES measurements of monolayers of several molecules - tetracene, pentacene, pentaphenyl and sexiphenyl - on Ag(110) and Cu(110) surfaces, performed using various polarizations of the incident light.

[1] P. Puschnig et al. Science 326, 702 (2009)
[2] S. Weiß et al. Nature Comm. 6, 8287 (2015)
[3] M. Dauth et al. Phys. Rev. Lett. 117, 183001 (2016)

O 46.20 Tue 18:30 P1A

Ab-initio investigation of the interface $\boldsymbol{\alpha}$-$\mathbf{Al_2O_3/Al}$ — •Lilit Amirkhanyan and Jens Kortus — TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany

Ceramic materials are used in industry to remove non-metallic inclusions from metallic melts like iron or aluminum. The filtration effect depends on interactions at the interface of the ceramic filter material. Interestingly, different ceramic materials show different filtration efficiency. Therefore, a detailed understanding of the processes at the interface are of interest.

We investigated the interface of the stable phase α-Al_2O_3 with surface (0001). A model of the Al melt has been derived from bulk Al using the (111) plane. All calculations are based on density function theory as implemented in the Quantum Espresso code. In order to investigate the effect of oxygen or aluminum termination we carried out calculation on Al_2O_3 with these two terminations using the Effective Screening Medium Method with open boundary conditions. As a result we find that both terminations will give positively charged surfaces.

Further, we created interface structures and obtained from these models an interface energy. The interface energy depends on the termination of α - Al_2O_3. In particular, the oxygen terminated interface of α - Al_2O_3/Al is more stable compared to the aluminum terminated case.

O 46.21 Tue 18:30 P1A

The geometric and electronic properties of the tetracene/Ag(110) interface studied by density functional theory — •Jana Fuchsberger[1], Daniel Lüftner[1], Xiaosheng Yang[2], Georg Koller[1], Michael Ramsey[1], Vitaliy Feyer[3], Serguei Soubatch[2], Stefan Tautz[2], and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [3]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Germany

Recently, the puzzling question of tetracene monolayers on Ag(110) has been revisited by means of photoemission tomography experiments. Thereby the azimuthal orientation of the molecules has been studied and several molecular emissions have been identified. However, the origin of two distinct emissions separated by almost 1 eV that appear to have the photoemission distribution of the highest occupied molecular orbital (HOMO) could not be explained. In this contribution, we use density functional theory to shed light on this problem. First, we determine the optimal adsorption geometry for two molecular orientations, namely parallel and perpendicular to the close-packed Ag-rows. We further analyze their electronic structures in terms of work function modifications, charge rearrangements and projected density of states. Finally, we compare simulated photoemission momentum maps for the two structures with experimental data.

O 46.22 Tue 18:30 P1A

DFT calculations of energy dependent XPS valance band spectra — •Mahdiyar Bagheri and Peter Blaha — Institute of

Materials Chemistry,Technical University Vienna, Vienna, Austria

In the past few years it became regularly possible to measure valance band X-ray photoelectron spectra (XPS) using variable excitation energies. In order to explain the observed variations in intensity with respect to the excitation energy, we performed XPS calculations using the WIEN2k code. The new module computes the XPS spectra using a combination of partial density of states times excitation-energy-dependent atomic cross-sections, and considers as additional correction the fraction of the corresponding orbital contained inside the atomic spheres. The resulting XPS spectra are compared with experimental data for SiO2, PbO2 and NiO at different excitation energies.

O 46.23 Tue 18:30 P1A

Local effects of self-assembled monolayers on NiO thin films — •Wenlan Liu[1,2], Shuangying Ma[1,2], Sabina Hillebrandt[2], Florian Ullrich[2], Sebastian Hietzschold[2], and Andreas Köhn[1,2] — [1]Institut für Theoretische Chemie, Universität Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart — [2]InnovationLab GmbH, Speyerer Straße 4, D-69115 Heidelberg

Due to the large band gap and the p-type character, NiO has been used as hole transmission and electron blocking layers in enhancing bulk heterojunction (BHJ) organic photovoltaic (OPV) cell performance. The performance of electronic devices can be further improved by applying self-assembled monolayer (SAM) on the NiO surface, such that one can easily tune the work function of the surface, and achieve other functions e.g. passivation and better wettability.[1]

As this work is closely cooperated with experiments based on solution-processed NiO thin films, we consider not only the idea NiO(111) surface, but also different variation of non-idea surfaces either with surface reconstruction or defect in buffer. Such local effects are taken care of by the periodic electrostatic embedded cluster model (PEECM).[2] The energetically stable conformations of the SAMs on NiO(111) surfaces have been examined. The corresponding properties have been calculated and compared carefully with the experimental results.

[1] S. A. DiBenedetto et al., Adv. Mater., *21* (2009), 1407
[2] M. Sierka et al., J. Chem. Phys., *120* (2009), 174710

O 46.24 Tue 18:30 P1A

Self-assembled monolayers on NiO thin films: a first-principles study — •Shuangying Ma[1,2], Wenlan Liu[1,2], Sabina Hillebrandt[2], Florian Ullrich[2], Sebastian Hietzschold[2], and Andreas Köhn[1,2] — [1]Institut für Theoretische Chemie, Universität Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart — [2]InnovationLab GmbH, Speyerer Straße 4, D-69115 Heidelberg

The study of the organic solar cells (OSC)[1]has received increasing attention due to its low cost and compatibility with the present well developed technologies[2]. NiO is good anode interlayer candidate owing to its wide band gap and p-type character[3]. By forming self assembled monolayers of certain organic molecules, e.g. 4-cyanophenyl phosphonic acid (CYNOPPA) on the NiO surface, can further modify the energy-level alignment between the semiconducting organic/inorganic interfaces, which is critical for efficient charge separation and significantly affects the open-circuit voltage as well[4].

In the present study, first-principles calculations are performed for different neat and SAMs modified hydroxylated and reconstructed NiO(111) surfaces. The related electronic and optoelectronic properties, e.g. band gaps, density of states, work functions, XPS and IR spectrums are compared with each other and with the experimental results. The corresponding dehydration mechanism between the CYNOPPA and NiO(111) hydroxylated surface is also studied with ab initio molecular dynamics.

[1] Nat. Photon., 3 (2009), 649; [2] Chem. Mater., 23 (2011) 2218; [3] Phys. Rev. B, 75 (2007), 241203; [4] Adv. Mater., 21 (2009), 1450

O 47: Electronic Structure of Surfaces: Magnetism and Spin Phenomena

Time: Tuesday 18:30–20:30 Location: P1A

O 47.1 Tue 18:30 P1A

A silicon-based room temperature spin source without magnetic layers — •Debkumar Bhowmick, Matthias Kettner, Manfred Bartsch, and Helmut Zacharias — Physikalisches Institut, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Controlling the electron spin orientation and spin injection into functional electronic devices is of central importance in the field of spin transport electronics or spintronics. So far ferromagnetic metal/semiconductor junctions have been used to develop for spintronics which works only under low-temperature. Self-assemble chiral molecular monolayer (like dsDNA, Lysine) on gold shows promising in the direction of development of room temperature spintronic devices. In this present study, electron spin filtering by DNA on silicon, covalently bound by a 3-isothiocyanatopropyl triethoxy silane linker have been shown. This provides a means for developing room temperature spintronics. Electrons from silicon passing through double-stranded DNA acquire a longitudinal spin polarization. This enables the integration of helical molecules as spin filters in modern electronics for spin control, injection, and detection.

O 47.2 Tue 18:30 P1A

A Riccati equation based model for chiral spin filters — •Daniel Nürenberg, Matthias Kettner, and Helmut Zacharias — Physikalisches Institut, Uni Münster, Germany

The spin selective transport of electrons in chiral molecules is currently under intense research in theory and experiment. These experiments include studies of the dependence of the spin polarization on the length of the molecules and on the starting spin polarization from the substrate. We show that the evolution of the spin polarization of an ensemble of electrons during propagation can be described by a Riccati equation, which can be fitted to experimental data. We propose that the coefficients in this model are suitable to characterize the efficiency of spin filters and help to distinguish spin-flip and perturbation from spin-dependent extinction effects. These perturbations also limit the spin polarization for long molecules. We apply our model to fit previous experimental data from DNA, oligopeptides and [7]-helicene.

O 47.3 Tue 18:30 P1A

Enantiomer-dependency of spin orientation in photoelectron transmission through heptahelicene — •Matthias Kettner[1], Daniel Nürenberg[1], Johannes Seibel[2], Karl-Heinz Ernst[2], and Helmut Zacharias[1] — [1]Physics Institute und Center for Soft Nanoscience, University of Münster, Germany — [2]Nanoscale Materials Science, EMPA, Switzerland

Spin transport electronics (spintronics) enables a new generation of efficient electronic and non-volatile memory devices. Though the concept of spintronics is well known, the field still lacks devices that work under ambient conditions. Experiments on self-assembled monolayers of double stranded DNA [1,2] and oligopeptides [3] indicated a very efficient spin filtering behavior of the molecules at room temperature. In present experiments enantiopure M- and P-heptahelicene molecules are evaporated onto noble metal single crystal surfaces. The molecules arrange themselves to a highly ordered monolayer [4]. Samples are then irradiated with $\lambda = 213\,\mathrm{nm}$ laser radiation to generate photoelectrons from the substrate. These electrons are transmitted through the heptahelicene layer and analyzed with regard to their average longitudinal spin orientation by a Mott polarimeter. The sign of the spin polarization is related to the helicity of the enantiomer whereas an influence of substrate on the spin-filter effect has not been observed.

[1] Göhler, B. et al., Science 2011, 331, 894. [2] Kettner, M. et al., Adv. Mater. Interfaces, 2016, 3, 1600595. [3] Kettner, M. et al., J. Phys. Chem. C 2014, 119, 26. [4] Ernst, K.-H., Acc. Chem. Res. 2016, 49, 1182.

O 47.4 Tue 18:30 P1A

Laser induced photocurrents in a Topological Insulator thin film analyzed by 2D maps for VIS and NIR — •Thomas Schumann[1], Helena Reichlová[3], Gregor Mussler[4], Eva Schmoranzerová[2], Pertr Němec[2], Tobias Kampfrath[5], Christian Heiliger[6], and Markus Münzenberg[1] — [1]IfP, University of Greifswald, Germany — [2]MFF, Charles University, Prague, Czech Republic — [3]FZU, Prague, Czech Republic — [4]PGI-9, Jülich, Germany — [5]FHI Berlin, Germany — [6]University of Gießen, Germany

Topological Insulators (TI) open up a new route to influence the transport of charge and spin in a surface film via spin-momentum locking [1,2]. It has been demonstrated experimentally [2] that illumination by circularly polarized light can result in excitation of a helicity-dependent photocurrent. We report our recent results on laser induced photocurrents in a terniary 3D TI thin film. The resulting photocurrents have been studied by 2D photocurrent maps for different dopings and for VIS to NIR laser excitation. We although discuss the effects of contacts and edges if they are illuminated by the laser.

[1]S.D.Ganichev,W.Prettl,J.Phys.: Condens. Matter 15 (2003) R935-R983

[2]J.W.McIver,D.Hsieh,H.Steinberg,P.Jarillo-Herrero and N.Gedik, Nature Nanotechnology 7, 96-100 (2012)

We acknowledge the funding of the DFG via the SPP 1666 Topological Insulators and the joint DAAD PPP Czech Republic project FemtomagTopo.

O 47.5 Tue 18:30 P1A

Inelastic Excitations on Fe-TPyP on Au(111) — •Daniela Rolf, Christian Lotze, Benjamin W. Heinrich, and Katharina J. Franke — Freie Universität Berlin

Prophyrin molecules constitute a class of well-investigated molecules, due to their versatility in terms of self-assembly and electronic and magnetic properties. Numerous studies have been performed with different central metal atoms on different metal surfaces, showing that by a suitable choice of metal center and surface, the molecular properties can be tailored. Interesting phenomena were observed, including the Kondo effect, vibronic coupling and negative-differential resistance.

Here, Fe-tetra-pyridil-porphyrin (Fe-TPyP) molecules were investigated on a Au(111) substrate. Employing a low-temperature STM, we show that a multitude of steps in the dI/dV-signal up to 135meV can be observed symmetrically around the Fermi level. These inelastic excitations were observed both on the Fe-center of the molecule as well as on the organic TPyP ligand, with some of the steps on the ligand being visible only at positive bias polarity. As none of the inelastic excitations could be observed on chlorine-coordinated Fe-TPyP-Cl molecules, molecular vibrations were excluded as the origin of the inelastic excitations. Instead, a contribution of magnetic origin is assumed.

O 47.6 Tue 18:30 P1A

Yu-Shiba-Rusinov states and inelastic excitations in Iron Porphine molecules on Pb(111) — •Laëtitia Farinacci, Gaël Reecht, Benjamin W. Heinrich, and Katharina J. Franke — Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

When adsorbed on a superconductor, magnetic impurities couple to the quasi-particles of the substrate. This interaction induces Yu-Shiba-Rusinov (YSR) states within the BCS gap of the superconductor whose energy depends on the coupling strength. In case of a vanishing coupling, they merge with the gap edge and it may be possible to observe inelastic excitations outside of the BCS gap.

Using STM we investigate the properties of Iron Porphine molecules on a Pb(111) surface. After deposition, the molecules form islands with a hexagonal pattern. Within these islands, two different types of molecules can be identified. Type I molecules show a clover shape with a central protrusion while type II molecules have a square-like appearance. YSR states are observed above type I molecules. Depending on their surroundings type II molecules can display inelastic excitations outside the BCS gap of Pb(111).

By approaching the tip closer to the molecules we are able to tune the energies of these YSR states and inelastic excitations. In particular, the YSR states can be suppressed.

O 47.7 Tue 18:30 P1A

Investigation of Ferromagnetism on Graphite due to Swift Heavy Ion Irradiation — •Eren Güvenilir[1], Cem Kincal[1], Umut Kamber[1], Dilek Yildiz[1,2], Clara Grygiel[3], Cornelis J. Van Der Beek[4], and Oğuzhan Gürlü[1] — [1]Istanbul Technical University, Istanbul, Turkey — [2]University of Basel, Basel, Switzerland — [3]Universite de Caen, Caen, France — [4]Ecole Polytechnique, Palaiseau

Defect induced ferromagnetism have been reported on carbon based materials. In this work we investigated the magnetic properties of highly ordered pyrolytic graphite (HOPG) samples after irradiation with swift heavy ions (SHI). Samples were irradiated under 80° and 87.5° angle of incidence using highly charged and highly energetic Pb and U ions. Such SHI irradiation generates comet-like defects on the sample surfaces. We performed magnetic force microscopy under atmospheric ambient conditions. Our measurements revealed that comet-like defects caused by SHI irradiation have significantly higher magnetic signal compared to native defects on HOPG surfaces.

O 47.8 Tue 18:30 P1A

Spin-resolved electron transmission through self-assembled layers of PNA — •Paul Möllers[1], Matthias Kettner[1], Daniel Nürenberg[1], Francesco Tassinari[2], Tal Z. Markus[2], Catalina Achim[3], Ron Naaman[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Chemical Physics, Weizmann Institute, Rehovot, Israel — [3]Department of Chemistry, Carnegie Mellon University, Pittsburgh, Pennsylvania, United States

The yield of electrons transmitted through chiral molecules can depend on the electron's spin; chiral molecules can therefore act a spin filters. This effect is referred to as the chirality-induced spin selectivity (CISS). Previous experiments have e.g. been performed with monolayers of double-stranded DNA [1]. In this contribution, we present results of our spin-resolved photoemission experiments performed at room temperature. The samples consist of self-assembled monolayers of helical molecules – various types of double-stranded peptide nucleic acid (PNA) – on polycrystalline gold surfaces. The samples are irradiated by a laser at $\lambda = 213\,\mathrm{nm}$ to generate photoelectrons from the gold substrate which are then transmitted through the adsorbed monolayer. Subsequently, the electrons are analyzed by a Mott polarimeter. We found longitudinal spin polarizations of $-5\,\%$ for PNA and $+4\,\%$ for γ-PNA. The results indicate that the adsorbed molecules act as a spin filter.

[1] B. Göhler et al., Science 331, 894 (2011)

O 48: Oxide and Insulator Surfaces: Structure, Epitaxy and Growth

Time: Tuesday 18:30–20:30 Location: P1A

O 48.1 Tue 18:30 P1A

Epitaxy of Fe_3O_4/CoO bilayers and formation of cobalt ferrite on $SrTiO_3$(001) — •Jannis Thien, Jari Rodewald, Martin Hoppe, Karsten Küpper, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

Thermoelectric generation using magnetic insulators such as ferrites has recently turned into a field of interest. In these materials the thermoelectric generation is initiated by a heat-mediated pure-spin-current, called the spin-Seebeck effect [1]. Furthermore, ferrites are of large interest for spin filters due their spin-dependent band gap [2].

One approach of preparing the ferrite $CoFe_2O_4$ is the interdiffusion of Fe_3O_4/CoO bilayers. Hence, Fe_3O_4/CoO bilayers were grown by reactive molecular beam epitaxy (RMBE) on $SrTiO_3$(001) consecutively. Afterwards the samples were post-annealed to start the diffusion process. The structural characterization of the surface was realised by low energy electron diffraction (LEED). X-ray photoelectron spectroscopy (XPS) was used to examine the chemical composition. Additionally, hard x-ray photoelectron spectroscopy (HAXPES) was carried out to be more sensitive to the bulk and interface composition. Further investigations of magnetic properties by vibrating sample magnetometry (VSM) are going to be performed.

[1] T. Niizeki et al., AIP Advances 5, 053603 (2015)

[2] J.-B. Moussy, J. Phys. D: Appl. Phys. 46, 143001 (2013)

O 48.2 Tue 18:30 P1A

NiO growth on Ag(001): A layer-by-layer vibrational study — •Florian O. Schumann[1], Krasimir L. Kostov[2], Sebastian Polzin[1], and Wolf Widdra[1,3] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria — [3]Max Planck Institute for Microstructure Physics, 06120 Halle, Germany

The vibrational properties of NiO(001) films on Ag(001) with thicknesses up to 50 monolayers (ML) are characterized with high-resolution electron energy loss spectroscopy (HREELS). The film-thickness-dependent Fuchs-Kliewer (FK) phonon frequency shifts and intensity changes are identified from the NiO monolayer to bulklike thick films. Characteristic changes of the vibrational properties are analyzed to resolve restructuring processes during annealing and thermal decomposition of NiO films. A quantitative comparison of the experimental data with the calculated loss function based on dielectric theory reveals an excellent agreement between the bulk and the NiO phonon properties for film thicknesses above 15 ML. In contrast, a strong FK phonon softening is observed for thin films below 5 ML that cannot be explained by dielectric theory nor phonon standing waves. This softening is attributed to the presence of surface stress, which results from the -2 % lattice mismatch between NiO and Ag. Furthermore the dispersion of six different phonon branches in the $\overline{\Gamma X}$ direction for a fully relaxed 25 ML and a pseudomorphically 4 ML film will be compared.

O 48.3 Tue 18:30 P1A

High quality surfaces of perovskite oxides for photoemission spectroscopy — •Marten Düvel, Marius Keunecke, Sabine Steil, Daniel Steil, Vasily Moshnyaga, and Stefan Mathias — Georg-August-Universität Göttingen

In correlated materials, e.g., perovskite oxides, the overall behavior is governed by the interaction between charge, spin, orbit and lattice degrees of freedom. We plan to follow energy conversion processes in perovskite oxides, after optical excitation, using different time-resolved spectroscopy techniques. As a first step, $La_{0,3}Sr_{0,7}MnO_3$ thin films were prepared by metalorganic aerosol deposition (MAD) technique on $SrTiO_3$ (001) substrates and characterized by XRR, XRD, AFM, STM, SQUID, PPMS and SEM. From these oxide materials, we evaluate different methods to obtain high quality surfaces under ultra-high vacuum conditions, suitable for surface-sensitive methods like low-energy electron diffraction (LEED) and spin-,time- and angle-resolved photoemission spectroscopy (trARPES). Financial support of the SFB 1073 (TPB07) is acknowledged.

O 48.4 Tue 18:30 P1A

First stages of growth of SrxLa(1-x)MnO3 on SrTiO3(110) by PLD — •Giada Franceschi, Michele Riva, Ulrike Diebold, and Michael Schmid — IAP, TU Wien

Among energy conversion devices, solid-oxide fuel-cells (SOFCs) are attracting worldwide interest, being extremely efficient and environmentally friendly. Electricity is generated through electrochemical oxidation of fuels, which is initiated by incorporating oxygen at the cathode surface of the device. The state-of-the-art cathode material is strontium-doped lanthanum manganite (LSM), and current research on SOFCs aims at understanding the mechanisms behind the oxygen incorporation at its surface. As recently demonstrated, the latter must be addressed through atomic scale investigation, but to do so, a well-defined single-crystalline model system needs to be established in advance: within our project, we aimed at obtaining such a single-crystalline model system in the form of thin, atomically flat LSM films, grown by pulsed laser deposition onto SrTiO3(110) substrates. First, we home-prepared and characterized the target for pulsed laser deposition growth. After the optimization of the growth parameters, we incrementally grew LSM on different SrTiO3(110) substrates, and investigated the first stages of growth by employing in-situ STM, LEED, and XPS. For a proper set of growth parameters, LSM realized an ordered growth, resulting in atomically flat surfaces. We observed a changing periodicity with the film thickness, related to some non-trivial interaction mechanisms with the substrate. Atomic scale investigations were used to study the morphology of the grown films.

O 48.5 Tue 18:30 P1A

Electric field induced desorption of oxygen adatoms from the MoO_{2+x}/Mo(110) surface — •Killian Walshe[1], Sergey I. Bozhko[2], Olaf Lübben[1], Brian Walls[1], Barry E. Murphy[1], and Igor V. Shvets[1] — [1]Trinity College Dublin, Dublin, Ireland — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow District 142432, Russia

Nanoscale writing on the MoO_{2+x}/Mo(110) surface has been demonstrated previously by Krasnikov *et al.* [1]. Pulsing with the scanning tunneling microscopy (STM) tip leads to the removal of oxygen adatoms. Here, in the zero tunneling current regime, STM measurements illustrate how the resolution of the nanoscale writing depends on the applied bias voltage and tip-surface distance. STM measurements and the theoretical modelling (COMSOL Multiphysics) of the electric field generated between the STM tip and metallic surface provides insight into the mechanism behind this process; the electric field generated by a negatively biased STM tip leads to anion oxygen adatoms penetrating the surface. The energetic barrier for this process has been estimated to be 0.45 eV. Density functional theory (DFT) calculations [1] demonstrate that the oxygen adatoms locally deform the underlying molybdenum oxide structure. It is suggested that this deformation, which leaves a gap below the oxygen adatom, reduces the barrier for the adatom to penetrate the surface.

1. A. Krasnikov *et al.*, *Nano Res.* **2013**, 6(12), 929-937

O 48.6 Tue 18:30 P1A

Single-crystalline growth of EuO on Cu (001) — •Tristan Heider[1], Timm Gerber[1], Patrick Lömker[1], Claus Michael Schneider[1,2], Lukasz Plucinski[1,2], and Martina Müller[1,2] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [2]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, 47048 Duisburg, Germany

The ferromagnetic insulator EuO shows very high spin polarization exceeding 90% which makes this material a prototype candidate for research in the field of spintronics. We studied MBE growth of EuO on Cu(001), because Cu is both a very good electrical and thermal conductor. Thus, Cu is also ideally suited as a substrate for photoemission experiments at low temperatures. Since the magnetic properties of EuO are strongly influenced by strain [1] Cu is an ideal substrate because it allows for nearly strain-free heteroepitaxy of EuO films, with the orientation EuO(100)||Cu(110) .

We systematically studied the growth of EuO on Cu(001) by performing synthesis in (a) temperature and (b) oxygen pressure series. We could restrict the EuO synthesis to a very small parameter window, in which single-crystalline growth is mastered. The crystalline quality was confirmed in situ by RHEED and LEED, while the chemical composition was analyzed by in situ XPS. An additional Eu capping layer was found to be a good protection from overoxidization of the highly reactive EuO film during vacuum transfer to the ARPES chamber, where high resolution spin-ARPES measurements are performed.

Reference: [1] Ingle et al. Phys. Rev. B 77, 121202(R) (2008)

O 49: Oxide and Insulator Surfaces: Adsorption

Time: Tuesday 18:30–20:30 Location: P1A

O 49.1 Tue 18:30 P1A

Synthesis of conjugated organic nanowires on the TiO_2(110) surface — •Jens Brede[1,2], Mikel Abadia[1], Marek Kolmer[3], Guillaume Vasseur[1,2], Łukasz Zajac[3], Alberto Verdini[4], Luca Floreano[4], Jose Enrique Ortega[1,2,5], and Celia Rogero[1,2] — [1]Centro de Física de Materiales CFM–MPC(CSiC-UPV/EHU), Paseo Manuel Lardizabal 5, E-20018 San Sebastián, Spain — [2]Donostia International Physics Center, Paseo Manuel Lardizabal 4, E-20018 San Sebastián, Spain — [3]Centre for Nanometer-Scale Science and Advanced Materials, NANOSAM, Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University Łojasiewicza 11, 30-348 Kraków (Poland) — [4]CNR-IOM, Laboratorio Nazionale TASC, I-34149 Trieste, Italy — [5]Departamento Física Aplicada I, Universidad del País Vasco, E-20018 San Sebastián, Spain

We have recently demonstrated the synthesis of poly(p-phenylene) nanowires from dibromoterphenyl precursors on the reduced TiO_2(110) surface[a]. Here, we summarize our findings and present new data were we used X-ray photoelectron spectroscopy to correlate the behavior of surface anchored hydroxyl groups with changes in the C 1s and Br 3d core levels as a function of annealing temperature. Thus, we obtained clear evidence for the proton-transfer mediated dehalogenation reaction as proposed by Kolmer *et al.*[b] In a second experiment we deposited trace amounts of different metals together with the molecular precursors and found highly uniform and ordered arrays of nanowires covering the entire surface. [a] JACS **138**, 5685-5692 (2016) [b] Kolmer *et al.* Angew. Chem. Int. Ed. **52**, 10300-10303 (2013)

O 49.2 Tue 18:30 P1A

On the Photocatalytic Activity of Metal Oxide Surfaces: Adsorption and Decomposition of N_2O on TiO_2(110) — •Marvin Quack, Max Kauer, and Karina Morgenstern — Chair of Physical Chemistry I, Ruhr-Universität Bochum, Germany

The role of N_2O as a greenhouse gas has been a major issue regarding global warming. In addition, N_2O is known to be responsible for stratospheric ozone depletion. A possible solution to decrease the emission of N_2O is the catalytic decomposition into molecular oxygen and nitrogen using metal oxides. In order to understand the principle of this catalytic process, we investigated adsorption and photocatalytic decomposition of N_2O on a rutile TiO_2(110) single crystal surface by Fourier transform infrared spectroscopy (FTIR) in ultra high vacuum at temperatures from 100 to 150 K. These studies show N_2O adsorbs on the surface in a linear configuration, binding to surface Ti^{4+} species via the O-end of the molecule. The effect of UV light irradiation on the catalytic decomposition of the adsorbed molecule has been investigated by *in-situ* infrared spectroscopic measurements. This contribution will discuss the time-resolved depletion of the absorption signals during irradiation in detail.

O 49.3 Tue 18:30 P1A

The acetone/TiO_2 (110) rutile interface: geometry, energetics and vibrational modes — Tim Würger, Wolfgang Heckel, •Kai Sellschopp, Stefan Müller, and Gregor Feldbauer — Hamburg University of Technology, Institute of Advanced Ceramics

Acetone is often present in chemical reactions during the formation of hybrid interfaces, and thus is a potential competitor to coupling agents like carboxylic acids. Therefore, we studied the adsorption geometry and energetics of acetone molecules on the TiO_2 (110) rutile surface with density functional theory (DFT). The focus lies on identifying and quantifying differences between molecular and dissociated adsorption modes. It turnes out, that saturation coverage is reached at 0.5 molecules per undercoordinated surface Ti atom. Furthermore, η^1-acetone binds $\approx 0.23\,\mathrm{eV}$ stronger then η^1-enolate, and 0.70 eV weaker than acetic acid. Corresponding vibrational spectra are presented and compared to IR spectroscopy experiments.[1]

[1] H. Noei, A. Stierle, DESY Hamburg, private communication.

O 49.4 Tue 18:30 P1A

Micron sized dendritic structures due to water ice on oxide surfaces under ambient conditions — •Kivanc Esat[1,2], Özgür Birer[3], and Oguzhan Gürlü[1] — [1]Istanbul Technical University, Department of Physics, Turkey — [2]ETH Zürich, Laboratory of Physical Chemistry, Switzerland — [3]Koç University, Chemistry Department, Turkey

Water is one of the most studied yet the least understood molecule at the fundamental level. Its magnificent characteristics can give rise to unexpected phenomena when adsorbed on surfaces. In our work we studied water adsorption on nanoscale chromium oxide particles those had been growth on glass and silicon oxide surfaces. We found out that dendritic structures can form spontaneously on these surfaces due to ambient water. Our systematic studies of dosing such surfaces with humidified air revealed formation of further fractal structures due to water condensation and evaporation. The growth of these structures was observed under an ambient optical microscope in real time. When these samples were transferred to an atomic force microscope (AFM) dendrites due to water ice could still be observed. AFM data showed that these structures could be as high as several hundredths of nanometers, proving them to be three dimensional. Depending on the density of the oxide particles on glass or silicon oxide surfaces, shapes, coverage areas and thicknesses of the dendrites were observed to differ. An explanation could be brought to their formation by use of Electrostatic Force Microscopy measurements.

O 49.5 Tue 18:30 P1A

DFT study of charged O_2^- adsorbed on $Ca_3Ru_2O_7$(001) — Wernfried Mayr-Schmölzer, Florian Mittendorfer, and •Josef Redinger — Institute of Applied Physics, TU Vienna, Wiedner Hauptstrasse 8-10/134, 1040 Vienna, Austria

An atomic scale knowledge of the surface chemistry of perovskite oxides is surprisingly poor, despite their use in a wide range of important applications, like in sensors, or fuel cells, or even in catalytic processes. Here we present a DFT study of O_2 adsorption on the (001) surface of Ruddelsden-Popper type $Ca_3Ru_2O_7$. Experimentally $Ca_3Ru_2O_7$ cleaves nicely, yielding an almost ideally flat rocksalt-like CaO(001) surface. However, due to the tilting and rotation of the RuO_6 octahedra in the bulk different Ca-O distances are present, creating preferred adsorption sites for an O_2 molecule. Upon adsorption O_2 does not dissociate, but rather gets negatively charged. This charging is predicted both for the metallic and the insulating anti-ferromagnetically ordered substrate state, which exists below $T_N < 50\mathrm{K}$. We investigate the origin of the charge transfer using standard PBE, PBE+U and hybrid-functionals and find distinct differences concerning the local magnetic configuration for metallic and insulating states.

O 49.6 Tue 18:30 P1A

Adsorption geometry and infrared absorption of CO_2 molecules on the KCl(100) surface — •Jochen Vogt — Chemisches Institut der Otto-von-Guericke Universität Magdeburg, Germany

The system CO_2/KCl(100) is an example of a physisorption system where a moderate lattice mismatch induces a variety of phases at different coverage, both with and without long-range order. Results of diffraction experiments (LEED, HAS) and infrared spectroscopy have revealed essential adsorbate properties [1]. Simulations of the adsorbate structure on different levels of theory [1,2] are useful to complete the picture by providing suitable structure models as starting points for a LEED structure analysis, and the assignment of observed features in IR spectra. This contribution presents results of plane wave DFT calculations on the structure and infrared absorption of the saturated monolayer phase CO_2-$(6\sqrt{2} \times \sqrt{2})R45°$/KCl(100). In accordance with diffraction experiments, the relaxed geometry containing 12 tilted inequivalent molecules exhibits glide-plane symmetry, caused by a modulation of the azimuthal orientation of the molecules. The simulated IR spectrum based on a Γ-point phonon calculation is dominated by a strong red-shifted mode in the region of the CO_2 asymmetric stretch vibration, as observed in IR experiments. However, the DFT result markedly overestimates the experimentally observed exciton band width. [1] F. Traeger et al., J. Phys. Chem. A115 (2011), 6986 [2] T. Wu et al., Appl. Surf. Sci. 339 (2015), 1

O 50: Semiconductor Substrates: Structure, Epitaxy, Growth and Adsorption

Time: Tuesday 18:30–20:30 Location: P1A

O 50.1 Tue 18:30 P1A

Mask aligner for shadow mask evaporation of nanostructures — •Simon Mathioudakis, Priyamvada Bhaskar, Tim Olschewski, Marcus Liebmann, Marco Pratzer, and Markus Morgenstern — II. Inst. Phys. B and JARA-FIT, RWTH Aachen University, Germany

In order to arrive at an experiment for detecting Majorana fermions using scanning tunneling microscopy, we aim at evaporating superconductors with pierced holes onto a topological insulator ($(Bi_{x-1}Sb_x)_2Te_3$). This structure is produced by evaporating the superconductor through a shadow mask. The goal is an in-situ process of creating an array of pierced holes and thus keep the interface free of resists or residues. Therefore, a mask aligner operating in ultra-high vacuum (UHV) is developed. It uses three piezo-drives to align the mask relative to the sample. Three capacitive sensors are used to determine the sample-mask distance down to a precision of 100 nm each. This technique has been successfully tested and as a first proof, gold has been evaporated onto HOPG and Si substrates. AFM and SEM characterizations reveal an edge width below 100 nm, however also indicate assymetry in the deposited holes due to a drift during evaporation.

O 50.2 Tue 18:30 P1A

Hydrogen etching of SiC(0001): Route to an epitaxy template — •Maximilian Bauernfeind, Felix Reis, Victor Rogalev, Marius Will, Ralph Claessen, and Jörg Schäfer — Physikalisches Institut and Röntgen Center of Complex Material Systems (RCCM), Universität Würzburg, 97074 Würzburg, Germany

The hexagonal (0001) surface of silicon carbide offers a huge playground for the epitaxy of a variety of different materials. An intriguing aspect is the growth of honeycomb lattices made of high-Z elements, such as Sn or Bi, predicted to exhibit topological protected edge states. To enable successful epitaxy of such materials, one has to focus on the substrate quality, and prepare defect-free and well-ordered flat surfaces. In-situ gas phase etching in a hydrogen atmosphere makes it possible to achieve these required qualities.

Here we demonstrate the effects of different etching parameters studied by scanning tunneling microscopy. The results are analyzed regarding large-scale terrace formation and defect density. In general, the etched substrate surface becomes hydrogen-passivated which, however, impedes the bonding of the admitted high-Z atoms. One approach to hydrogen desorption from SiC(0001) discussed in the literature is a photoinduced process with synchrotron UV light.

In addition, we present the succesful thermal desorption of hydrogen and the formation of a dangling bond (DB) state, as inspected by photoemission. The surface density of the DB state is analyzed in an annealing study. This finally renders SiC as a versatile growth template.

O 50.3 Tue 18:30 P1A

Halbleiterheterostrukturen - Analyse und Interpretation kapazitätsspektrokopischer Messungen — •Martin von Sprekelsen und Wolfgang Hansen — Jungiusstraße 9, 20355 Hamburg

Mit Rasterkapazitätsmikroskopie können Ladungsträgerkonzentrationen bei fester Probenbias-spannung abgebildet und daraus Rückschlüsse auf zugrundeliegenden Dotierungsprofile gezogen werden. Bei heterogenen Halbleitern wird die räumliche Lage von Dotierungsübergängen mit Hilfe der Rasterkapazitätsspektroskopie ermöglicht. Messungen und Verfahren werden vorgestellt.

O 50.4 Tue 18:30 P1A

Reaction channels of methanol on Si(001) studied by means of STM and XPS — •Patrick Kirsten, Christian Länger, and Michael Dürr — Institut für Angewandte Physik, Justus-Liebig-Universität, 35392 Giessen

Adsorption of organic molecules on silicon typically proceeds via an intermediate state. For diethyl ether, e.g., a dative bond between oxygen and silicon is formed in this intermediate, which was isolated at low surface temperatures on Si(001)[1]. A similar adsorption via a datively bonded intermediate state is proposed for alcohols on Si(001), however, the proton transfer associated with the transition from the intermediate into the final state is expected to proceed much faster than the energetically less favourable ether cleavage [2].

Indeed, when we performed XPS measurements after adsorption of methanol on Si(001) at different surface temperatures, the C 1s and O 1s spectra recorded both at 90 K and room temperature indicate dissociative adsorption and covalent bonding of the H atom and OCH_3 fragment. In STM images taken after adsorption at room temperature, the end-bridge adsorption configuration is predominant. Changes in the adsorption configurations with surface temperature are interpreted in terms of a precursor-mediated reaction channel.

[1] Reutzel, et al., J. Phys. Chem. C **119**, 6018 (2015).
[2] Kato, et al., J. Phys. Chem. B **105** 10340 (2001).

O 50.5 Tue 18:30 P1A

HREELS of Ammonia Adsorbed on a Water Reacted Si(001)-(2x1) Surface — •Niklas Fornefeld[1], Felicitas Scholz[1], Ulrich Köhler[1], Stefan Kubsky[2], and Francois Rochet[3] — [1]Arbeitsgruppe Oberflächenphysik, Ruhr-Universität-Bochum, Germany — [2]Synchrotron Soleil, St. Aubin (Paris), France — [3]Laboratoire de Chimie Physique Matière et Rayonnement, Univ. P. et M. Curie, Paris, France

Surface bound hydroxyl-groups on silicon surface became an interesting topic for research due to the use as interface between an anorganic and an organic semiconductor. To investigate the binding properties on those silanol-groups we studied the adsorption of ammonia (NH_3) as an example for a Lewis base. In order to determine the adsorption kinetics and geometry and the behavior during the process of unfreezing, we studied the NH_3/(H/OH)/Si(001)-(2x1) system with High Resolution Electron Energy Loss Spectroscopy (HREELS) in the temperature range between 100K and 300K.

We report the self-limited adsorption of molecular ammonia on surface silanols in a proton-acceptor geometry (ammonia giving its lone pair to Si-OH) below 140K. Around 160K the molecularly adsorbed ammonia desorbs within seconds. Taking temperature dependent spectra, the desorption kinetics was quantitatively determined. In addition, there are indications for the growth of a small amount of dissociated ammonia on isolated dangling bonds of the water covered surface.

O 50.6 Tue 18:30 P1A

As-modification of vicinal Si(100) surfaces for III-V-on-Si heteroepitaxy in CVD ambient — •Agnieszka Paszuk[1], Oliver Supplie[1], Sebastian Brückner[1], Peter Kleinschmidt[1], Anja Dobrich[1], Andreas Nägelein[1], Matthias M. May[2], and Thomas Hannappel[1] — [1]Institute of Physics, Technische Universität Ilmenau, Germany — [2]Department of Chemistry, Cambridge University, UK

Compound semiconductors grown on Si substrates are attractive for high efficiency solar cells, optoelectronic and microelectronic devices. Growth of III-V materials with low defect densities on Si is challenging due to lattice mismatch and different thermal expansion coefficients, as well as polar-on-nonpolar epitaxy. Arsenic (As) enables growth of ternary compounds, such as GaAsP, and As is mostly present in application-relevant III-V MOCVD reactors. We previously showed that dedicated As-modification of the heterointerface is suitable to control the III-V sublattice orientation [1]. Here, we will study the dimer orientation on vicinal Si(100) surface prepared in As-rich MOCVD ambient. The entire process is controlled by in situ reflection anisotropy spectroscopy (RAS) and the obtained RA spectra are benchmarked by LEED and XPS. We show that the RAS signal is not only terrace-related (As-coverage, type and orientation of the dimers) but it also can contain contributions from the step structure. We achieve in situ control of the majority dimer orientation on As-modified Si(100) surfaces and can thereby choose the sublattice orientation of the subsequently grown, single-domain III-V epilayer. [1] A.Paszuk et al., APL 106, 231601 (2015); O. Supplie et al., APL Mater.3,126110 (2015).

O 50.7 Tue 18:30 P1A

Adsorption of acetone on TiO2 rutile(110) — •Jessica Kräuter, Milena Osmić, and Katharina Al-Shamery — Carl von Ossietzy University of Oldenburg, 26129 Oldenburg, Germany

For increasing selectivity and activity of heterogeneous catalysts it is necessary to get a fundamental understanding of the interactions between adsorbate and catalyst. Therefore, as a model system for chemical reactions the adsorption of aldehydes/ketones on a common catalyst like TiO2 rutile(110) is studied. Recently, an influence of the temperature dependent mobility of bulk defects on the reductive coupling of benzaldehyde was concluded from own work.[1] In previous coverage dependent studies on the ketone acetone and co adsorbed molecular oxygen the occurrence of a diolate species has been identified on a medium reduced rutile single crystal at liquid nitrogen temperatures.[2,3] Here we present the influence of bulk defects from studies on temperature dependent adsorption of acetone co adsorbed with molecular oxygen and oxygen ad atoms. On a more strongly reduced rutile single crystal a diolate species can be observed even without oxygen co adsorption. Furthermore, in TPRS an additional surface species appeared from 235 to 274 K when co adsorbing acetone with molecular oxygen which has not been reported before. Changes of the molecular orientation of acetone on the surface were also proven by polarization dependent IRRAS measurement. [1] P. M. Clawin, C. M. Friend, K. Al-Shamery, A European Journal, 2014, 90, 7665. [2] M. A. Henderson, J. Phys. Chem. B, 2008, 108, 18932. [3] N. G. Petrik, M. A. Henderson, G. A. Kimmel, J. Phys. Chem. C., 2015, 119, 12273.

O 51: Nanostructures at Surfaces: 1D and 2D Structures and Networks

Time: Tuesday 18:30–20:30 Location: P1C

O 51.1 Tue 18:30 P1C

growth of covalently bonded Sierpiński triangles up to the second generation — gaochen gu, na li, and •yongfeng wang — key laboratory for the physics and chemistry of nanodevices, department of electronics, Peking University, Beijing, China.

Growth of covalently bonded Sierpiński triangles (CB-STs) on metal surfaces was investigated by scanning tunneling microscopy (STM). Three synthetic strategies (namely, dehydration condensation, cyclotrimerization coupling and Schiff-base reactions) were used to fabricate CB-STs. Second generation CB-STs were obtained at the solid-vacuum interface utilizing the Schiff-base reaction between 4,4"-dialdehyde-1,1':3',1"-terphenyl (TPDAL) and 1,3,5-tris(4-aminophenyl)benzene (TAPB) on Au(111). The CB-ST patterns persist at annealing temperatures as high as 500 K. Homotactic three-fold motifs, insufficient migration and irreversible covalent reaction are the main limitations for growing higher-generation STs. The present results provide new insights on the growth of STs on metal surfaces.

O 51.2 Tue 18:30 P1C

self-assembly of L-tryptophan on Cu(111) studied by LT-STM — qiang xue and •yongfeng wang — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China.

The chiral nanoclusters and one-dimensional chains of L-tryptophan on Cu(111) were investigated by ultrahigh vacuum scanning tunneling microscopy at 4.4 K. Small isolated clusters and chains coexisted on Cu(111) when molecules were deposited onto the substrate at around 30 K with a coverage of 0.25 monolayer. Then almost all the molecules self-assembled into chiral hexamers after being annealed at room temperature. When increasing molecular coverage to the full layer, only chains were found on the surface. High resolution STM images revealed that chains were composed by neutral, zwitterionic and anionic molecules. Chiral hexamers were formed by anionic tryptophan molecules. The structure difference was attributed to the competition between intermolecular and molecule-substrate interactions.

O 51.3 Tue 18:30 P1C

robust Sierpiński triangle fractals on symmetry-mismatched Ag(100) — yawei wang and •yongfeng wang — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China.

Sierpiński triangle fractals were constructed on both Ag(111) and symmetry-mismatched fourfold Ag(100) surfaces through chemical reaction between H3PH molecules and Fe atoms under vacuum. Density functional theory calculations revealed that the fractals were stabilized by the strong coordination interaction between Fe and O atoms. In comparison, pure H3PH molecules formed fractals via moderately strong hydrogen bonds only on Ag(111), not on Ag(100).

O 51.4 Tue 18:30 P1C

charging single Co atoms on ultrathin NaCl films — chenyang yuan and •yongfeng wang — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China.

Single Co adatoms adsorbed on a double-layer NaCl film supported by Cu(111) were negatively charged after applying a positive voltage pulse to the sample in a scanning tunnelling microscope.Density functional calculations showed that the magnetic moment of Co changed from 3μB to 2.2μB after charge state manipulation.

O 51.5 Tue 18:30 P1C

Spin related transport of single molecule studied by LT-STM — •Yajie Zhang and Yongfeng Wang — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing, China

A revolution in electronics is with the contemporary evolution of the two novel disciplines of spintronics and molecular electronics. A fundamental link between these two fields can be established using organic magnetic materials. Using a low-temperature scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS), we are able to study the single molecules under ultrahigh vacuum conditions at 4.2 /0.4 K. In this talk, we measured the magnetic properties of retinoic acid molecules, FePc and DyPc2 adsorbed on metal surface with corresponding spin carries of 2s, 3p, and 4f electrons. Unlike the pre-existing metal ion in FePc or DyPc2, retinoic acid molecules can be switched reversibly to a special state by placing the tip over the neck of the bulky heads at an appropriate sample voltage. The generation of a stable cationic radical makes the molecule have an unpaired electron. The dI/dV spectrum confirms the appearance of spin in switched states. In addition, we proposed that the two Pc ligands in the same double-decker DyPc2 molecules molecule rotate by 45 degrees against each other, which can be directly deduced from the STM imaging.

O 51.6 Tue 18:30 P1C

Plasma Assisted Synthesis and Mechanism of Rare V2O5 Nanostructured Thin Films — •Megha Singh, Prabhat Kumar, and Gade B. Reddy — Thin Film Laboratory, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016

Two rare nanostructures of V2O5 using facile plasma assisted sublimation process (PASP) have been synthesized. V2O5 nanoflakes and nanoplates assembled in microspheres (NPMSs) were obtained on large area over nickel coated glass substrate. The temperature of growth is varied along with time duration of deposition in order to obtain the different kinds of nanostructure as well as to understand the role of Ni-seed layer playing in controlling the morphology of nanostructures.

The morphological, structural, and vibrational properties of V2O5 nanostructured thin films are systematically investigated systematically as a function of time and deposition temperatures. Structural analysis carried out using the XRD shows the pure orthorhombic phase of V2O5 and revealed the dependence of crystallinity on the temperature and duration of growth. The Raman study of vanadium and oxygen atoms in nanostructured thin films (NTFs) is carried out by micro-Raman, which evidences the presence of single orthorhombic phase of V2O5 and accorded with XRD results. HRTEM analysis with SAED confirms that NFs and NPMSs are polycrystalline in nature. The stoichiometry ratio obtained from XPS analysis is ˜2.4, shows the compositional purity and stoichiometric nature of V2O5 NTFs. Based on the observed results a three steps growth mechanism is proposed.

O 51.7 Tue 18:30 P1C

6-Mercaptopurine self-assembled monolayers on Au(100)-hex: revealing the fate of gold ad-atoms — •Kathrin Müller[1], Pilar Carro[2], Flavia Lobo Maza[3], Carolina Vericat[3], Roberto C. Salvarezza[3], Ulrich Starke[1], Klaus Kern[1,4], and Doris Grumelli[3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Área de Química Física, Departamento de Química, Universidad de La Laguna, Tenerife, Spain — [3]Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas, UNLP- CONICET- La Plata, Argentina — [4]Institut de Physique, Ecole Polytechnique Fédéerale de Lausanne, Switzerland

Self-assembled monolayers (SAMs) can be used as inexpensive surface coatings for applications in sensors, surface protection and many more. Especially interesting is the interaction of the anchoring group (thiol, silane, phosphate) with the metallic substrate (e.g. gold, copper, silver), which determines the main properties of the SAMs. Here, we report on the adsorption of 6-mercaptopurin (6MP) on (100)-orientated reconstructed gold. The SAM was investigated with STM, LEED, XPS, electrochemical techniques and DFT calculations. We show that 6MP is unable to form vacancy islands in contrast to other thiol-gold SAMs, although its adsorption lifts the hex reconstruction. Thus, there is a large excess of gold adatoms in contact with the thiol molecules, which form disordered molecule-gold clusters. The remaining molecules arrange in two different well-ordered adatom-free domains. Our results show that the formation of ordered thiol-gold adatom complexes is not a general process and depends strongly on the thiol molecule.

O 51.8 Tue 18:30 P1C

New atomic models for Au-induced wire structures on Ge(001) surfaces at higher Au coverages — •Kaori Seino[1], Simone Sanna[1], Wolf Gero Schmidt[1], and Friedhelm Bechstedt[2] — [1]Lehrstuhl für Theoretische Physik, Universität Paderborn, Paderborn, Germany — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Jena, Germany

One-dimensional (1D) electronic systems have been investigated extensively because of the interest both in fundamental physics and in nano or atomic scale devices. The atomic structure of Au-induced nanowires on Ge(001) substrates, which arguably belong to the most interesting quasi 1D systems, is still under discussion despite intensive research.

We have studied the structural, energetic and electronic properties of Au-induced nanowires on Ge(001) surfaces by means of density functional theory calculations [1,2]. We start the investigations from the original and a modified giant missing row structure, the Au-trimer stabilized Ge ridge model [3]. Three new structures for a higher Au coverage in the range between 1.25 monolayer (ML) and 1.75 ML are proposed. It it found that the new models are energetically more favorable than the models proposed previously. Moreover, they are able to explain several features of the experimental results.

[1] K. Seino and F. Bechstedt, Phys. Rev. B **93**, 125406 (2016).

[2] K. Seino and F. Bechstedt, J. Phys.: Condens. Matter **28**, 284005 (2016).

[3] S. Sauer *et al.*, Phys. Rev. B **81**, 075412 (2010).

O 51.9 Tue 18:30 P1C

Continuously changing incommensurate adlayer: Coronene on Graphene — •Falko Sojka, Matthias Meissner, Tobias Huempfner, Lars Matthes, Roman Forker, and Torsten Fritz — Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

It has been reported previously that coronene (C24H12) grows on graphite in a commensurate manner [1]. However, by means of distortion-corrected low-energy electron diffraction (LEED) measurements we find that this is the case only under very special conditions. Rather, C24H12 grows preferably incommensurate on graphene as well as on graphite. Upon variation of temperature or coverage this well-defined structure changes continuously. On the basis of our experimental results we show how the lattice constant and the rotation angle of the layer are related. We further show that this type of incommensurate epitaxy is also accompanied by energy gain. Theoretical calculations are performed based on force-field calculations scaled by density functional theory (DFT) results as introduced recently [2]. The main claim here is to assume a flexible adlayer lattice instead of a rigid one. [1] M. Lackinger et al., Anal. Bioanal. Chem. 374 (2002) 685. [2] M. Meissner et al., ACS Nano 10 (2016) 6474-6483.

O 51.10 Tue 18:30 P1C

Epitaxy of Flexible 2D Crystals — •Matthias Meissner[1], Falko Sojka[1], Lars Matthes[1], Friedhelm Bechstedt[1], Xinliang Feng[2], Klaus Müllen[2], Stefan C. B. Mannsfeld[3], Roman Forker[1], and Torsten Fritz[1] — [1]Uni Jena Germany — [2]MPI für Polymerforschung Mainz, Germany — [3]cfaed, TU Dresden, Germany

The epitaxy of many organic films on inorganic substrates can be classified within the framework of rigid lattices which helps to understand the reproducible film orientations. For incommensurate systems, however, this classification fails as an explanation for an epitaxial alignment. Tiny shifts in atomic positions away from ideal lattice points, so-called static distortion waves (SDWs), had been proposed to be responsible for the orientational epitaxy in such cases. Using low-energy electron diffraction and scanning tunneling microscopy, we provide direct evidence for SDWs in the incommensurate monolayer of the molecule hexa-*peri*-hexabenzocoronene on graphite. They manifest as sub-Ångström molecular displacements away from an ideal, yet incommensurate lattice. By means of a density-functional-theory based gradient approach, we show that flexibility in the adsorbate layer is crucial to provide a total energy minimum for the observed domain orientation, constituting orientational epitaxy. While structural relaxation at an interface is a common assumption, the combination of the precise determination of the incommensurate epitaxial relation, the direct observation of SDWs in real space, and their identification as the sole source of epitaxial energy gain constitutes a comprehensive proof of this effect. [M. Meissner et al.: ACS Nano **10**, 6474-6483 (2016).]

O 51.11 Tue 18:30 P1C

Self-assembly of MoMo-Methyl molecules on Au surfaces — •Lu Lyu[1], Zheng Wei[1,2], Jobynson Kollamana[1], Manuel Zimmer[3], Markus Gerhards[3], Benjamin Stadtmüller[1], Mirko Cinchetti[4], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]College of Material Science and Engineering, Chongqing University, 400044 Chongqing, People's Republic of China — [3]Department of Chemistry, University of Kaiserslautern, Erwin-Schrödinger-Straße 52, 67663 Kaiserslautern, Germany — [4]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

We systematically investigated the self-assembly and ordering of MoMo-Methyl (3M) molecules on Au(111) and Au(788) surfaces with variable-temperature scanning tunneling microscopy (STM) at substrate temperature of 106 K. On Au(111), most of the molecules form two-dimensional ordered superstructures preserving the herringbone reconstruction of the substrate. In addition, one-dimensional zig-zag molecular chains were observed, in contrast to the straight chains that we previously studied for 3M grown on Cu(111) On the vicinal Au(788), two types of one-dimensional (1D) molecular chains were observed. On more narrow terraces, 2D-like molecular ribbons are formed. These differences indicate that the coordination of Au substrate atoms with 3M molecules can be ignored on Au(111) but not on Au(788).

O 51.12 Tue 18:30 P1C

STM imaging and spectroscopy of diindeno-pyrene: theoretical modeling — •Seddigheh Nikipar[1], Thomas Lehmann[1], Frank Eisenhut[1], Dmitry A. Ryndyk[2], Francesca Moresco[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Germany

One of the most promising experimental techniques to build new atomic scale materials is surface assisted synthesis in UHV condition. For its characterization and analysis, scanning tunnelling microscopy and spectroscopy are main tools. Recently our group observed the synthesis of diindeno-pyrene molecules by deposition of dibromo-diphenyl-pyrene on Au(111). Our current research focuses on exploring the structure and electronic properties of this new molecule on Au(111) by STM imaging and finite-voltage spectroscopy. To support the experimental results, we developed a computational method based on the CP2K computational package, by combining the density functional theory (DFT), first principle molecular dynamics, and electron transport approach starting from the Tersoff-Hamann approximation. We also used the Elastic scattering quantum chemistry approach (ESQC) for molecular transport to simulate the STM topography and dI/dV spectroscopy images. Using the localized/projected molecular orbital method, we analyze the molecular orbitals, energy alignment and electron density of states. The results of the theoretical modelling indicate good agreement with the experimental results.

O 51.13 Tue 18:30 P1C

Vibrational Eigenmodes of the Au-$(\sqrt{3} \times \sqrt{3})$/Si(111) surface reconstruction examined by Raman spectroscopy and first-principles calculations — •Benedikt Halbig[1], Martin Liebhaber[1], Utz Bass[1], Jean Geurts[1], Eugen Speiser[2], Jochen Räthel[2], Sandhya Chandola[2], Norbert Esser[2], Sergej Neufeld[3], Marvin Krenz[3], Simone Sanna[3], and Wolf Gero Schmidt[3] — [1]Uni. Würzburg, Exp. Physik III, Würzburg, Germany — [2]Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Berlin, Germany — [3]Uni. Paderborn, Dep. Physik, Paderborn, Germany

Submonolayer coverages of metal adatoms on semiconductor surfaces show particular reconstructions, e.g., (5×2) and $(\sqrt{3}\times\sqrt{3})$ for the Au/Si(111) system. Raman spectroscopy proves to be a sensitive probe analysing vibration eigenmodes of these material systems, as demonstrated for Au-(5×2)/Si(111) [1]. We report on the investigation of Au-$(\sqrt{3}\times\sqrt{3})$R30°/Si(111) by polarized *in situ* Raman spectroscopy in combination with first-principle calculations within Density Functional Theory. The Raman spectra, taken at 300 K and $\approx$ 20 K, reveal a main peak at 73 cm^{-1} accompanied by adjacent peaks on the low-energy side, a singular peak at 30 cm^{-1}, and a group of three peaks around 115 cm^{-1}. Density Functional Theory Frozen-Phonon calculations were carried out for three structural models labeled twisted-trimer, conjugate honeycomb-chained-trimer and honeycomb-chained-trimer [2]. [1] M. Liebhaber et al., PRB, accepted (2016). [2] J. Y. Lee et al., JKPS, 55, 6 (2009), and references therein.

O 51.14 Tue 18:30 P1C

Fabrication and investigation of near-surface spin centers in high-purity single crystal diamond — •Nicolas Wöhrl[1], Reinhard Remfort[1], Stefan Borgsdorf[2], Tanmoy Chakraborty[3], Ulrich Köhler[2], Dieter Suter[3], and Volker Buck[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — [2]Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum, Germany — [3]Experimentelle Physik IIIA, Technische Universität Dortmund, Germany

Photons from ideal single-photon sources exhibit quantum mechanical characteristics and therefore allow applications in novel fields including quantum cryptography and spintronics. One promising candidate for this task is the nitrogen-vacancy (NV) center in diamond. The main aim of this project is the fabrication and investigation of near-surface NV–centers in high-purity single-crystal diamond films. Preparation of these active elements is still challenging, especially when read-out is desired to be by optical as well as electronic means. In this work, pure single-crystal diamond films are homoepitaxially grown by microwave-plasma-assisted chemical vapor deposition, and the film quality is characterized. PL-measurements show, that the purity of these films surpasses the quality of commercially available electronic grade diamonds ($N < 5$ ppb) significantly. NV centers are created by ion implantation and their properties are investigated spectroscopically.

O 51.15 Tue 18:30 P1C

Electron beam induced surface activation - a novel method to study and reduce proximity effects — •Christian Preischl, Martin Drost, Fan Tu, and Hubertus Marbach — Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen, Germany

We apply different focused electron beam-based nanolithographic techniques in an ultra-high vacuum (UHV) environment. Recently, we explored Electron Beam Induced Surface Activation (EBISA), in which a surface is first chemically activated by the highly focused electron beam. In a second step, the activated regions can be developed with certain precursor molecules, resulting in the catalytic decomposition and eventually autocatalytic growth of the latter [1]. Suitable substrates for EBISA are oxide surfaces, thin organic films or surface anchored metal-organic frameworks. EBISA does not only allow for the controlled fabrication of well-defined nanostructures but also enables detailed insights into electron back-scattering processes by exploring and visualizing the corresponding proximity effects. Along with the presentation of these results, we will also discuss strategies to reduce proximity effects in electron beam lithography.

[1] H. Marbach, Appl. Phys. A, 117 (2014), 987;

O 51.16 Tue 18:30 P1C

The influence of low energy electron irradiation on the work function of aromatic self-assembled monolayers investigated by Kelvin Probe Force Microscopy — •Paul Penner[1], Marcin Kisiel[2], Sascha Koch[1], Thilo Glatzel[2], Ernst Meier[2], and Armin Gölzhäuser[1] — [1]Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany — [2]Department of Physics, University of Basel, 4056 Basel, Switzerland

Carbon Nano-Membranes (CNMs) are two-dimensional materials that are made by e.g. low- energy-electron irradiation induced cross-linking of Self-Assembled Monolayers (SAMs) of aromatic and organic molecules. The variation of different precursor molecules for the SAM and CNM formation allows not only to tune the properties of the final CNM but also to study the influence on the surface properties due to the specific SAM modification. Here we investigate the change in the work function of pristine SAMs and CNMs on a Au(111) substrate by means of Kelvin Probe Force Microscopy (KPFM) for different precursor molecules. The SAMs were partially cross-linked using a TEM-grid as a mask in order to compare the morphology and the work function of SAMs and CNMs simultaneously. Whereas no significant difference on the morphology due to the electron irradiation was observed, the analysis of the work function of pristine and cross-linked SAMs revealed a molecule dependent increase of the work function. On the one hand, this could be attributed to the modification of the dipole moment of the SAM and of the Au-S interface but also to the influence of different headgroups (H, NO2, CN) on the other hand.

O 51.17 Tue 18:30 P1C

"Nunchakus"molecules on metallic surfaces investigated by scanning tunneling microscopy — •lacheng liu[1,2], hong-ying gao[1,2], philipp held[3], armido studer[3], and harald fuchs[1,2] — [1]Center for Nanotechnology, Heisenbergstr.11, 48149 Muenster, Germany — [2]Physikalisches Institut, Westfaelische Wilhelms-Universitaet, Wilhelm-Klemm-Straße 10, 48149 Muenster, Germany — [3]Organisch-Chemisches Institut and Center for Mutiscale Theory and Simulation, Westfaelische Wilhelms-Universitaet, Corrensstr.40, 48149 Muenster

Scanning tunneling microscopy(STM) is demonstrated to be a promising tool to investigate the molecular conformation on metallic surfaces with atomic precision. In this work,we studied the adsorption conformations and self-assembly structures of four different *nunchakus* shaped molecules: Bis(2-naphthyl) peroxide, 2-Naphthoic anhydride, Bis(2-naphthyl)ethanedione and trans-1,2-Bis-(2-naphthyl)ethene. Different metal substrates Au(111), Ag(111) and Cu(111) were tested to reveal the interaction between organic molecules and metal surfaces. For these *nunchakus* shaped molecules, different adsorption conformations even on the same metallic surface were identified. The center to center distances of 2-Naphthyl groups in single molecules were measured, which are shorter than the ones in gas phase due to the specific interaction between O atoms and metallic surface atoms which leads to the tortuosity of the molecules.

O 51.18 Tue 18:30 P1C

Highly ordered 3D nanostructure arrays with improved electrochemical performance for sodium-ion battery anodes — •Liying Liang, Yang Xu, Chengliang Wang, Min Zhou, Liaoyong Wen, Huaping Zhao, Yaoguo Fang, Yan Mi, and Yong Lei — Institute for Physics and IMN MacroNano, Ilmenau University of Technology, Ilmenau 98693, Germany

Due to the lower cost and larger abundance of Na, Na-ion batteries have been a potential alternative to Li-ion batteries for energy storage devices. The development of electrode materials or structures with good electrochemical performance is currently key task in Na-ion batteries research. In this work, we presented a highly ordered 3D nanostructure array with large-scale high ordering, well vertical alignment, and large interval spacing, fabricated by a facile and cost-effective nanoimprinted AAO templating technique, might be successfully used as an electrode and showed an excellent electrochemical performance. This arrays conceptual design is universal to most of electrode materials. In return for this electrode design, high ion accessibility, fast electron transport, and strong electrode integrity are presented. Used as additive- and binder-free anode for Na-ion batteries, the electrochemical performances are greatly enhanced. This work may open up more applications of such highly ordered 3D nanostructure arrays in energy storage systems.

O 51.19 Tue 18:30 P1C

Tip-enhanced near-field optical microscopy on single-walled carbon nanotubes — •Sonja Tauchert, Xian Shi, Nicolai F. Hartmann, and Achim Hartschuh — Department Chemie and CeNS, LMU Munich, Germany

Tip-enhanced near-field optical microscopy (TENOM) [1] is a scanning probe technique with highest detection sensitivity. It is capable of providing a broad range of spectroscopic information on single objects and structured surfaces with nanometer spatial resolution. We utilized TENOM to investigate the photoluminescence (PL) of (6,5) SWCNT/PFO-BPy conjugates. PL images reveal the spatial homogeneity of both emission intensity and energy along individual nanotubes. The images provide detailed information on several key phenomena influencing the excited state properties of SWCNTs including the interaction with the environment, nanotube-nanotube coupling and defect density. Specifically, we focus on the photophysics of excitons at local dopant sites [2].

[1] Mauser, N. et al., Chem. Soc. Rev., Vol. 43, No. 4, 2014.
[2] Hartmann, N. et al., Nanoscale, Vol. 7, No. 48, 2015.

O 51.20 Tue 18:30 P1C

Analysis of molecular wire formation of cyano-functionalized porphyrins on Cu(111) by calculation of STM images — •Martin Gurrath[1], Wolfgang Hieringer[2], Michael Lepper[3], Tobias Schmitt[4], Alexander Schneider[4], Hubertus Marbach[3], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Lehrstuhl für Theoretische Chemie, FAU Erlangen-Nürnberg — [3]Lehrstuhl für Physikalische Chemie II, FAU Erlangen-Nürnberg — [4]Lehrstuhl für Festkörperphysik, FAU Erlangen-Nürnberg

The structure of adsorbed cyano-functionalized free-base tetraphenyl porphyrins (2H-TCNPP) on Cu(111) and their appearance in scanning tunneling microscopy (STM) is investigated by density-functional theory (DFT) calculations. In experiment, a formation of one-dimensional 2H-TCNPP chains in which the molecules are strongly distorted along the chain axis is observed after annealing. The DFT calculations support that the molecular wire formation is triggered by Cu adatoms and they provide insights into the cause of the strong distortion of the 2H-TCNPP molecules.

O 51.21 Tue 18:30 P1C

Simulation of reversibly interlocked SWCNTs — •Sebastian Gsänger and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

In chemical functionalization of single-walled carbon nanotubes (SWCNTs), usually one has to compromise between altering the structure of the nanotube via covalent attachment of the adsorbates or by forming rather fragile supramolecular complexes. An alternative, which combines having only non-covalently bound species but leads to very stable structures, is the concept of mechanically interlocking the CNT inside the adsorbate molecule. Specifically, we explore adsorbates which allow for a reversible ring closure in the rotaxane-forming step, therefore promising greater yields and a better control of the target structure. By performing molecular dynamics simulations with the generalized AMBER force field, we identified suitable structures and geometries and analyzed their behaviour and the reaction conditions.

O 51.22 Tue 18:30 P1C

On-Surface Synthesis of Low-Dimensional Nanostructures from Haloarenes — •Qitang Fan[1], Tao Wang[2], Cici Wang[2], Junfa Zhu[2], Min Chen[1], Claudio K. Krug[1], Malte Zugermeier[1], Julian Kuttner[1], Gerhard Hilt[1], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]National Synchrotron Radiation Laboratory, University of Science and Technology of China

The fabrication of low-dimensional nanostructures via on-surface synthesis has attracted tremendous attention due to their potential applications in nano-scale electronics and devices. Robust zero-dimensional (0D) cycles and one-dimensional (1D) chains are fabricated on metal surfaces from 4,4”-dibromo-m-terphenyl (DBMTP) molecules. Hyperbenzene, a hexagon consisting of 18 phenyl rings, forms ordered arrays on Cu(111), Ag(111) and Au(111) with maximum yield under pseudo-high dilution conditions. Organometallic tetragons and hexagons with C-Cu-C bonds were obtained on Cu stripes (with width from 2.6 nm to 3.6 nm) of a Cu(110)-(2x1)O supergrating surface. Zigzag organometallic chains and the corresponding oligophenylene chains form from DBMTP on Cu(110), Cu(111), Ag(111) and Au(111) with different yields and length distributions. The comparison of the outcomes on different substrates may shed light on the control of the topologies of nanostructures.

O 51.23 Tue 18:30 P1C

Halogen bonding in molecular self-assemblies of functionalized triphenylamines on Au(111) and Ag(111) — •Sachin Raj Menon[1], Christian Steiner[1], Tim Sander[1], Natalie Hammer[2], Milan Kivala[2], and Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, Germany — [2]Chair of Organic Chemistry I, Department of Chemistry and Pharmacy, Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, Germany

Halogen-substituted molecules are frequently used as precursors in the on-surface synthesis of carbon-based molecular architectures. It is therefore important to understand how they self-assemble on metal surfaces, because it might affect the structure of the covalent reaction products. Halogen bonds are comparatively weak and often compete with other interactions such as hydrogen bonds.

Herein, we report on the self-assembly of halogen-substituted, carbonyl-bridged triphenylamines on Au(111) and Ag(111) by high-resolution scanning tunneling microscopy at low temperatures. We studied the binding motifs of various triphenylamine networks that result from competing halogen bonding and hydrogen bonding interactions. In addition, we discuss the influence of the molecule-substrate interactions on the self-assembly as well as the strength of the sigma-hole bonding by comparing chlorine and iodine substituted moieties.

O 51.24 Tue 18:30 P1C

The electronic structure of the Si(553)-Au surface functionalized by small molecules — •Svetlana Suchkova[1], Eugen Speiser[1], Sandhya Chandola[1], Conor Hogan[2], and Friedhelm Bechstedt[3] — [1]Leibnitz-Institut fuer Analytische Wissenschaften - ISAS - e.V., Department Berlin, Schwarzschildstr. 8-10, 12489 Berlin, Germany — [2]Universita di Roma ”Tor Vergata”, Via della Ricerca Scientifica 1, 00133 Roma, Italy — [3]Friedrich-Schiller-University Jena, Institut fuer Festkoerpertheorie und optik, Helmholtzweg 3, 07743 Jena

We propose a method for surface modification and tuning the electronic structure of the stepped Si(553)-Au surface by site-specific adsorption of toluene-3,4-dithiol (TDT) molecules. We continue our research on the adsorption of the molecule using density functional theory (DFT) simulations. Hydrogen is used to passivate the step edge dangling bonds, and various orientations/adsorption geometries of TDT on terrace sites are analysed. In spite of expectations, that molecular thiol groups will interact with Au chains, it was shown that the most reactive surface adsorption sites are Si double bonds on the honeycomb chains. On the basis of the analysis of the electronic band structure it was shown that depending on the selective adsorption geometry, metallic or insulating phases of the surface are observed. Our approach offers microscopic manipulation and fine tuning of surface geometry and electronic properties, preparation of nanopatterned surface templates with controllable molecular adsorption sites, and suggests a switch of chemical reactivity on such surfaces

O 52: Nanostructures at Surfaces: Dots, Particles, Clusters

Time: Tuesday 18:30–20:30 Location: P1C

O 52.1 Tue 18:30 P1C

A Neural Network Potential for the Simulation of Copper Clusters on Zinc Oxide — •Martín Leandro Paleico and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Germany

A catalyst composed of large copper and zinc oxide nanoparticles is utilized in the industrial synthesis of methanol. Studying this system requires a simulation method capable of handling thousands of atoms with ab-initio accuracy, but with computational efficiency comparable to classical force fields. For this purpose Neural Network Potentials (NNP) are trained using DFT reference data, to reproduce the potential energy surface of the system.

The current work focuses on the first results for the ternary copper-zinc oxide system. In particular, the growth of copper clusters on zinc oxide surfaces is studied through combined molecular dynamics and Monte Carlo simulations, utilizing a NNP to provide the energies and forces.

O 52.2 Tue 18:30 P1C

Mobility and apparent height of mass selected copper clusters on well ordered Al_2O_3 layers studied with STM — •Dominik Wolter[1], Raphael Floegel[1], Matthias Bohlen[1,3], Christoph Schröder[1], Conrad Becker[2], and Heinz Hövel[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Aix-Marseille Université, CNRS, CINaM UMR 7325, 13288 Marseille, France — [3]Now at: Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany

Oxide layers are commonly used for industrial purposes (e.g. microelectronics) but also a topic of current research. It was shown previously, that an Al_2O_3 film on a clean $Ni_3Al(111)$ surface can provide a template for metal cluster growth [1,2,3]. The quality of the oxidized surface was investigated with LEED and STM. We evaluate the next-neighbor (NN) distances of deposited Cu clusters in order to learn more about their arrangement on the oxidized surface as well as their apparent height, which strongly depends on the applied bias voltage. First Z(V) single point spectroscopy data is shown. Furthermore the mobility of the clusters at various coverages is analyzed by incremental heating procedures. The normalized NN distances are then compared to Monte Carlo simulation data for various lattices to check whether the clusters attach to the oxide's template structure. We found strong indication for the fixation of clusters on the so called dot sites of the surface. [1] S. Degen et al., Faraday Discuss. **125**, 343-356 (2004) [2] A. Wiltner et al., Thin Solid Films **400**, 71-75 (2001) [3] C. Becker et al., New J. Phys. **4**, 75.1-75.15 (2002)

O 52.3 Tue 18:30 P1C

Optische und elektronische Eigenschaften wasserabgesättigter Rutil-Nanopartikel — •Walter Pfäffle — Institute of Physical Chemistry University of Hamburg

Halbleitende Metalloxide in Form von Nanokristallen oder Nanopartikel sind in letzter Zeit unverzichtbar für viele Anwendungen geworden. Mit einer Bandlücke von 3,23 eV für Anatas und 3,0 eV für Rutil ist Titandioxid ein halbleitendes Metalloxid, das insbesondere in Verbindung mit photoktalytischer Wasserspaltung immer häufiger untersucht wird und industriell von großer Bedeutung ist. Man kann sich die Partikel in der Theorie so zurecht bauen, dass sie die gewünschten optischen und elektronischen Eigenschaften besitzen. Der quantum-size Effekt besagt, dass kleine halbleitende Partikel verschiedene Absorptionseigenschaften haben. Wenn also der Radius des Elektron-Loch-Paars größer wird, als die Größe des Partikels verbreitert sich die Bandlücke. Wasser abgesättigte Rutil Nanopartikel werden zunehmend im Hinblick auf ihre photokatalytische Wasserspaltung und elektronische *Fallen* Zustände untersucht. Es wurden in dieser Arbeit strukturelle, optische und elektronische Eigenschaften von verschiedenen mit Wasser abgesättigten Rutil Nanopartikeln mit verschiedenen Methoden berechnet und diese mit dem Festkörper, dessen Oberflächen und nicht abgesättigten Partikeln verglichen. Insbesondere wird auf die Berechnung der absoluten Orbitallagen und die Visualisierung der Grenzorbitale Wert gelegt, da sie für photokatalytische Wasserspaltung von großem Interesse sind. Dabei benutzte ich zur Strukturoptimierung, dass semi empirische Programm MSINDO , GPAW und CRYSTAL.

O 52.4 Tue 18:30 P1C

Formation and stabilization of silver and gold nanoparticles in room temperature ionic liquids. — •Alexander Kononov, Stefanie Roese, Florian Lippert, and Heinz Hövel — Fakultät Physik/DELTA, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany

Room temperature ionic liquids (RTILs) are chemically stable salts in the liquid phase at room temperature (RT) with negligible vapour pressure, which makes them suitable for vacuum applications. RTILs form a self organized structure of cations and anions by hydrogen bonds, which allow steric and electronic stabilization of metallic nanoparticles (NPs) [1].

Deposition of metal atoms on the RTIL surface leads to the formation of metal NPs in the RTIL [2,3]. For a better understanding of the formation mechanism of silver and gold NPs, several samples were prepared by magnetron sputter deposition into an RTIL (BMIM PF_6) under different sputter conditions. Formation and aggregation processes of NPs stored at different temperatures were detected (after sputtering at RT) by UV/Vis absorption measurements. Afterwards the sputtered Ag RTIL samples are compared to samples produced by deposition of clusters preformed in a supersonic expansion [4].

[1] J. Dupont, J. D. Scholten, Chem. Soc. Rev. **39**, 1780, (2010). [2] K. Richter, A. Birkner, A. Mudring, Phys. Chem. Chem. Phys. **13**, 7136, (2011). [3] T. Torimoto, K. Okazaki, T. Kiyama, K. Hirahara, N. Tanaka, S. Kuwabata, Appl.Phys.Lett. **89**, 243117, (2006). [4] D. C. Engemann, S. Roese, H. Hövel, J. Phys. Chem. **120**, 6239, (2016).

O 52.5 Tue 18:30 P1C

Metal-enhanced fluorescence of oriented emitters in plasmonic nanostructures — •Fabian Gossler[1], Matthias Stöter[2], Thorsten Schumacher[3], Markus Lippitz[3], Josef Breu[2], Andreas Fery[1], and Tobias A.F. König[1] — [1]Institute of Physical Chemistry and Polymer Physics, Leibniz Institute of Polymer Research (IPF), Hohe Str. 6, 01069 Dresden — [2]Dept. of Inorganic Chemistry 1, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth — [3]Dept. of Experimental Physics 3, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth

For implementation of nanophotonic devices, a tunable life-time and controllable enhancement of the spontaneous emission is necessary. We fabricate a gold film coupled anisotropic silver nanocube cavity to systematically study the fluorescence enhancement of oriented fluorophores. For a rational design, the plasmonic properties of the silver nanocubes are designed to match with the emission spectrum of a selected fluorophore. Silicate bilayers with intercalated fluorophores are used as emitting spacer due to their regular height of 4 nm on large scales and orientation of the dye molecules. Finite-difference time-domain (FDTD) simulations, atomic force microscopy (AFM), dark field spectroscopy, confocal and time-resolved photoluminescence measurements have been used to characterize the tailormade nanocavity. Significant emission enhancement and a strong influence on life-times are observed inside the nanocavity. FDTD simulations support the results and demonstrate the potential of this cavity enhancement as building block for application in plasmonic lasers or metamaterials.

O 52.6 Tue 18:30 P1C

Deposition and temperature dependent surface interaction of Co nanoparticles on W(1 1 0) — •Jens Schubert, Hendrik Bettermann, and Mathias Getzlaff — Institute of Applied Physics, Heinrich-Heine-Universität Düsseldorf

Our research involves supported nanoparticles of 3d-metal alloys. Temperature dependent behavior is interesting for fundamental research and possible technological applications. These properties depend strongly on the nanoparticles' size.

The nanoparticles are produced under UHV conditions by a magnetron sputter source (Haberland-type), which gives access to sizes ranging from 3nm to >12nm.

Our approach is to measure surface structure and cleanliness with LEED (low energy electron diffraction) and the temperature dependent interaction of cobalt nanoparticles on a W(110) surface with spatial resolution by scanning tunnelling microscopy (STM) before and after heating.

O 52.7 Tue 18:30 P1C

Nanoparticle Adhesion and Optical Particle Motion Control — •Michaela Schmid[1], Daniel Geiger[1], Clara Wanjura[1], Irina Schrezenmeier[1], Matthias Roos[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Carl Zeiss SMT GmbH, Rudolf-Eber-Strasse 2, 73447 Oberkochen, Germany

The adhesion of nanoparticles on substrates like silicon wafers is of high interest for a variety of scientific and industrial applications. To determine adhesion, a method based on lateral pushing of nanoparticles by an atomic force microscope (AFM) tip was used. The lateral force acting on the cantilever by the particle is then a function of its adhesion force to the substrate.

However, the nature of the detachment and moving process remains unclear. Additional experiments are necessary to distinguish between rolling, sliding or jumping motion. These processes are investigated by simultaneous optical observation. Using total internal reflection (TIR) illumination, the scattering intensity of the bead contains the distance information from bead to substrate. Partially fluorescent particles allow to distinguish between rolling and sliding motion [1].

[1] S. Schiwek et al, Evidence of a rolling motion of a microparticle on a silicon wafer in a liquid environment, J. of Appl. Phys. 119, 194304 (2016)

O 52.8 Tue 18:30 P1C

Nanoparticle Adhesion on Flat Surfaces - an AFM Lateral Force Study — •Clara Wanjura[1], Daniel Geiger[1], Michaela Schmid[1], Irina Schrezenmeier[1], Matthias Roos[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Carl Zeiss SMT GmbH, Rudolf-Eber-Strasse 2, 73447 Oberkochen, Germany

Understanding how nanoparticles adhere to surfaces is relevant, since in many applications, as for example in photolithography, such nanoparticles can already cause defects. In other settings, the adhesion of nanoparticles might be desirable. In all of these cases, it is important to understand how strongly particles stick to the surface and how to influence that interaction.

The lateral force needed to move nanoparticles with an AFM tip is sampled at discrete points in time over several weeks for probes stored in different environments to understand the aging process of silicon surfaces decorated by nanoparticles. As well as an increase in lateral force in certain environments, the formation of layers of a hard material, possibly silicon oxide, around the particles is shown. In addition, the height of these layers is examined with an AFM and compared to a published model for the growth of silicon oxide layers through oxidation, the Deal-Groves model [1].

[1] General Relationship for the Thermal Oxidation of Silicon, Deal, B. E. and Grove, A. S., Journal of Applied Physics, 36, 3770-3778 (1965), DOI:http://dx.doi.org/10.1063/1.1713945

O 52.9 Tue 18:30 P1C

Noncollinear spin arrangement in size-selected FeV clusters on Cu(100) — •Fridtjof Kielgast[1], Ivan Baev[1], Friederike Albrecht[1], Christina Ossig[1], Michael Martins[1], and Wilfried Wurth[1,2] — [1]Physics Department, University of Hamburg — [2]DESY Photon Science, Hamburg

Deposited clusters constitute interesting model systems for fundamental as well as applied research, as their electronic and magnetic properties tend to change nonlinearly with cluster size and composition. Here, we present investigations on small, size-selected V_nFe_m adsorbates produced by high energy sputtering. The clusters were deposited onto a Cu(100) surface using a soft landing scheme to avoid fragmentation. X-Ray magnetic circular dichroism (XMCD) measurements were carried out up to sizes of n+m=3. The XMCD signal was obtained by switching an external magnetic field (±7T) and scanning the $L_{2,3}$ edges of V and Fe respectively with circular polarized light at the P04 beamline at PETRA III, DESY. By changing the incidence angle between the incoming light and the sample, the axis of easy magnetization could be found. This work is supported by the DFG in the framework of the SFB 668.

O 52.10 Tue 18:30 P1C

Synthesis of transition metal oxide nanoparticles by thermal decomposition of metal oleate precursors — •Aladin Ullrich, Mostafizar Mohammad Rahman, and Siegfried Horn — Institut für Physik, Universität Augsburg, D-86159 Augsburg, Germany

Iron oxide nanoparticles are currently one of the most interesting materials due to unique properties and potential applications. The size, shape and size distribution of iron oxide nanoparticles have great influence on their physical properties and therefore on their application potential.

We have investigated the influence of synthesis parameters like the heating rate or surfactants on particle size, shape and size distribution of iron oxide nanoparticles applying the method of thermal decomposition of iron oleate precursor. The particle size varies from 14-24 nm for different heating rates (from 1 to 35°C/min) in our experiments. Spherical nanoparticles were obtained in the presence of oleic acid as surfactant, cubic nanoparticles were obtained using a mixture of oleic acid and Na-oleate as surfactants. Different size distributions are observed for different heating rates. Magnetic properties of different sized particles were investigated using SQUID magnetometry. In addition, manganese ferrite nanoparticles with varying Fe:Mn ratio were synthesized. The influence of the Fe:Mn ratio on the Curie temperature and saturation magnetization of the nanoparticles was investigated.

O 52.11 Tue 18:30 P1C

Characterization of Ag clusters in ionic liquids with DLS — •Florian Lippert, Stefanie Roese, and Heinz Hövel — Fakultät Physik / DELTA, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund

Ag clusters produced in a supersonic expansion [1] can be deposited without coalescence into room temperature ionic liquids (RTILs), which are salts of weakly coordinating cations and anions being liquid at room temperature controlled by UV/Vis spectroscopy [2].

To get an insight into the process of stabilization and aggregation, we investigate Ag clusters in EMIM-FAP and BMIM-PF_6 by dynamic light scattering (DLS) [3].

The time-dependent change of the scattered light intensity depends on the Brownian motion of the nanoparticles. By means of that it is possible to receive the size distribution of the particles given by their hydrodynamic radius.

For proper measurement the material properties as viscosity and refractive index are indispensable. To determine the refractive index of the RTIL an Abbe refractometer and extrapolation to other wavelengths is used.

Measurements for storage at different temperatures show how stable the clusters in the ionic liquid are over time scales of several days.

[1] H. Hövel, S. Fritz, A. Hilger, U. Kreibig and M. Vollmer, Phys. Rev. B 48, 18178, 1993 [2] D. Engemann, S. Roese and H. Hövel, J. Phys. Chem. C 120, 6239, 2016 [3] B.J. Berne and R. Pecora, Dynamic Light Scattering, Dover Publications, New York, 2000

O 52.12 Tue 18:30 P1C

Ultrafast vibration and cooling of ultrathin gold nanotriangles studied by ultrafast X-ray Diffraction — •J. Pudell[1], A. von Reppert[1], R. M. Sarhan[1], F. Stete[1], M. Reinhard[1,4], M. Rössle[1], W. Koopmann[1], F. Zamponi[1], N. Del Fatti[2], A. Crut[2], J. Koetz[3], F. Liebig[3], C. Prietzel[3], and M. Bargheer[1,4] — [1]Institut für Physik, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [2]FemtoNanoOptics group, Institut Lumière Matière, Univ Lyon, Université Lyon 1, CNRS, 69622 Villeurbanne, France — [3]Institut für Chemie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [4]Helmholtz-Zentrum Berlin, Wilhelm-Conrad-Röntgen Campus, BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

We study the vibrations and subsequent thermalization of ultrathin gold nanotriangles upon optical excitation of the electron gas by ultrafast x-ray diffraction (UXRD). Our measurements yield an accurate determination of the structural response of an asymmetric nanoparticle including amplitude and phase of the excited vibrational motion. The amplitude of the fastest mode with 3.6 ps period measures the instantaneous rise of electronic pressure and the phonon-pressure rising within 6 ps. Slower symmetric in-plane modes of the particle contribute less to the signal. The nanosecond relaxation time of the expansion yields a direct measure of heat flow out of the nano-object, which is limited by the molecular connection to the substrate. We report data recorded at the laser-driven Plasma X-ray Source (PXS) in Potsdam and at the XPP-KMC3 Beamline at the synchroton radiation facility Bessy II.

O 52.13 Tue 18:30 P1C

Selective nucleation of MnSb Islands on GaAs Substrates — •Christian Klump[1], Bo Zhang[1], Julian Ritzmann[2], Arne Ludwig[2], Andreas Wieck[2], and Ulrich Köhler[1] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany

For future spintronic semiconductor devices, spin polarization and injection is one important prerequisite. Ferromagnetic or half-metallic materials can be used as efficient spin-injectors. As with the underlying semiconductor quantum dots, it is necessary to be able to grow the spin-injector material site-selectively. Prestructuring the substrate and strain-driven nucleation are two approaches for site-selective growth.

Prestructuring the substrates introduces defects to the surface and may deteriorate the quality of subsequent island growth. Examples of growth on a prestructured substrate are shown.

Strain-driven nucleation, on the other hand, opens the prospect of pin-pointing exactly one spin-injector island to one semiconductor QD by using the inherent strain induced by the underlying semiconductor QD, so spin-injection can be studied for each QD, individually.

MnSb is an interesting material for spin-injection with its high Curie temperature of 587 K and its compatibility with semiconductor substrates. The strain induced pairing of MnSb islands with InAs QDs is studied. MnSb islands were grown on different GaAs substrates by MBE. Structural and magnetic properties have been studied by STM, LEED and MOKE.

O 53: Nanostructures at Surfaces: Other Aspects

Time: Tuesday 18:30–20:30 Location: P1C

O 53.1 Tue 18:30 P1C

Modelling of surface properties of beryllium-tungsten alloys — •Alexander Kaiser[1], Ivan Sukuba[1,2], Lei Chen[1], Jan Urban[2], and Michael Probst[1] — [1]Institute for Ion Physics and Applied Physics, University of Innsbruck, Innsbruck, Austria — [2]Technikerstraße

The high melting of tungsten and its resilience against physical sputtering make it a favorable material for plasma facing components with high heat loads. Beryllium is a very light, low-Z material and a neutron multiplier and also has other favorable properties such as a low tritium solubility. In the ITER thermonuclear fusion experiment, beryllium will be used for the first wall and tungsten for the divertor. Sputtering, transport, and deposition of these materials can lead to alloy formation in the device. With quantum chemical methods, we try to shed some light on the stability and the reactivity of Be, W, and selected alloys of Be and W, including their sputtering properties.

O 53.2 Tue 18:30 P1C

Surface Modifications of Various Ionic Fluoride Single Crystals by Slow Highly Charged Ions — •Ayman S. El-Said[1], Richard A. Wilhelm[2,3], René Heller[2], Friedrich Aumayr[3], and Stefan Facsko[2] — [1]Physics Department, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Institute of Applied Physics, TU Wien, 1040 Vienna, Austria

The creation of surface nanostructures is of high importance for today's nanoelectonics and nanophotonics applications. Slow highly charged ions (HCI)have demonstrated their uniqueness and effectiveness in the formation and control of nanostructures in various materials. Here, we focus on the surface modifications induced by HCI in alkali (LiF) and alkaline-earth (CaF2 and BaF2) fluoride single crystals. The surfaces were irradiated with HCI of different charge states and kinetic energies. In case of CaF2 and BaF2, only one type of nanostructures (hillocks) was observed after surpassing certain potential energy thresholds for the incident HCI. For LiF, HCI were able to create three types (pits, calderas, and hillocks) of nanostructures by varying the impinging ions' charge states, or microscopically the locally deposited potential energy. The results are discussed in terms of defect-mediated desorption and thermal spike models.

O 53.3 Tue 18:30 P1C

Controlling charge fluctuations of a few donor system — •Ole Bunjes, Philipp Kloth, Judith von der Haar, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Combining a low temperature Scanning Tunneling Microscope with optical excitation, we have investigated temporal charge fluctuations within the tip induced space charge region. Our studies on the (110) surface of n-doped GaAs have shown that the system can be driven into different non-equilibrium states due to optically induced minority charge carriers [1]. Analysis of the noise characteristic of the tunnel current reveals the influence of photo-generated holes on dynamical charging processes. The presence of these free charges allows us to change and control the noise characteristic of the system. The noise level depends on the laser intensity as well as the tunnel current, controlled by the tip-sample-distance. Most surprisingly, the overall noise can even be reduced compared to the non-illuminated system. We attribute the optically induced modification of the noise characteristic to temporal charging and discharging of dopant atoms within the space charge region [2]. We acknowledge the financial support by the SFB1073 C04. [1] P. Kloth et al., Nat. Commun. 7, 10108 (2016) [2] K. Teichmann et al., Nano Lett. 11, 3538-3542 (2011)

O 53.4 Tue 18:30 P1C

Controlling charge dynamics in a space charge region under optical excitation — •Judith von der Haar, Philipp Kloth, Ole Bunjes, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

By combining laser excitation and Scanning Tunneling Microscopy we have investigated the charge dynamics of a few donor system at the n-doped GaAs(110) surface. When a STM-tip is positioned close to the GaAs a SCR is induced inside the sample. In equilibrium it is screened by ionized donors at the surface. We force the system out of equilibrium by illuminating the sample and generating free charge carriers. The photo-generated holes can be addressed by tunneling electrons, leading to an additional transport channel. Using the tunnel current as a control parameter we are able to actively change the hole concentration at the surface [1]. The temporal evolution of the photo-generated holes was studied for different laser intensities, tunnel currents and bias voltages using pulsed optical excitation with nanosecond time resolution [2]. This gives access to the screening dynamics of the tip-induced potential. Furthermore, we have measured the charging and discharging processes of single donors. Atomically resolved data proof that the relaxation time depends on the relative depth of the donors to the surface. This work was supported by the DFG via the SFB1073 C04. [1] P. Kloth et al., Nat. Commun. 7, 10108 (2016) [2] P. Kloth et al. A versatile implementation of pulsed optical excitation in Scanning Tunneling Mircroscopy. Rev. Sci. Instr. (acc. 2016)

O 53.5 Tue 18:30 P1C

Neon ion beam induced pattern formation on amorphous carbon surfaces — •Omar Bobes, Hans Hofsäss, and Kun Zhang — II. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

We investigate the ripple pattern formation on amorphous carbon surfaces at room temperature during low energy Ne ion irradiation as a function of ion incidence angle. Monte Carlo simulations of the curvature coefficients applied to the Bradley-Harper and Cater-Vishnyakov models, including the recent extensions by Harrison-Bradley and Hofsäss and taking into account the incorporation of the ions into the film predict that pattern formation on amorphous carbon should be possible for low energy Ne ions from 250 eV up to 5 keV. Moreover, simulations are able to explain the absence of pattern formation in certain cases. Our experimental results are compared with prediction using current linear theoretical models and applying the crater function formalism as well as Monte Carlo simulations to calculate curvature coefficients using SDTrimSP program.

O 53.6 Tue 18:30 P1C

Treatments of high-density polyethylene (HDPE) with atomic hydrogen - a surface study — •Torben Schlebrowski, Christian B. Fischer, and Stefan Wehner — Department of Physics, University of Koblenz-Landau, 56070 Koblenz, Germany

The deposition of diamond-like carbon (DLC) films on materials like polymers is a well-established method for substrate surface modification and its refinement. The interaction of atomic hydrogen with polymers in contrast is not well studied, although it is part of the most techniques used for DLC depositions. For a complete description of the carbon deposition process it is inescapable to study this aspect, since the hydrogen is supposed to change and modify the polymeric substrate surface by impinging. Measurements by in situ thermal desorption spectroscopy (TDS) during hydrogen treatment are performed to analyze process products and by atomic force microscopy (AFM) surface changes due to the hydrogen processing are revealed. The contribution shows first results for the interaction of atomic hydrogen with common polymers as HDPE.

O 53.7 Tue 18:30 P1C

Investigating the switching behaviour of a Tetraphenylmethane-Derivative on Au(111) with STM — •Timo Frauhammer[1,2], Lukas Gerhard[2], Kevin Edelmann[2], Marcin Lindner[2], Michal Valasek[2], Marcel Mayor[2], and Wulf Wulfhekel[1,2] — [1]Physikalisches Insitut, Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe, Germany

The adsorption and switching behaviour of a Tetraphenylmethane-derivative adsorbed on Au(111) have been studied using scanning tunneling microscopy (STM) at 5.3 K. This derivative consists of a Tetraphenylmethane-core where the four Hydrogen atoms in para-position with respect to the central sp3-Carbon atom are substituted by three Thioacetate-groups and one Triflate-group. The molecules have been deposited on Au(111) from a Dichloromethane solution by using a spray technique. The tip of the STM induces a characteristic switching behaviour between two metastable states. Moreover, Random Telegraph Noise (RTN) can be observed at certain tunneling parameters. The functional dependence of this RTN on bias voltage and tip-sample distance indicates that the switching is induced by the electrical field in the tunnel junction.

O 53.8 Tue 18:30 P1C

Universal readers based on hydrogen bonding or π-π stacking for identification of DNA nucleotides in electron tunnel junctions — •Suman Sen[1], JongOne Im[2], Peiming Zhang[2], and Stuart Lindsay[2] — [1]Max Planck Institute, Stuttgart, Germany — [2]Arizona State University, Tempe, USA

A universal reader molecule, which recognizes all the naturally occurring nucleobases in a tunnel junction, is required for sequencing DNA by a recognition tunneling (RT) technique. We have designed a series of heterocyclic carboxamides based on hydrogen bonding and a large-sized pyrene ring based on a π-π stacking interaction as reader candidates. RT measurements were carried out in a scanning tunnel microscope. All of these molecules generated electrical signals with DNA nucleotides in tunneling junctions under physiological conditions. Using a support vector machine as a tool for data analysis, we found that these candidates distinguished among naturally occurring DNA nucleotides with the accuracy of pyrene > azole carboxamides. In addition, the pyrene reader operated efficiently in a larger tunnel junction. However, the azole carboxamide could read abasic monophosphate, a product from spontaneous base hydrolysis or an intermediate of base excision repair. Thus, we envision that sequencing DNA using both π-π stacking and hydrogen-bonding-based universal readers in parallel should generate more comprehensive genome sequences than sequencing based on either reader molecule alone.

O 53.9 Tue 18:30 P1C

Hyperuniformisation by Lloyd's algorithm for Centroidal Voronoi diagrams — •Jakov Lovrić[1,2], Philipp Schoenhoefer[3,4], Sebastian Kapfer[3], Fabian Schaller[3], Michael Klatt[5], Bruce Gardiner[4], Ana-Sunčana Smith[1,2], and Gerd Schröder-Turk[4] — [1]Institute Ruđer Bošković, Division of Physical Chemistry, Group for Computational Biosciencies, Zagreb, Croatia — [2]Institute for Theoretical Physics, PULS Group and Cluster of Excellence: EAM, FAU Erlangen-Nürnberg, Germany — [3]Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [4]School of Engineering and Information Technology, Murdoch University, Western Australia 6150, Australia — [5]Karlsruhe Institute of Technology (KIT), Institute of Stochastics, Karlsruhe, Germany

We study an application of centroidal Voronoi diagrams and Lloyds algorithm. The simple idea is that the evolution of points under Lloyd's algorithm leads to more uniform structures, in a loose sense. We investigated, and found an initial positive result, that Lloyd's algorithm can be used to achieve hyper-uniform structures when starting from several types of disordered point patterns. We havn't found a point pattern where Lloyd's algorithm does not lead to a hyper-uniform structure. An important question is whether Lloyd's algorithm induces crystalisation of the point configuration; one may have thought this possible, given that the body-centered cubic lattice is considered the configuration with lowest energy w.r.t. the functional used in Lloyd's algorithm.

O 53.10 Tue 18:30 P1C

Biopolymers in Vacuum and at Surfaces — •Stephan Rauschenbach[1], Sabine Abb[1], Elise Duquesne[1], Christian Schön[1], Ludger Harnau[1], Duy Le[2], Talat Rahman[2], and Klaus Kern[1] — [1]Max Planck Institute for Solid State Res., Stuttgart, Germany — [2]Univ. of Central Florida, Tampa FL, USA

Proteins, DNA, and sugars are the main classes of biopolymers. Each, with its unique properties, is essential for living organisms. Thus their thorough characterization is essential to improve our understanding of the complex molecular interactions underlying to the supreme functionality. With soft-landing electrospray ion beam deposition[1], we are able to control the transfer of said classes of polymers onto surfaces in vacuum such that high resolution imaging by scanning tunneling microscopy (STM) can reveal structural details at the submolecular level. This enables unprecedented insights, such as detection of saccharide subunits, sequence controlled assembly and folding of peptides, controlled formation of peptide-metal complexes, or conformation control of proteins. With this work we open routes to new materials based on complex, specific, molecular interaction and enable high resolution structural analysis of individual biopolymers.

[1] S. Rauschenbach et al. **Annu. Rev. Anal. Chem.** 9, 16.1-16.26 (2016)

O 53.11 Tue 18:30 P1C

Simulation of high energy XPD-patterns — •Robert Rauter, Christopher Kohlmann, Tobias Lühr, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Germany, Otto-Hahn-Str. 4, 44221 Dortmund

Photoelectron diffraction (XPD) is a powerful tool to examine surface and interlayer structures of solids. In order to extract the structural information from the experimental data, simulated XPD patterns are compared to experimental XPD patterns. For determining the correct structure a multiplicity of different surface and interface layer structures must be considered within the simulation.

The XPD pattern simulation is performed by the EDAC (Electron Diffraction in Atomic Clusters) package [1]. Reducing the quantity of simulations is achieved by utilizing a genetic algorithm [2]. We report on the improvement of convergence by applying the genetic algorithm in comparison to a deterministic approach.

[1]F.J. Garcia de Abajo, M.A. Van Hove and C.S. Fadley, Phys. Rev. B **63**, 075404 (2001).

[2]Pancotti, A. et al., J. Appl. Phys. **106**, 34104 (2009).

O 53.12 Tue 18:30 P1C

Considering the Convergent Beam in a Quantitative LEED Analysis — •Tilman Kisslinger, Pascal Ferstl, M. Alexander Schneider, and Lutz Hammer — Lehrstuhl für Festkörperphysik, Universität Erlangen–Nürnberg, D–91058 Erlangen, Germany

In a conventional LEED experiment the primary electron beam is not parallel, but slightly convergent (opening angle typically $2 \times 0.6°$), in order to focus the beam on the screen. Thus, experimental LEED intensity spectra are in fact a superposition of spectra belonging to all angles within that cone of incidence, therefore, model calculations performed for the central cone angle are just an approximation of the experimental situation.

For nominally normal incidence of the primary beam, which is the common experimental alignment, as it preserves a maximum of symmetry elements of the surface, we performed a pseudo–experiment, in which for a Rh(100)–(2×2)–O surface intensity spectra were calculated for various angles within a cone of $\Theta_{max} = 0.75°$, weighted according to their corresponding solid angle and averaged. A comparison with the set of spectra calculated for normal incidence yields a R_P of 0.036. It is further shown that using an average cone angle $\Theta_{av} = \Theta_{max}/\sqrt{2}$ instead fits the pseudo-experiment with high accuracy ($R_P = 0.0003$). Fitting the (average) angle of incidence for real experimental data of various and structurally very different systems taken nominally at normal incidence always led to an improvement of the R-factor by about 0.02 - 0.03. Consistently, all fits result in the same value for Θ_{av}, because it is solely determined by the experimental geometry.

O 54: Metallic Nanowires on Semiconductor Surfaces

Time: Tuesday 18:30–20:30 Location: P1C

O 54.1 Tue 18:30 P1C

Quasi-one-dimensional plasmons in Si(hhk)-Au: a crossover of dimensions — •Timo Lichtenstein[1], Zamin Mamiyev[1], Marvin Detert[1], Julian Aulbach[2], Jörg Schäfer[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Physikalisches Institut and RCCM, Universität Würzburg

For future plasmonic devices one-dimensional (1d) plasmons offer unique properties: an inherently predetermined direction, a wavelength much shorter than those of photons, and an almost linear dispersion. Au induced wires on regularly stepped Si(hhk) are a playground for quasi-1d structures. Therefore, they were prepared at coverages where the surfaces host single or double atomic gold chains parallel to the steps. This allows studying the influence of spacing and wire width. The wire quality was checked with spot profile analysis in low energy electron diffraction, in combination with an electron energy loss spectrometer providing both high energy and momentum resolution it gave access to the plasmon dispersion. Although 1d metallicity is observed, the plasmon dispersion strongly depends on two-dimensional properties: the lateral distribution of the 1d electron density within one terrace (intrawire correlation) and the spacing of the wires (interwire correlation). We obtained effective widths considerably smaller than the terrace width. A quantitative description is possible by a modified wire array plasmon model, claiming extensions of theory. Also, STM gives a modulated DOS of comparable width. Both the chain type as well as the terrace size seem to be of influence.

O 54.2 Tue 18:30 P1C

Au-chains grown on Ge(100): A detailed SPA-LEED and EELS-LEED study — •Timo Lichtenstein, Zamin Mamiyev, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover

Ge(100) is known as a substrate for self-organized growth of one-dimensional quantum wires by adsorption of Au, highly interesting for future plasmonic devices. In this study, the morphology has been investigated by means of spot profile analysis low energy electron diffraction. Using LEED in combination with an energy electron loss spectrometer we measured the plasmon dispersion relation with both high energy and momentum resolution. First, we systematically measured the properties on variously prepared surfaces. From G(S)- and H(S)-analyses on ex-situ chemically treated Ge-samples followed by multiple in-situ Ar^{+}-sputtering and high-temperature annealing cycles, we were able to obtain surfaces with a terrace width of around 100 nm and low roughness After the growth of the Au-wires, this analysis favors a giant missing row structure. For Au coverages higher than 0.7 ML low-dimensional plasmon modes appear in the loss spectra. Their dispersion relation increases linearly for parallel momentum $> 0.1\,\text{Å}^{-1}$, but deviates from the typical dispersion of a quasi-one-dimensional plasmon for $< 0.1\,\text{Å}^{-1}$. These effects are possibly attributed to the strong electronic correlations of the system due to the Luttinger-liquid-like behavior inside the wires as well as the strong coupling between. Peak widths and heights of the plasmon excitations in the loss spectra reveal a low excitation probability and very short lifetimes.

O 54.3 Tue 18:30 P1C

Tin nanowires on vicinal Si(111) surfaces — •Monika Jäger, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

Si(111) surfaces covered by 0.3 ML Sn are known to form a $\sqrt{3}\times\sqrt{3}$ reconstruction and reveal a Mott transition upon cooling below 70 K [1]. This system is now confined to a wire like one-dimensional structure using vicinal Si(111) substrates and investigated by means of STM and LEED.
Adsorption of Sn at 900 K gives rise to a refacetting of the Si(557) surface into a local (223) orientation with an average spacing of 1.58 nm similar to the isoelectronic Pb/Si(557) system (e.g. [2]). This change in orientation ist compensated by wider (111) terraces exhibiting a $\sqrt{3}\times\sqrt{3}$ reconstruction. In order to improve the long-ranged ordering, Si(223) surfaces are used additionally as a substrate. On both vicinal surfaces, the (223)-orientated parts consist of $4\frac{2}{3}\times 0.332$ nm wide (111) terraces which show a 0.75 nm periodicity along the terraces. This is consistent with the ×2 features seen in LEED measurements. Furthermore, the electronic structure is probed at different temperatures by STS.
[1] S. Modesti et al., PRL **98**, 126401 (2007).
[2] C. Brand et al., Nat. Comm. **6**, 8118 (2015).

O 54.4 Tue 18:30 P1C

Quantitative LEED studies on Si(111)-(5×2)-Au — •Andreas Alexander[1], Frederic Timmer[1], Joachim Wollschläger[1], Kaori Seino[2], and Friedhelm Bechstedt[2] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

The (5×2)-Au reconstruction on Si(111) has been in the focus of research for nearly 50 years now. Lately, in particular as a prototype for one-dimensional (1D) metallic chain structures. In order to understand the physical properties accompanying these 1D chains a profound knowledge of the atomic structure is needed. Historically, a plethora of atomic structures (EBH [1],AN [2],KK [3]) with varying Au coverages were discussed. More recently Shirasawa et al. [4] were able to show that Surface X-ray Diffraction experiments favor the KK-model slightly. Due to the higher surface sensitivity of Low Energy Electron Diffraction (LEED) as compared to SXRD we carried out quantitative LEED experiments in order to assess this observation.

[1] S. Erwin et al., Phys. Rev. B **80**, 155409 (2009)
[2] T. Abukawa and Y. Nishigaya, Phys. Rev. Lett. **110**, 036102 (2013)
[3] S. G. Kwon and M. H. Kang, Phys. Rev. Lett. **113**, 086101 (2014)
[4] T. Shirasawa et al., Phys. Rev. Lett. **113**, 165501 (2014)

O 54.5 Tue 18:30 P1C

Gold-induced Surfaces on Stepped Germanium: Growth and Characterization — •Tim Wagner, Julian Aulbach, Ralph Claessen, and Jörg Schäfer — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg

Adsorption of gold atoms on stepped Ge(hhk) surfaces leads to the formation of atomic wires via self-organization. Inspired by interesting physics such as spin chains on the step edges of similar gold-induced Si(hhk) surfaces [1], we establish recipes for the preparation of several gold-induced Ge(hhk) surfaces. Therefore, the preliminary sputter and anneal treatment of the stepped Ge(335), Ge(557) and Ge(553) substrates as well as the adsorption procedure of gold atoms provided by an electron beam evaporator have been optimized to achieve well-ordered surfaces. Due to the adsorption of gold atoms some Ge(hhk) surfaces undergo a refacetting in order to form a stable gold-induced surface. Based on scanning tunneling microscopy and low energy electron diffraction we determine the formation of surface reconstructions on the atomic scale on the Ge(hhk)-Au surfaces. In particular, we have characterized these surfaces regarding the formation of atomic wire structures, such as those formed by the Au and Ge atoms, and will present first indications for the occurence of superstructures.

[1] J. Aulbach et al., Nano Lett. 16(4) (2016).

O 55: Graphene

Time: Tuesday 18:30–20:30 Location: P2-EG

O 55.1 Tue 18:30 P2-EG

Inelastic electron tunnelling into graphene bilayers on Ir(111) — •Alexander Tries, Johannes Halle, Nicolas Néel, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

Physical vapour deposition of C onto graphene-covered Ir(111) has been used to fabricate graphene nanoflakes. Due to C atom intercalation the flakes form underneath graphene. Scanning tunnelling microscopy with atomic resolution reveals that the lattices of the upper graphene layer and the flakes are rotated with respect to each other. Spectra of the differential conductance show the hole-like Ir(111) surface resonance on top of the graphene-flake stackings. Graphene phonons with wave vectors comparable to the Brillouin zone dimensions leave their signatures in inelastic electron tunnelling spectra. Funding by the Deutsche Forschungsgemeinschaft through Grant No. KR 2912/10-1 is acknowledged.

O 55.2 Tue 18:30 P2-EG

The effect of defects on the band structure of graphene near the Dirac point — •Piotr Kot[1,2], Jonathan Parnell[2], Sina Habibian[2], and Christian R. Ast[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of British Columbia, Vancouver, Canada

Using a simple real-space tight-binding model, we present the effect of defects on the band structure of graphene in momentum space near the Dirac point. While several of the calculated defects strongly alter the band dispersion and line width near the Dirac point, we find that a band gap forms only in systems where atoms are missing from one sublattice. Another finding of note is that some specific defects open a band gap with broadened, but not entirely delocalized, states in the gap. These band gaps with broadened states strongly resemble "elongated" Dirac points that have been experimentally found by photoemission spectroscopy and have been discussed in the literature. We surmise that these "elongated" Dirac points are, at least in part, due to specific defects in the graphene. Our findings also point to obstacles to opening a band gap in graphene, which have to be considered.

O 55.3 Tue 18:30 P2-EG

Scanning tunneling microscopy and spectroscopy on graphene/*h*-BN/SiO$_2$/Si devices — •Lena Stoppel, Fabian Paschke, Julia Tesch, Samuel Bouvron, Yuriy S. Dedkov, and Mikhail Fonin — Department of Physics, University of Konstanz, Germany

Exceptional transport properties of graphene, a two-dimensional honeycomb lattice of sp^2-bonded carbon atoms, make it a promising material for applications in microelectronics and sensing.

Here, we present a systematic scanning tunneling microscopy (STM) study of graphene on *h*-BN/SiO$_2$/Si substrates. We use wet chemical transfer of CVD-grown multilayer hexagonal boron nitride (*h*-BN) and CVD-grown monolayer graphene onto a silicon chip with a thin insulating silicon dioxide layer. The transfer method was optimized in a way that STM measurements reveal large surface areas of clean graphene, showing the honeycomb atomic lattice and a Moiré pattern due to the underlying *h*-BN. We also perform scanning tunneling spectroscopy measurements to investigate the electronic properties of graphene. In a similar procedure graphene was transferred onto metal dichalcogenides, and the electronic properties were investigated.

O 55.4 Tue 18:30 P2-EG

Novel preparation technique for high quality graphene on boron nitride samples for combined electrical transport and STM measurements — •Tjorven Johnsen, Michael Weimer, Peter Nemes-Incze, and Markus Morgenstern — II. Physikalisches Institut B, RWTH Aachen, Otto-Blumenthal-Straße, 52074 Aachen

Whereas in electrical transport experiments suspended graphene samples or samples sandwiched between to boron nitride flakes show the highest mobility due to low charge disorder they are not accessible for scanning tunneling microscopy (STM). STM requires a graphene flake that is supported by a substrate and features an exposed surface. Here we present a novel technique to prepare such graphene samples on boron nitride substrates. A mica support is used to pick up boron nitride and graphene flakes from SiO$_2$ substrates. The graphene flake is contacted by gold evaporation through a shadow mask. In contrast to other fabrication methods we avoid any polymers in the process that works without any wet chemistry leading to a dry and polymer free transfer and contacting process for 2D materials. In addition to the low density of adsorbates on the graphene surface the clean and flat boron nitride substrate leads to high quality graphene samples.

O 55.5 Tue 18:30 P2-EG

Graphene growth on SiC(0001) without step bunching — •Jakob Lidzba, Martina Wanke, Florian Speck, and Thomas Seyller — Professur für Technische Physik, Institut für Physik, TU Chemnitz, Reichenhainer Straße 70, 09126 Chemnitz, Germany

Epitaxial growth of graphene on SiC(0001) is a well-established method for the production of high-quality graphene layers [1]. The growth process ist accompanied by a step bunching of the SiC and the concomitant formation of so-called macrosteps. Since the growth of graphene layers starts at the step edges, this prevents the formation of uniform graphene films. Therefore it is crucial to find a way of controlling their development. Kruskopf et al. stated, that the H-etch pretreatment is responsible for strong step bunching. However, the formation of high steps at the surface can be suppressed by separating the processes of buffer layer and graphene growth [2,3]. In this study we test different parameters for the growth process of monolayer graphene to avoid step bunching and therefore improve the growth process. Thickness of the graphene layers and chemical composition of the surface were determined from XPS spectra, while AFM was used to examine the topography of the sample surfaces.

[1] K.V. Emtsev et al., Nature Mater. **8**, 203 (2009).
[2] M. Kruskopf et al., J. Phys.: Condens. Matter **27**, 185303 (2015).
[3] M. Kruskopf et al., 2D Mater. **3**, 041002 (2016).

O 55.6 Tue 18:30 P2-EG

Preparation of epitaxial graphene on 4H-SiC(0001) — •Hassan Kakag, Florian Speck, Martina Wanke, and Thomas Seyller — Professur für Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany

The growth of epitaxial graphene (EG) on 6H-SiC(0001) in argon under atmospheric pressure provides high-quality graphene layers at large scale [1]. The present study is focused on the optimization of hydrogen etching and growth of EG on the (0001) surfaces of the other commonly available polytype 4H-SiC. Etching in hydrogen as well as sublimation growth is carried out in a hot-wall reactor [2]. The dependence of the etching behavior on the hydrogen flow rate and annealing temperature was studied in the range of 0.2-3.0 slm and 1350-1500 °C, respectively. Furthermore, the influence of process temperature and annealing time on the graphene growth was investigated. Surface composition and graphene thickness were obtained from XPS. The surface morphology after hydrogen etching and graphene growth was investigated by AFM. The onset of graphitization is witnessed by the formation of the $(6\sqrt{3}\times6\sqrt{3})R30^\circ$ reconstruction at 1450 °C for an annealing time of 15 min. The best result of monolayer graphene growth was achieved with an annealing time of 15 min at a temperature of 1700 °C. In addition, bilayer graphene growth at step edges of the terraced SiC substrate was observed at 15 and 30 min annealing time. The substrate steps are mostly ordered and of similar height.

[1] K. V. Emtsev et al., Nature Mater. **8**, 203 (2009).
[2] M. Ostler et al., Phys. Status Solidi B **247**, 2924 (2010).

O 55.7 Tue 18:30 P2-EG

Role of the tunnelling junction elements in photon emission from Au/Mica, Au/Cr/Mica, graphene/Cu systems — •Hakki Tunç Çiftçi[1], Berk Zengin[1], Umut Kamber[1], Cem Kincal[1], Dilek Yildiz[1,2], and Oğuzhan Gürlü[1] — [1]Istanbul Technical University, Istanbul, Turkey — [2]University of Basel, Basel, Switzerland

Photon emission occurrence from the tunnel junction relies on the material, apex and the cleanness of the tip of a scanning tunnelling microscope (STM). Certainly the surface electronic properties of the sample as well as its morphology directly determines the nature of the emitted photons. Minute and almost untraceable variance of chemical composition of the surfaces has a serious effect on the same phenomenon. For instance, chromium diffusion on to the surface in the Au/Cr/Mica system was shown to affect the local photon emission properties of the Au surface due to tunnelling injected electrons. The knowhow gathered from such studies was employed in the investigation of the photon emission measurements performed with a photon STM on Graphene/Copper system. Being able to identify the influence of tip effects and the local chemistry of the surface paved the way to a deconvoluted method of investigation of the correlation between photon emissivity of Graphene/Cu interface to the local surface orientation.

O 55.8 Tue 18:30 P2-EG

Graphene formation on thin epitaxial grown Cu(111)-foils by chemical vapor deposition of acetone — •Jens Neurohr[1], Samuel Grandthyll[1], Michael Weinl[2], Matthias Schreck[2], Karin Jacobs[1], and Frank Müller[1] — [1]Experimental Physics, Saarland University, 66041 Saarbruecken, Germany — [2]Experimental Physics 4, University of Augsburg, 86135 Augsburg, Germany

In comparison to the standard growth of graphene on copper via the CVD-process, an oxygen containing precursor (acetone) has been used for graphene formation on thin single crystalline Cu(111-foils. In contrast to some literature reports, graphene formation can be obtained at quite low temperatures of about 700°C [1,2]. Graphene growth on the Cu(111)-foils was investigated by X-ray photoelectron spectroscopy (XPS), X-ray photoelectron diffraction (XPD), low energy electron diffraction (LEED), Fermi surface mapping(FSM), and scanning tunnel microscopy (STM) revealing nearly one monolayer coverage of mostly ±1.65° rotated domains.

References:

[1] L. Gao, J. R. Guestand N. P. Guisinger Nano Letters 10.1021/nl1016706

[2] H. K. Yu, K. Balasubramanian, K. Kim, J.-L. Lee, M. Maiti, C. Ropers, J. Krieg, K. Kern and A. M. Wodtke ACS Nano 10.1021/nn503476

O 55.9 Tue 18:30 P2-EG

Analysis of local variations of the electronic properties of monolayer and bilayer graphene/HOPG — •Anne Holtsch and Uwe Hartmann — Universität des Saarlandes, P.O. Box 151150, 66041 Saarbrücken

Cleaving a hopg bulk material can occasionally result in formation of graphene. Compared to other substrates hopg has the advantage that occurring Moiré patterns solely have their origin in rotation of the graphene lattice with respect to the hopg lattice orientation. We investigate the topography of the Moiré superstructure by scanning tunnelling measurement (STM) and changes of the electronic properties of graphene induced by the Moiré pattern and variation in amount of graphene layers using scanning tunnelling spectroscopy (STS).

The formation of a Moiré pattern goes along with corrugation of the graphene sheet. But STM measurements of bilayer graphene where both layers are aligned without rotation but the system itself is rotated towards the substrate do not show any corrugation. A possible Moiré pattern in the lower layer does not permeate to the top layer leading to the conclusion that the occurrence of a Moiré pattern is an effect restricted to the topmost graphene layer.

In a monolayer graphene with corrugation due to a Moiré pattern the distance of the graphene layer to the substrate adjusts the size of a band gap opening. For small distance the monolayer can behave bilayer-like. With increasing distance the size of the band gap decreases.

O 55.10 Tue 18:30 P2-EG

Sulfur intercalation of epitaxial graphene on 6H-SiC(0001) — •Santha J. Panigrahi, Florian Speck, Adrian Schütze, Martina Wanke, and Thomas Seyller — Professur für Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany

During the initial stages of the sublimation growth of epitaxial graphene on SiC(0001), a carbon-rich $(6\sqrt{3} \times 6\sqrt{3})R30^\circ$ reconstruction, also referred to as buffer layer (BL), is formed at the interface to the SiC. Despite being structurally graphene-like, covalent interaction with the topmost Si atoms of the substrate renders the BL electronically inactive. Upon intercalation, these bonds to the substrate are broken. The BL is decoupled from the SiC substrate and the electronic properties of graphene are restored.

In this contribution, we show that upon annealing in a CVD-like setup at temperatures between 600 and 850 °C in the presence of sulfur, the BL can be decoupled from the SiC substrate. We investigate the sulfur intercalation employing a combination of experimental techniques such as X-ray photoelectron spectroscopy, low energy electron diffraction and atomic force microscopy to study chemical composition and structural properties.

O 55.11 Tue 18:30 P2-EG

Dimerization of activated Coronene on HOPG — •Jürgen Weippert[1], Julian Bachmann[1], Jean-Francois Greisch[1,2], Artur Böttcher[1], and Manfred M. Kappes[1,2] — [1]Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

We have studied the dimerization of Coronene (Cor) as a model reaction for the fabrication of tailored graphene nanoribbons (GNR). Low energy ion beam deposition of both intact monomers as well as dehydrogenated congeners was used to grow the corresponding films. The composition of the incident cationic beam can be tuned by changing the electron impact energy and by varying the selected mass range. Thermal desorption measurements indicate that this leads to the on-surface formation of Cor dimers presumably already during the film growth. We find two different reaction channels: (a) 2(Cor-2H)*(Cor-2H)2 and (b) (Cor-2H)+Cor*(Cor-H)2. While the monomers sublime at 460K the dimers (Cor-2H)2 sublime around 800K. The thermal desorption spectra indicate that the binding energy and the pre-exponential factor (EB=2.9 eV, v=1017 s-1) of on-surface-formed dimers (Cor-2H)2 are comparable to that of directly deposited Dicoronylene. We have also explored the structures of the corresponding (Cor-2H)2 and (Cor-H)2 species using a combination of laser ablation and ion mobility measurements.

O 55.12 Tue 18:30 P2-EG

Response of the electronic structure of graphene to pressure, temperature and humidity — •Haydar Altuğ Yildirim, Umut Kamber, Cem Kincal, and Oğuzhan Gürlü — Istanbul Technical University, Istanbul, Turkey

Since its first isolation, the detection of gas molecules as well as humidity and temperature by use of graphene have been a matter of interest. We have used atmospheric pressure Chemical Vapor Deposition (AP-CVD) grown graphene and various transfer techniques to produce graphene based sensors on dielectric substrates. A controlled atmosphere chamber was designed and built to investigate the response of the resistivity of graphene to varying pressure, temperature and humidity. Comparison of the measurements taken by custom made graphene devices and a precise commercial sensor have shown similar responses. Upon changing the surface temperature of the graphene device we were able to control the adsorption of the water molecules. Effects of graphene growth parameters and transfer processes on to dielectrics, as well as ageing and temperature over humidity sensing capacity of graphene based devices will be presented.

O 55.13 Tue 18:30 P2-EG

A comparative study of the oxidation of PAHs using atomic oxygen — •Jürgen Weippert[1], Vincent Gewiese[1], Philipp Huber[1], Artur Böttcher[1], and Manfred M. Kappes[1,2] — [1]Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

We have studied the oxidation of PAH films (Coronene, Hexabenzocoronene, Rubrene) as model systems for fabrication of tailored nanographene oxides. The corresponding PAH films were grown by low energy ion beam deposition. The as-prepared PAH films were then exposed to a flux of atomic oxygen at room temperature. UPS and XPS based analysis of the chemical composition of the resulting oxidized films reveals a broad spectrum of PAH oxides dominated by epoxy and ether species. The interaction of flat PAHs with the substrate modifies the oxidation pathways in submonolayers cf. multilayers: epoxides are replaced by lactones as the dominating oxide with the exception of non-planar Rubrene. According to theoretical predictions we attribute this specific influence of theHOPG substrate to mobile epoxy functionalities which are produced by reaction of HOPG with incident O atoms. These can approach the adsorbed PAH molecules along the surface * thus destabilizing their molecular rims.

O 55.14 Tue 18:30 P2-EG

Intercalated porphines at the BN/Cu(111) interface: structure, electronic properties and function — •Jacob Ducke[1], Alexander Riss[1], Alejandro Pérez Paz[2], Angel Rubio[3], Johannes V. Barth[1], and Willi Auwärter[1] — [1]Physik-Department E20, Technische Universität München, 85748 Garching, Germany — [2]ETSF, Universidad del País Vasco, 20018 San Sebastián, Spain — [3]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

The technological applicability of surface-supported molecular materials is often restricted by their limited stability. While covalent bonding can potentially enhance thermal stability, many of the currently researched molecular functionalities are sensitive to and impaired by the gaseous or liquid environment.

In this work we present the fabrication of heterostructures consisting of porphines that are sandwiched between a copper surface and an insulating BN monolayer. Due to the electronic transparency of the BN layer, the intercalated molecules can be characterized and manipulated using scanning tunneling microscopy (STM). While the presence of the capping BN layer influences the self-assembly, we show that intrinsic molecular functionalities as switching between different tautomers or self-metalation are preserved. Such metal/molecule/insulator structures provide an opportunity to protect organic materials from atmospheric pressure, and might also be used to control chemical reactions through geometric confinement.

O 56: 2D Materials beyond Graphene

Time: Tuesday 18:30–20:30 Location: P2-EG

O 56.1 Tue 18:30 P2-EG

Effect of different sulfur environment on sulfurization of MoO3 into MoS2 nanoflakes — •Prabhat Kumar, Megha Singh, and Gade B Reddy — Thin Film Laboratory, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016

In present work, Molybdenum disulfide (MoS2) nanostructured thin films (NTFs) were synthesized by sulfurizing MoO3 NTFs in three different non-conventional methods (named methods 1-3). Method 1 uses sulfur vapors, second utilizes H2S/Ar gas and third adopts plasma of H2S/Ar gas. The effect of sulfurizing ambient on its efficiency to convert MoO3 into MoS2 has been studied. And parameters such as crystallinity, purity, uniformity and stoichiometry control have been basis of this study. The samples showed uniform nanoflakes (NFs) structures throughout sample, revealed by SEM, same as their precursor MoO3. XRD and Raman disclosed crystalline MoS2 in all three methods, however the degree of crystallinity was greater in case of sulfurization in H2S/Ar plasma ambient. HR-TEM revealed formation of core-shell nanostructures comprising of MoO2 in core and MoS2 making shell. Quantitative analysis of sulfurized films carried out by XPS, shows the presence of MoS2 in methods 1,2 and 3 with percentage found to be 18%, 87% and ~100% respectively. Plasma ambient has resulted in high quality of MoS2 NTFs based on parameters such as crystallinity and stoichiometry control. Hydrogen sulfide plasma provides reducing environment as well as source of reactive sulfur species for sulfurization. The advantage of using plasma is reduced temperature and time.

O 56.2 Tue 18:30 P2-EG

X-ray absorption spectroscopy studies on transition metal dichalcogenide heterointerfaces — •Florian Rasch[1], Sage Bauers[2], Danielle Hamann[2], Gavin Mitchson[2], Kyle Hite[2], Javier Herrero-Martín[3], Manuel Valvidares[3], David Johnson[2], Bernd Büchner[1], and Jorge Hamann-Borrero[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Dresden, Germany — [2]Department of Chemistry and Materials Science, University of Oregon, Eugene, Oregon, United States — [3]ALBA Synchrotron Light Source, Cerdanyola del Vallès, Barcelona, Spain

Transition metal dichalcogenides (TMD) are layered quasi 2D materials that exhibit exciting physical phenomena such as superconductivity (SC) and charge density waves (CDW), which strongly depend on the TMD dimensionality. In order to study the effect of dimensionality on the electronic properties of TMD a series of ferecrystal heterostructures with chemical formula $[(\mathrm{MSe})_m/(\mathrm{TSe}_2)_n]_k$ (M = Sn, Pb, Bi and T = V, Nb, Ti) were synthesized with precise control of the dimensionality, i.e. m and n. Additionally, study of the charge transfer (CT) into the dichalcogenide layer is possible by changing the M cation. Here we present a X-ray absorption spectroscopy (XAS) study at the transition metal $L_{2,3}$ edges for $(\mathrm{PbSe})_1/(\mathrm{VSe}_2)_n$ (with n = 1, 3), as well as $(\mathrm{MSe})_1/(\mathrm{NbSe}_2)_1$ and $(\mathrm{MSe})_1/(\mathrm{TiSe}_2)_1$ (with M = Sn, Pb, Bi) heterostructures at temperatures below and above T_{CDW}. Our experiments clearly show strong changes of the transition metal XAS spectra by changing the M ion. Moreover, X-ray magnetic circular dichroism reveals weak magnetism for samples containing Ti and V.

O 56.3 Tue 18:30 P2-EG

Synthesis and Spectroscopy of Bismuthene — •Felix Reis[1], Gang Li[2,3], Lenart Dudy[1], Maximilian Bauernfeind[1], Stefan Glass[1], Werner Hanke[3], Ronny Thomale[3], Jörg Schäfer[1], and Ralph Claessen[1] — [1]Physikalisches Institut and RCCM, Universität Würzburg, Würzburg, Germany — [2]Institute for Solid State Physics, Vienna University of Technology, Vienna, Austra — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Würzburg, Germany

The search for quantum spin Hall materials with large band gap has become one of the major research thrusts of solid state physics. Despite other approaches, graphene with its honeycomb lattice geometry always fascinated the community. Here, we report the realization of so-called "bismuthene", which is synthesized on the wide-bandgap substrate SiC(0001). Scanning tunneling microscopy imaging clearly displays the honeycomb structure. Using tunneling spectroscopy, we find a huge bulk gap of $\sim 800\,\mathrm{meV}$, with the Fermi level positioned well inside this gap. Interestingly, metallic edge states are observed when the bismuthene film edge is approached. A comparison of angle-resolved photoemission measurements and density functional theory band structure calculations is a further manifestation of the formation of bismuthene. To understand the empirical electronic properties, a detailed theoretical analysis is performed. A low-energy effective model demonstrates that the substrate not only stabilizes bismuthene, but plays a crucial role in the formation of the observed huge band gap, which is driven by the large on-site spin-orbit coupling.

O 56.4 Tue 18:30 P2-EG

Thermodynamic stability, electronic and optical properties of graphene oxide dependence on oxidation level. — •Ivan Guilhon[1], Lara K Teles[1], Marcelo Marques[1], Friedhelm Bechstedt[2], Jürgen Fürthmuller[2], and Silvana Botti[2] — [1]Grupo de Materiais Semicondutores e Nanotecnologia, Instituto Tecnológico de Aeronáutica, DCTA, 12228-900 São José dos Campos, Brazil — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, D-07743 Jena, Germany

Graphene oxide is a two-dimensional material with potential applications in ultra-thin electronic, optoelectronic and sensor devices. It is an intermediate compound in the graphene synthesis through chemical route. Despite the fact that the chemical composition of such system have strong influence on its electronic and optical process, these interesting features have not been investigated until now.

We propose a statistical model for graphene oxide based on the cluster expansion of the disordered system based on the generalized quasi-chemical approximation (GQCA). Epoxide and hydroxyl groups are considered. Thermodynamic stability of the system is investigated and the known tendency of the system to decompose into highly oxidized domains and pristine graphene is explained and discussed in the light of binodal and spinodal decomposition. We calculate the energy gap as a function of the degree of oxidation considering composition fluctuation effects in the whole composition range, showing tunable electronic properties in a wide range interval. Optical absorbance spectra are predicted for different chemical compositions.

O 56.5 Tue 18:30 P2-EG

Low Temperature Scanning Tunneling Spectroscopy on MoS_2 nanoflakes on Au(111) — •Daniela Dombrowski[1,2] and Carsten Busse[1,2] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster

We perform low temperature scanning tunneling spectroscopy at 5 K of MoS_2 nanoflakes grown on Au(111) by a combination of physical and chemical vapour deposition. We find a band gap of approx. 1.9 eV and pronounced peaks, originating from the MoS_2 bands. The Shockley-surface state at 0.5 eV is present on the bare gold surface, but absent below the MoS_2 islands.

Furthermore, we take advantage of the spatial resolution of scanning tunneling spectroscopy to measure the influence of the moiré superstructure arising from the lattice mismatch between the MoS_2 layer and the underlying gold substrate. We observe a significant shift of the valence band edge, whereas the conduction band remains almost unchanged, hence leading to a variation of the gap energy induced by the moiré pattern.

Finally, we find a new state right above the valence band, which is associated with the edge of the MoS_2 flakes.

O 56.6 Tue 18:30 P2-EG

Structural dynamics of TMDC heterostructures studied by femtosecond electron diffraction — •Daniela Zahn, Thomas Vasileiadis, Lutz Waldecker, and Ralph Ernstorfer — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Vertical heterostructures of two-dimensional (2D) crystals offer intriguing new perspectives for the fabrication of novel nanodevices [1]. Especially for optoelectronic devices, it is important to understand their relaxation dynamics after optical excitation, which are governed by the interplay of electronic and phononic coupling across the interface and electron-phonon coupling in the individual materials. One experimental technique that can directly observe the structural response to photoexcitation is femtosecond electron diffraction [2]. The evolution of the atomic mean-square-displacement can be experimentally accessed by means of the Debye-Waller effect. Our focus lies on heterostructures with staggered (type II) band alignment, which exhibit photo-induced charge separation across the interface. We present results on bulk WSe_2/WS_2 heterostructures revealing sub-picosecond transfer of hot charge carriers across the interface and intralayer energy transfer from the charge carriers to the lattice on a timescale of few picoseconds in both materials. The results suggest that the equilibration between the two materials is carried out primarily by hot charge carrier transfer while vibrational coupling plays a minor role.

[1] A. Geim, I.V. Grigorieva, Nature 499, 419-425 (2013).

[2] L. Waldecker, R. Bertoni, R. Ernstorfer, JAP 117, 044903 (2015).

O 56.7 Tue 18:30 P2-EG

Growth of ultrathin MoS_2 films - Temperature dependency — •Vanessa Zeuner, Lukas Madauss, and Marika Schleberger — Universität Duisburg-Essen, Deutschland

Molybdenum disulfide (MoS_2) is an important representative of transition metal-dichalcogenides (TMDCs).With a direct bandgap it is an interesting candidate for a variety of electronic and optoelectronic applications. Therefore, the growth of large area, two dimensional films is investigated. We synthesized the MoS_2 films by chemical vapour deposition on SiO_2/Si substrates and used MoO_3 and S powders as the reactants. The influence of the temperature during the process on the morphology of the two dimensional MoS_2 flakes is studied.

O 56.8 Tue 18:30 P2-EG

Electronic Structure of surface-doped FeTe bulk crystals and epitaxial FeTe thin films on Bi_2Te_3 — •Fabian Arnold[1], Jonas Warmuth[2], Jan Fikáček[3], Matteo Michiardi[1], Marco Bianchi[1], Jan Honolka[3], Tim Wehling[4], Philip Hofmann[1], and Jens Wiebe[2] — [1]Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark — [2]Department of Physics, Hamburg University, Hamburg, Germany — [3]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [4]Institut für Theoretische Physik, Universität Bremen, Bremen, Germany

The realization of unconventional superconductivity in iron-based superconductors (SCs) has attracted growing attention in the physics community in the recent years, especially after the discovery of high temperature superconductivity in systems involving thin layers. Iron-chalcogenides have the simplest crystal structure in this materials class which turns them into good candidates for fundamental studies of the electronic structure and its relation to the superconductivity. It is especially interesting that for strongly correlated high-Tc SC materials like Fe-based SCs, a transition to the SC phase upon chemical doping is observable. Here we present an angle-resolved photoemission spectroscopy study of bulk FeTe and thin films of FeTe grown on the topological insulator Bi_2Te_3 [1,2], surface-doped with alkali atoms, and compare to ab-initio calculations. Interestingly, there is almost no change in the electronic structure upon surface doping. [1] S. Manna et al., arXiv:1606.03249 (2016), Nat. Commun. (in press). [2] T. Hänke et al., arXiv:1606.09192 (2016), Nat. Commun. (in press).

O 56.9 Tue 18:30 P2-EG

Near-surface dynamics of hot carriers in $2H$-MoS_2: momentum-dependent relaxation and spin- and valley-polarized excitation — •Hauke Beyer, Petra Hein, Gerald Rohde, Ankatrin Stange, Marcel Behrendt, Kerstin Hanff, Lexian Yang, Kai Rossnagel, and Michael Bauer — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany

Time- and angle-resolved photoelectron spectroscopy (trARPES) is employed to study different aspects of ultrafast near-surface carrier dynamics in $2H$-MoS_2. Momentum-dependent population and relaxation processes within the conduction-band energy landscape are monitored following photoexcitation with 395 nm laser pulses. Our results indicate that surface-localized defect states play a key role in the final depopulation of the conduction band [1]. Furthermore, we are able to selectively address K and K' valleys in the trARPES experiment using circularly polarized 590 nm laser pulses owing to the lack of inversion symmetry in the top layer of $2H$-MoS_2. Similar to recent trARPES results reported for $2H$-WSe_2 [2], dichroism is observed in excited state intensity as well as dynamics.

[1] P. Hein et al., Phys. Rev. B **94**, 205406 (2016).

[2] R. Bertoni et al., arXiv:1606.03218.

O 56.10 Tue 18:30 P2-EG

Ultra-thin Bi2Te3 films on semiconductor substrates — •Mert Taşkin and Oğuzhan Gürlü — Istanbul Technical University, Department of Physics, Maslak, 34469, Istanbul, Turkey

Bi2Te3 has a rhombohedral crystal structure and it consists of quintuple layers (QLs) along c-axis. QLs bind with van der Waals interaction. Consequently, the crystal can be cleaved from this interface and the resulting Te1 terminated (0001) surface can be investigated with scanning probe techniques. Bi2Te3 was shown to be a topological insulator (TI) besides being a thermoelectric material; yet, the knowledge on the electronic structure of this material at ultra-thin limit is still incomplete. Before making any attempt at an application with Bi2Te3 in the 2D limit, it is quite important to understand its general physical properties. We modified chemical vapor deposition (CVD) technique to grow ultra-thin Bi2Te3 films on semiconductor/metal-oxide surfaces. In this process we obtained ultra-thin films and microparticles of Bi2Te3. The heights of obtained Bi2Te3 films are measured to be a few QLs. The radius of Bi2Te3 micro-particles are 1-5 micrometers. Here the structural and spectroscopic characteristics of these ultra-thin films will be discussed.

O 56.11 Tue 18:30 P2-EG

The interaction of the calcium-intercalated silicene (CaSi2 - R15) surface with a H2 molecule, a DFT study — •Pingo Mutombo, Petr Brázda, Martin Ondráček, and Lukáš Palatinus — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, CZ-16200, Prague, Czech Republic

First-principles calculations have been used to investigate the silicene intercalated CaSi2-R15 compound and discuss the adsorption of H2 at its silicon-rich surface. We assess the stability of the surface by calculating the surface energy. We further determine the band structure of the compound, the surface work function, and charge redistribution both inside the compound and near the surface. It was found that there is a charge transfer from Ca to Si atoms. Moreover, the silicene-related Dirac cone shifts from high symmetric point of the hexagonal Brillouin zone and moves below the Fermi level,due the presence of the Ca atoms. DFT calculations suggest that a hydrogen molecule undergoes a dissociative adsorption on the topmost Si atoms, indicating a high reactivity of the silicene surface layer.

O 56.12 Tue 18:30 P2-EG

Structural modifications of 2D hexagonal boron nitride caused by ion irradiation — Lara Bröckers, •Henry Bohnen, and Marika Schleberger — Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany

Single layers of hexagonal boron nitride (hBN) – often called *white graphene* – are a two-dimensional insulating material, which is interesting as a building block for heterostructures with graphene or other 2D semiconducting materials. Its atomic structure is similar to the structure of graphene. That makes it interesting to test if one can cause the same structural modifications of hBN by ion irradiation, as shown for graphene.[1,2] Therefore we irradiated ultrathin hBN layers with swift heavy ions under grazing incidence. We investigated the efficiency (i.e. number of ions needed to create one folding on average) for different number of layers and different substrates. As a result we found a higher efficiency for the folding of thicker layers hBN in comparison to graphene.

[1] Akcöltekin S. et al. *Applied Physics Letters* 98 (2011) 101063

[2] Ochedowski O. et al. *NimB*, 340 (2014) 39-43.

O 56.13 Tue 18:30 P2-EG

Nanostructuring 2D Materials by Ion Irradiation — •Andre Maas[1], Roland Kozubek[1], Lukas Madauss[1], Ursula Ludacka[2], Mukesh Kumar Tripathi[2], Henning Lebius[3], Marko Karlusic[4], Jani Kotakoski[2], and Marika Schleberger[1] — [1]Universität Duisburg and Cenide, Fakultät für Physik, 47048 Duisburg, Germany — [2]Universität Wien, Boltzmanngasse 5, 1090 Vienna, Austria — [3]CIMAP, (CEA-CNRS-ENSICAEN-UCN), blvd Henri Becquerel, F-14070 Caen, France — [4]Ruder Bošković Institute, Bijenićka cesta 54, 10000 Zagreb, Croatia

To fully exploit the colossal technological potential of 2D materials, methods to introduce defects in a controlled way are a key factor. We have investigated energetic ion irradiation induced defects and nanostructures in 2D materials like graphene and single layer MoS2. We show that apart from the well-known binary collisions caused by singly charged keV projectiles, the dense electronic excitation triggered by highly charged ions as well as swift heavy ions may be used to create various characteristic nanostructures each of which may be fabricated by choosing the proper irradiation conditions.

Our experiments, including optical spectroscopy techniques and atomic resolution STEM, reveal unique morphologies such as closed bilayer edges with a given chirality, nanopores of round shape as well as chemical modifications like hydrogenation of the 2D material. By controlled variation of ion parameters like kinetic energy, charge state, angle of incidence, etc., this wide spectrum of modifications in 2D materials can be accessed.

O 56.14 Tue 18:30 P2-EG

Investigation of sputter processes on metalic surfaces and 2D-Materials using Time-of-Flight mass spectroscopy — •Stephan Sleziona[1], Philipp Ernst[1], Matthias Herder[2], Andreas Wucher[2], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, AG Schleberger, Germany — [2]Universität Duisburg-Essen, AG Wucher, Germany

We have investigated the sputtering processes and ionization probability of metallic surfaces (Indium and Molybdenum) irradiated by two different kinds of ions. We used highly charged ions (HCI), i.e. Xe^{30+} Ions (E$_{\mathrm{pot}}$= 15 keV and E$_{\mathrm{kin}}$= 180 keV) , and singly charged Ar-Ions with kinetic energy of E$_{\mathrm{kin}}$= 4 keV. While the interaction of the latter with the solid is dominated by nuclear stopping the interaction of HCIs consist partly of electronic stopping, too. To study the differences, the Indium surface was irradiated by both types of ions and Time-of-Flight (ToF) mass spectra were recorded. In order to do so we optimized the spatial positions of the Argon-Gun, the HCI source,the spectrometer, and the laser, which was used to post-ionize secondary neutral particles . In addition, the operating voltages and timings of the different components were optimized. With this new set-up we obtained ToF spectra which show a significant difference between the two types of ions. Most recently we used this technique to investigate sputter processes of 2D-Materials.

O 56.15 Tue 18:30 P2-EG

Influence of the Charge Density Wave Order on Quasiparticle Excitations in 2*H*-NbSe$_2$ — •Eva-Maria Liebhaber[1], Olof Peters[1], Michael Ruby[1], Kai Rossnagel[2], Benjamin W. Heinrich[1], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany. — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany.

The transition metal dichalcogenide (TMDC) 2*H*-NbSe$_2$ is a layered material with interesting properties of strongly correlated electrons at low temperatures. A superconducting phase with a critical temperature of T$_{\mathrm{c,SC}} \approx 7.2\,\mathrm{K}$ coexists with a threefold symmetric charge density wave (CDW) with T$_{\mathrm{c,CDW}} \approx 33\,\mathrm{K}$. Although the material has been studied intensively for a long time, the exact interplay between superconductivity and CDW order is still under debate. Recently, Soumyanarayanan *et al.* observed a quantum phase transition from the familiar triangular CDW to a stripe charge order which they assigned to local strain caused by subsurface defects [1].
Here, we investigate the influence of the different CDW phases on the quasiparticle excitation spectra using low temperature scanning tunneling spectroscopy with superconducting tips. The quasiparticle spectra show variations with the periodicity of the CDW as well as on the atomic scale.

[1] A. Soumyanarayanan *et al.*, *Proceedings of the National Academy of Sciences* **110**, 1623-1627 (2013).

O 56.16 Tue 18:30 P2-EG

Structural analysis of PTCDA domains on an epitaxial hexagonal boron nitride (hBN) monolayer via SPA-LEED and STM — •Christine Brülke[1], Timo Heepenstrick[1], Moritz Sokolowski[1], and Sergey Subach[2] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstraße 12, 53115 Bonn, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52452 Jülich, Germany

Epitaxial monolayers of hBN on metal surfaces are of interest as two-dimensional insulating substrates as well as templates for the formation of epitaxial layers of organic molecules. Here, we report a structural analysis of one monolayer of PTCDA on hBN/Cu(111) by spot profile analysis low energy electron diffraction (SPA-LEED) and scanning tunneling microscopy (STM). hBN grows on the Cu(111) surface in an incommensurate structure with a lattice mismatch of 2.0 % (at 100 K) corresponding to an unstrained hBN layer. The films show rotational mosaicity, however, the majority of the hBN domains are in or close to alignment with the unit cell vectors of the Cu(111) surface (± 2°).

On this hBN layer PTCDA molecules form ordered domains with a herringbone structure with lattice constants a = (19.8 ± 0.3) Å and b = (12.4 ± 0.2) Å. This yields a size of the unit cell that deviates by 3.1 % and 2.2 % from that in the (102) plane of the α and β bulk crystals, respectively. The majority of PTCDA domains are statistically distributed in their azimuthal orientation. There is only a small preference for domains that are oriented along the unit cell vectors of the hBN layer.

O 56.17 Tue 18:30 P2-EG

Deposition of biphenylthiols on Au(111) by Electrospray Ionization — •Patrick Stohmann[1], Sascha Koch[1], Antoine Hinaut[2], Thilo Glatzel[2], Ernst Meyer[2], and Armin Gölzhäuser[1] — [1]Department of Physics, Universität Bielefeld, Universitätsstrasse 25, 33615 Bielefeld, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

When aromatic self-assembled monolayers (SAMs) are electron-irradiated, intermolecular cross-linking leads to the formation of Carbon Nano Membranes (CNM) with molecular thickness [1]. The preparation of SAMs requires clean surface conditions for the formation of well-defined molecular structures as well as for the analysis via scanning probe techniques. However, thermal evaporation under UHV conditions may lead to the fragmentation of molecules during the sublimation while the formation of wet-prepared SAMs may suffer from polluting adsorbates on the bare surface. Here we present the study of biphenylthiols on Au(111), prepared by Electrospray Ionization (ESI). ESI allows for the introduction of organic molecules in vacuum under controlled conditions on atomically clean surfaces and was successfully applied in previous experiments [2]. The molecular deposition on the surface is investigated by means of scanning tunneling microscopy (STM) and nc-atomic force microscopy (NC-AFM) combined with Kelvin probe force microscopy (KPFM). [1] A. Turchanin et al., A. Gölzhäuser, Adv. Mater., 2009, 21, 1233-1237 [2] A. Hinaut et al., E. Meyer, Beilstein J. Nanotechnol., 2015, 6, 1927-1934

O 56.18 Tue 18:30 P2-EG

Spectroscopic Mapping and Imaging Ellipsometry applied to Conducting, Semi-Conducting and Insulating 2D-Materials — Sebastian Funke[1], Ursula Wurstbauer[2,3], Aleksandar Matkovic[4], Avery Green[5], and •Peter H. Thiesen[1] — [1]Accurion GmbH, Stresemanstraße 30, 37079 Göttingen, Germany — [2]Walter Schottky Institute and Physics-Department, TU München, Garching 85748, Germany — [3]Nanosystems Initiative Munic 80799, Germany — [4]Centre for Solid State Physics and New Materials, Institute of

Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — [5]College of Nanoscale Science and Engineering, State University of New York, 253 Fuller Road, Albany, New York 12203

The poster will present the localization and characterization of Graphene Monolayer flakes and similar thicknesses regions of insulating hexagonal boron nitride (hBN) and on semiconducting transition metal dichalcogenide Molybdenum disulphide (MoS2).

Matkovic et al. characterized monolayers of graphene by spectroscopic imaging ellipsometry (SIE). The resulting Fano resonance modelling for the dispersion of Graphene can be used to search for flakes of graphene on different substrates, based on the spectroscopic mapping of the ellipsometric angles Δ and Ψ. This ellipsometric flakesearch is less dependent from the substrate compared to e.g. conventional light microscopy.

O 56.19 Tue 18:30 P2-EG

Imaging Mueller Matrix Ellipsometry for the Characterization of Microstructured Anisotropic Thin-Film Samples — Matthias Duwe[1], Sebastian Funke[1], Christian Röling[1], •Peter H. Thiesen[1], Aday J. Molina-Mendoza[2], and Andres Castellanos-Gomez[3] — [1]Accurion GmbH, Stresemannstr. 30, 37079 Göttingen, Germany — [2]Universidad Autonoma de Madrid. Departamento de Fisica de la Materia Condensada. Campus Universitario de Cantoblanco, 28049 Madrid, Spain — [3]IMDEA Nanoscience, C/ Faraday 9, Campus Universitario de Cantoblanco, 28049 Madrid, Spain

Imaging ellipsometry (IE) is an established technique for the characterization of structured thin-film samples with lateral resolutions down to the micron scale. In most cases, however, imaging ellipsometers featuring microscopic resolution only yield the ellipsometric angles Δ and Ψ. Thus, these ellipsometers mainly have been applied to isotropic samples so far. Here, we present imaging Mueller matrix ellipsometry (IMME) with high microscopic lateral resolution capable of measurements at a variable angle of incidence. By operating Accurion*s imaging ellipsometer EP4 (PCSA configuration) in a rotating-compensator mode, the ellipsometer yields Mueller matrix micrographs for the upper 3x4 matrix elements of the sample. We applied this imaging Mueller matrix ellipsometer to the characterization of microscopic flakes of anisotropic 2D-materials, such as black phosphorus.

O 56.20 Tue 18:30 P2-EG

Lateral heterostructures of MoS2 and carbon nanomembranes — •Antony George[1], Christof Neumann[1], Zian Tang[1], Andreas Winter[1], Uwe Hübner[2], Michael Mohn[3], Ute Kaiser[3], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, D-07743 Jena, Germany — [2]Leibniz-Institut für Photonische Technologien e.V., 07745 Jena, Germany — [3]Electron Microscopy Group of Material Science, Ulm University, 89081 Ulm, Germany

Atomically thin two dimensional (2D) materials are promising for future ultrathin electronic and optoelectronic devices. In order to realize such devices, it is highly desired to connect/stitch different 2D materials laterally. Here, we present our recent results of the fabrication of lateral heterostructures of molecular thin carbon nanomembranes (CNMs) with MoS2 by electron beam assisted crosslinking. To this end, MoS2 single layer crystals grown by chemical vapour deposition (CVD) were transferred onto gold films on mica substrates. Then, self-assembled monolayers of 4*-nitro-1, 1*-biphenyl-4-thiol (NBPT) were grown on the areas between the MoS2 crystals. Electron beam irradiation was employed to crosslink the SAM molecules with each and with the edges of the MoS2 crystals. The formed CNM-MoS2 lateral heterostructures were transferred onto new solid and holey substrates and characterized by complementary methods including Raman spectroscopy, atomic force microscopy (AFM), helium ion microscopy (HIM) and high resolution transmission electron microscopy (HRTEM).

O 57: Ultrafast Electron and Spin Dynamics

Time: Tuesday 18:30–20:30 Location: P2-EG

O 57.1 Tue 18:30 P2-EG

Excited Electron Dynamics in Thiophene-based Polymers — •Carsten Winter, Deb Kumar Bhowmick, Nils Fabian Kleimeier, and Helmut Zacharias — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Optically active thiophene-based polymers are promising candidates for solar cell, OLED or transistor applications. Several variants of thiophene polymers coupled with pyrrole or fluorene chains exist, and form an internal donor-acceptor system.

In this presentation we show the results of a time-dependent photoemission study on the three thiophene polymers PFTT (with a fluorene extension), PDPP4T and DTT (with a pyrrole extension) on a Si(100) substrate. The fundamental, second and third harmonics of a 6 kHz, 35 fs Ti:Sapphire laser system with a time-of-flight spectrometer are utilized for static 3PPE to determine the energetic positions of high lying occupied and intermediate unoccupied electronic levels. Dynamic 3PPE is then used to study the electron dynamics of the intermediate states directly in the time domain.

One-color 3PPE with 3 eV on PFTT shows intermediate lifetimes of 65 to 195 fs depending on the electron kinetic energy and the order of p- and s-pulse. On PDPP4T and DTT a two-color experiment (1.5 eV and 4.5 eV) can determine two distinct, longer electronic lifetimes between 1 and 10 ps for the faster channel and 20 to 100 ps for the slower channel.

O 57.2 Tue 18:30 P2-EG

Ultrafast Doublon Dynamics in $1T$-TaS$_2$ — •Manuel Ligges[1], Isabella Avigo[1], Denis Golež[2], Matthias Kalläne[3], Kai Rossnagel[3], Martin Eckstein[4], Phillip Werner[2], and Uwe Bovensiepen[1] — [1]Faculty of Physics, Universität Duisburg-Essen — [2]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — [3]Institute of Experimental and Applied Physics, Universität Kiel, 24098 Kiel — [4]Max Planck Research Department for Structural Dynamics, University of Hamburg-CFEL, 22761 Hamburg

Using time- and angle-resolved photoemission we study photo-induced electron dynamics in the (quasi-)2D Mott insulator $1T$-TaS$_2$. In the low excitation limit, we observe population and subsequent decay dynamics of the upper Hubbard band that are significantly faster than expected, indicating a characteristic time scale of $\hbar/J$ for the underlying scattering processes. Theoretical calculations based on dynamic mean field theory indicate that such dynamics only occur when the system is effectively hole-doped. We furthermore stress that on these time scales the electronic and phononic subsystems are decoupled.

O 57.3 Tue 18:30 P2-EG

Ultrafast electron dynamics in single crystals studied by time-resolved two-photon momentum microscopy — •Tobias Eul[1], Florian Haag[1], Benjamin Frisch[1], Philip Thielen[1], Martin Piecuch[1], Mirko Cinchetti[2], Martin Aeschlimann[1], and Benjamin Stadtmüller[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany — [2]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

Electron dynamics in solid state systems and at interfaces play a crucial role for the performance of nanoscale spintronic devices. Therefore, it is essential to investigate the electron dynamics in the materials used for such devices.

The inelastic lifetimes of electronic states can be directly obtained with time resolved two-photon photoemission, using a cross-polarized pump-probe setup. Combining this technique with momentum spectroscopy in a ToF-PEEM operated in K-space mode, we are able to observe the energy dependent electron dynamics for each point in the accessible momentum space. This allows us to analyze cross-correlation traces for different intermediate state energies and different positions in the k_x/k_y-plane. As first model systems, we focused on bulk states of simple noble metal surfaces using different angles of incide of laser light. Based on the observed behavior, we aim to tune the electron lifetime of the metal surface by adsorption of organic molecules

O 57.4 Tue 18:30 P2-EG

Ab initio approach to the ion stopping power at the plasma-solid interface — Karsten Balzer, •Niclas Schlünzen, Jan-

Philip Joost, Lasse Wulff, and Michael Bonitz — CAU Kiel, Germany

The energy loss of ions in solids is of key relevance for many applications of plasmas, ranging from plasma technology to fusion. Standard approaches are based on density functional theory or SRIM simulations, however, the applicability range and accuracy of these results are difficult to assess, in particular, for low energies. Here, we present an independent approach that is based on ab initio nonequilibrium Green functions theory, e.g. [1,2] that allows to incorporate electronic correlations effects of the solid. As first application of this method to low-temperature plasmas, we concentrate on proton and alpha-particle stopping in a graphene layer and similar finite honeycomb lattice systems. In addition to the stopping power we present time-dependent results for the local electron density, the spectral function and the photoemission spectrum [3] that is accessible in optical, UV or x-ray diagnostics [4].
[1] M. Bonitz, *Quantum Kinetic Theory, 2nd edition* (Springer, 2016)
[2] K. Balzer and M. Bonitz, Lect. Notes Phys. **867** (2013)
[3] M. Eckstein and M. Kollar, Phys. Rev. B **78**, 245113 (2008)
[4] K. Balzer, N. Schlünzen, and M. Bonitz, Phys. Rev. B, accepted for publication, arXiv:1602.06928 (2016)

O 57.5 Tue 18:30 P2-EG

Ultrafast transition to a hidden state in $1T$-TaS$_{2-x}$Se$_x$ single crystals — •Ljupka Stojchevska[1,2], Ebru Ekici[3], Kira Kolpatzeck[3], Christian A. Bobisch[3], Dragan Mihailovic[1], and Uwe Bovensiepen[2] — [1]Complex Matter Department, Jozef Stefan Institute, Ljubljana, Slovenia — [2]Faculty of Physics, University of Duisburg-Essen, Duisburg, Germany — [3]Faculty of Physics, Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, German

We report on femtosecond pump-probe spectroscopy study on the relaxation dynamics in $1T$-TaS$_{2-x}$Se$_x$ single crystals with 6%, 7.5%, 17% and 19% selenium doping. We observe a transition to a new hidden state [1] (H-state) which is inaccessible under normal equilibrium conditions and can only be reached after a quench with a single femtosecond laser pulse at 1.6-4.8 mJ/cm^2 fluence. Similarly as in [1], a notable change in the coherent phonon spectra plays the role of the fingerprint of the successful switching to a new state via optical path. The major output is observation of the significantly higher temperature stability of the H-state ($\sim$ 104 K) in comparison with the parent $1T$-TaS$_2$ material ($\sim$ 70 K). In addition, intense experimental efforts are currently undergoing in order to microscopically characterize H-state by means of scanning tunneling microscopy (STM) and to investigate the electronic structure with femtosecond time- and angle-resolved photoemission spectroscopy (trARPES). [1] Stojchevska, L. et al., Science, 344, 177 (2014).

O 57.6 Tue 18:30 P2-EG

Characterization of an ultrafast MHz electron point source — •Jannik Malter, Melanie Müller, Faruk Krecinic, and Ralph Ernstorfer — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Ultrafast electron point sources allow for electron microscopy and diffraction [1] as well as scanning probe techniques [2] with very high spatial and temporal resolution. The laser repetition rate is a crucial parameter as it directly influences statistics of the measurement, and taking the required laser pulse energy into account determines the thermal stress on the tip. We discuss photoemission from a metal tip using an optical parametric amplified laser in the low-MHz regime. Photoemission is either triggered by direct illumination of the apex, or by excitation and nanofocusing of surface plasmon polaritons [3]. Due to the better thermal response of the tip, the latter approach could possibly lead to femtosecond electron holography and contribute to laser-triggered ultrafast STMs.

[1] Müller et al. Femtosecond electrons probing currents and atomic structure in nanomaterials. Nature Comm. 5, 2014

[2] Cocker et al. Tracking the ultrafast motion of a single molecule by femtosecond orbital imaging. Nature 539, 2016

[3] Müller et al. Nanofocused Plasmon-Driven Sub-10 fs Electron Point Source. ACS Photonics 3 (4), 2016

O 57.7 Tue 18:30 P2-EG

Mahan cone formation and time-resolved two-photon photoemission of the adsorbate system Tin-Phthalocyanine on Ag(111) — •Stephan Jauernik, Petra Hein, Max Gurgel, Julian Falke, and Michael Bauer — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany

Recently, the adsorption of tin-phthalocyanine (SnPc) on Ag(111) has attracted considerable interest due to peculiarities in the adsorbate-substrate interaction and switching capabilities reported for the adsorbed SnPc [1]. Using Low Energy Electron Diffraction (LEED) and Photoemission/Two-Photon Photoemission (PES/2PPE) we address in this work the correlation of structural and electronic properties of this model-type system in the incommensurate adsorption phase which forms in the coverage regime between 0.90 ML and 1.0 ML. 1PPE data of 1ML SnPc on Ag(111) reveal the formation of Mahan cones [2,3] which we associate with a direct optical transition within the Ag sp-band modified by diffraction in the presence of the 2D adsorbate superstructure. Using time-resolved bichromatic 2PPE we focus on the electronic structure of the adsorbate layer and the characteristic relaxation dynamics of molecular resonances.
[1] C. Stadler et al., Nature Physics 5, 153 (2009)
[2] G. D. Mahan, Phys. Rev. B 2, 4334 (1970)
[3] Winkelmann et al., New Journal of Physics, Volume 14 (2012)

O 58: Surface Science: Misc.

Time: Tuesday 18:30–20:30 Location: P2-EG

O 58.1 Tue 18:30 P2-EG

Effect of the sub-surface on the surface revealed by Scanning Probe Microscopy on irradiated graphitic surfaces — •Cem Kincal[1], Dilek Yildiz[1,2], Umut Kamber[1], Clara Grygiel[3], Cornelis J. van der Beek[4], and Oğuzhan Gürlü[1] — [1]Istanbul Technical University, Istanbul, Turkey — [2]University of Basel, Basel, Switzerland — [3]Université dé Caen, Caen, France — [4]Ecole Polytechnique, Palaiseau, France

Comet-like and hillock like structures on swift heavy ion (SHI) irradiated HOPG surfaces have already been reported. We have shown that it is possible to obtain atomic resolution on the tail section of the comet-like structures with STM. Such STM data proved that the interaction of SHI with the bulk does not damage surface layers except for the entry point. Friction force microscopy showed complementary results to our STM measurements. Interestingly, we observed that the tail sections of the comet-like structures appeared on the friction maps, although they could not be observed in simultaneously taken topography maps. Intriguingly, tail sections showed less friction compared to the pristine HOPG surface. Our results indicate the friction between two surfaces can also be a function of the bulk material. Moreover, we have studied SHI irradiation of moiré zones formed on HOPG. Data revealed that irradiation of moiré zones under grazing incidence did not show any unzipping or folding of the top most graphene layer generating the moiré pattern.

O 58.2 Tue 18:30 P2-EG

Electrostatic, phononic and van der Waals friction on layered materials — •Dilek Yildiz, Marcin Kisiel, and Ernst Meyer — Universität Basel, Basel, Switzerland

An unintuitive friction is caused due relative motion of bodies with a few nanometres gap in-between. This non-contact friction phenomenon still awaits to be understood completely. Effects of such non-contact friction can be measured by oscillating a highly sensitive cantilever like a tiny pendulum over a surface. We studied with TaS2 and HOPG crystal surfaces, which are well known layered structures. Energy dissipation spectra measured on both materials have shown clear differences. While electrostatic interaction causes energy dissipation on TaS2 at low temperatures, van der Waals friction is observed on the same sample at high temperatures due to the phase transition. Rather, we observed the lack of electrostatic friction on HOPG and we measured phononic type of friction, which is due to the short range forces. Mechanism of energy dissipation on TaS2 depends on a temperature driven phase transition of the crystal. In this presentation we will discuss three different mechanisms of non-contact friction: Friction due to electrostatic, van der Waals and phononic interactions between tip and the sample.

O 58.3 Tue 18:30 P2-EG

Optical properties of laser-excited metals under nonequilibrium conditions. — •Pascal D. Ndione[1], Sebastian Weber[1], Dirk O. Gericke[2], and Baerbel Rethfeld[1] — [1]Department of Physics and Research Center Optimas, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany — [2]Centre for Fusion, Space and Astrophysics, Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

Improving our understanding of the response of materials under intense laser irradiation is critical for various applications. The modification of optical properties is also a key feature for fundamental science as reflectivity or transmission carry many information about the correlated many-body system. The present contribution investigates the behavior of metals subjected to short laser pulses of visible light. For metals, the laser directly excites the electrons which drives them out of equilibrium. On a time scale of a few tens to hundreds femtoseconds after laser irradiation, the electrons thermalize to a Fermi distribution at an elevated temperature. We are interested in the optical properties of metals under the nonequilibrium conditions during the relaxation process. Different approximations of the dielectric function are compared for thermalised metals. Then, we aim to include nonequilibrium electron distributions into the dielectric function.

O 58.4 Tue 18:30 P2-EG

Novel Reflection High-energy Positron Diffractometer at NEPOMUC — •Matthias Dodenhöft and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ) and Physics Department E21, Technische Universität München, Lichtenbergstr. 1, 85748 Garching b. München, Germany

The precise knowledge of the surface structure is essential to understand e.g. chemical reactions, optimize catalytic techniques or develop nanoelectronic devices. It has been shown that Total Reflection High-energy Positron Diffraction (TRHEPD) is a powerful tool to determine the positions of adatoms and topmost layers of reconstructed surfaces with unprecedented accuracy. In contrast to the application of high-energy electrons in RHEED, positrons exhibit the phenomenon of total reflection at surfaces due to their positive scattering potential. For this reason, TRHEPD shows outstanding surface sensitivity and thus provides information, which cannot be obtained with other techniques such as RHEED or SXRD.

In order to enable TRHEPD experiments, we intend to set up a new positron diffractometer coupled to the high-intensity positron beam NEPOMUC, located at the research reactor FRM II in Munich. Beside the identification of surface structures, this setup will also enable us to investigate surface related phenomena such as phase transitions, reconstruction or surface melting. This project is supported by the BMBF (funding number 05K16WO7).

O 59: Plasmonics and Nanooptics

Time: Tuesday 18:30–20:30 Location: P2-OG1

O 59.1 Tue 18:30 P2-OG1

Fabrication of nanoaperture arrays in a free standing gold film for electron energy-loss spectroscopy — •Mike Prämassing[1], Stephan Irsen[2], and Stefan Linden[1] — [1]Physikalisches Institut Universität Bonn, Nußallee 12, D53115 — [2]Forschungszentrum Caesar Bonn, Ludwig-Erhard-Allee 2, D53175

Periodic nanoaperture arrays in thin metallic films are well known to exhibit extraordinary optical transmission orders of magnitude higher than predicted by standard aperture theory [1]. In contrast, for thinner metal films a suppressed optical transmission has been reported [2]. Both effects can be explained by resonant coupling of the incident light to surface plasmon polaritons (SPPs) via the array. Scanning transmission electron microscopy (STEM) in combination with electron energy-loss spectroscopy (EELS) is a powerful tool for the spatial and spectral characterization of the SPPs. However, STEM-compatibility restricts us to fabricate the films either free-standing or on a membrane, transparent for the electron beam. We present two STEM-compatible fabrication approaches for nanoaperture arrays in metallic films with thicknesses from 10 nm to 100 nm: Focused ion beam milling in a free-standing film or electron beam lithography on an electron transparent SiN membrane. The chosen range of film thickness corresponds to the transition region between enhanced and suppressed optical transmission.

[1] Ebbesen et al., Nature 391, 667-669 (1998).
[2] Braun et al., Phys. Rev. Lett. 103, 203901 (2009).

O 59.2 Tue 18:30 P2-OG1

Optimizing Yagi-Uda antennas for high directivity and electrical driving in the visible regime — •Philipp Grimm, René Kullock, and Bert Hecht — NanoOptics & Biophotonics Group, Experimentelle Physik 5, Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Antennas are fundamental devices which couple localized fields to far-field radiation and vice versa. In radio technology, a widespread antenna geometry is found in Yagi-Uda antennas whose far-field emission is highly directional, thus enabling efficient communication between two instances.

In the optical regime metallic nanoparticles exhibiting plasmonic resonances can act as antennas for light. So far they have already been arranged to Yagi-Uda antennas and showed pronounced directivity [1,2]. However, while these attempts were based on optical pumping our aim is to electrically drive them similar to [3]. In order to obtain reasonable working antennas for this more complex case, here we use an analytic dipole interaction model and numerical boundary element simulations to characterize possible geometries and extract design rules. Using that we find fabricable Yagi-Uda antenna geometries which show high directivity and are still suitable for electrical driving.

[1] A. Curto et al., *Science 329, 5994 (2010)*
[2] T. Kosako et al., *Nat. Photonics 4, 5 (2010)*
[3] J. Kern et al., *Nat. Photonics 9, 9 (2015)*

O 59.3 Tue 18:30 P2-OG1

Near Field Investigation of Plasmonic Bowtie Antennas — •Jon Polensky, Bendix Ketelsen, Thomas Klings, Jens Ehlermann, Irene Fernandez-Cuesta, and Robert Blick — Center for Hybrid Nanostructures (CHyN), Hamburg, Germany

Single-molecule detection techniques are revolutionizing the way we understand (bio)chemical processes. But observing single molecules is a big technological challenge. One idea is using the hot-spot yielded by a plasmonic nanoantenna which confines and enhances optical fields. The hot spot can be focused down to less than tens of nanometers.

We have constructed a Scanning Near Field Optical Microscope (SNOM) to investigate the optical near fields of relevant structures. One proof of concept is the study of the optical properties of the aforementioned plasmonic nanoantennas. Two different geometries were characterized and compared. We used the SNOM to measure the intensity of the hotspot by changing the polarization of the incident laser beam.

We investigated triangular and circular antennas made of gold, with triangle side lengths of l = 140 nm and a radius of r = 80 nm, respectively. The antennas were made by nanoimprint lithography and lift-off. It was found out, that both antenna shapes lead to a field enhancement in the nanometric gap between the structures. The polarization change of the incident beam showed a significant effect: light that is parallel polarized to the long axis of the antenna induced a more intense hotspot than perpendicular polarized light. The factor between the two relative hotpot intensities is 1.5.

O 59.4 Tue 18:30 P2-OG1

Babinet principle and plasmonic antennas for enhanced optical processes — Martin Hrtoň[1,2], •Vlastimil Křápek[1,2], and Tomáš Šikola[1,2] — [1]Central European Institute of Technology, Brno University of Technology, Purkyňova 123, CZ-612 00 Brno, Czech Republic — [2]Institute of Physical Engineering, Brno University of Technology, Technická 2, CZ-616 69 Brno, Czech Republic

Babinet principle for localized surface plasmon resonance was theoretically studied in direct and indirect plasmonic antennas (particles and apertures). We focused on two-part antennas with a conductive or non-conductive junction exhibiting strongly localized and enhanced electric near field. We aim at a design of plasmonic antennas that can be used for the enhancement of optical processes.

O 59.5 Tue 18:30 P2-OG1

Fabrication and Characterization of Photonic Metasurfaces — •Alexander Fassbender, Felix Bleckmann, and Stefan Linden — Physikalisches Institut, Rheinische Friedrich-Wilhelms Universität Bonn, Nußallee 12, D-53115 Bonn, Germany

Photonic metasurfaces can be used to locally control the phase of incoming electromagnetic waves by scattering the wave from the subwavelength building blocks of the metasurface. In combination with the Generalized Snell's law this allows to nearly arbitrarily control the refraction at such surfaces. Depending on the exact structure of the used metasurface one can construct various optical elements, e.g., lenses and holograms.
Here, we want to demonstrate a metasurface that generates an optical vortex. For that purpose, we fabricate an antenna array using electron beam lithography. We employ gold antennas with a length of 200 nm to modify the properties of a circular polarized wave at 750 nm wavelength. More specific, we control the locally induced phase of light with the opposite helicity by rotating each antenna by a certain angle relatively to a reference axis. To achieve a radial phase gradient, necessary to generate an optical vortex, the orientation of the antennas rotates by π per turn. Using an interferometer we plan to demonstrate that our photonic metasurface generates an optical vortex exhibiting the characteristic spiral phase distribution.

O 59.6 Tue 18:30 P2-OG1

Far-field characterization of colloidal light management structures for PV — •Lutz Mühlenbein[1], Peter M. Piechulla[1], Alexander Sprafke[1], and Ralf B. Wehrspohn[1,2] — [1]FG Mikrostrukturbasiertes Materialdesign, MLU Halle-Wittenberg — [2]Fraunhofer IMWS, Halle

Light management strategies are object of extensive research in the field of thin film photovoltaics, with the primary goal of increasing the short circuit current J_{SC} of PV cells. However, while J_{SC} is the figure of merit in the final device, in order to optimize light management structures, we are interested in the more fundamental optical properties, e.g. angular and wavelength resolved scattering. Using conventional fabrication technologies, controlling those properties is either expensive (for example by photolithography) or severly limited (random etching processes). In contrast, layers of self-organized colloidal particles can be produced on a large scale at low cost and allow for a wide range of scattering properties. In the presented work, we are focussing on appropriate and practicable characterization techniques in order to link the optical response to the microstructure of these colloidal layers.

O 59.7 Tue 18:30 P2-OG1

Enhancement of the second harmonic signal of nonlinear crystals by nanoantennas — •Emre Gürdal[1], Markus Kalmutzki[2], Anke Horneber[3], Hans-Jürgen Meyer[2], Alfred J. Meixner[3], Dai Zhang[3], Dieter Kern[1], and Monika Fleischer[1] — [1]Applied Physics, Tübingen, Germany — [2]Inorganic Chemistry, Tübingen, Germany — [3]Physical and Theoretical Chemistry, Tübingen, Germany

In the last decade nonlinear crystals have become a common tool for frequency conversion. A commonly observed second order nonlinear optical process is the so-called second harmonic generation (SHG). The interaction of two photons with e.g. a nonlinear crystal allows the creation of one photon with twice the energy. The efficiency of this nonlinear process can be enhanced using localized surface plasmons (LSPs). At the resonant wavelength of LSPs excited within metallic nanostructures, a strong electric near-field is created in their close vicinity, which improves the nonlinear optical process. We investigate nonlinear crystals that are nanostructured with gold nanodiscs by electron beam lithography. We measure and simulate the optical properties of dimers. The scattered intensities and resonance frequencies depend on the size and distance of the respective discs. For excitation we use a pulsed femtosecond laser with a wavelength of 774 nm, to which the nanodimer resonances are matched. The spectrally resolved nonlinear intensity at the position of the nanostructures is compared with the nonlinear signal of the unstructured crystal surface.

O 59.8 Tue 18:30 P2-OG1

Raman enhancement due to gold nanoparticles on a graphene monolayer — •Marcel Weinhold, Sangam Chatterjee, and Peter J. Klar — Justus Liebig University Giessen, Institute of Experimental Physics I, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany

Tip-enhanced Raman spectroscopy (TERS) is a powerful technique for analyzing molecular vibrations as well as lattice dynamics in bulk materials with a high spatial resolution down to a few nanometers, and combines the advantages of ordinary Raman spectroscopy and atomic force microscopy.
Despite the huge progress in improving the achievable spatial resolution of tip-enhanced Raman spectroscopic techniques, there remain many questions unanswered regarding the mechanisms, that lead to the enhancement of Raman signals. The understanding of these effects is essential for improving the TERS techniques. We study the enhancement effects of gold nanoparticles (representing a TERS tip) deposited on a graphene monolayer. Graphene was employed because of its two-dimensionality, its strong Raman signals, and the opportunity of purchasing samples with coverages close to 100%. We used Raman mapping with different excitation lasers, and various laser powers to determine the influence on the Raman enhancement. The enhancement factor shows a dependence on the excitation wavelength and varies for the different graphene modes. Additionally, we obtain a systematic shift in the measured phonon-frequencies probably related to a plasmonic coupling between gold and graphene that correlates with the applied laser power.

O 59.9 Tue 18:30 P2-OG1

Polarization resolved microscopy of plasmonic nanoparticles — •Jasmin Schönzart, Markus Pfeiffer, and Klas Lindfors — Department of Chemistry, University of Cologne, Luxemburger Str. 116, 50939 Köln, Germany

The plasmon resonance of metal nanoparticles may be modified by changing the shape or material of the particle or the medium surrounding the nanostructure. Varying the shape of resonant metal nanoparticles allows controlling the optical properties of the structure. Using the polarization of the incident light the excitation of different plasmonic modes can be controlled. This is of great interest, as the localization of the near field enhancement can be controlled on a sub-wavelength scale. Here we present a microspectroscopy setup, which enables interference-contrast microscopy of very small plasmonic nanostructures using complex polarization states of the incident light such as radial and azimuthal polarization.
In initial experiments we determined the size-dependent interference scattering signal for spherical gold nanospheres down to particle sizes of 20 nm. In further studies we investigated gold nanorods. These show a longitudinal- and transversal plasmon mode, which can be excited separately, depending on illumination wavelength and orientation of the polarization with respect to the nanorod axis.We further show some first results on measurements with radial and azimuthal illumination polarizations. Here magnetic and electric modes of higher order can be excited.

O 59.10 Tue 18:30 P2-OG1

Magneto-plasmonic interactions in Ni/Au, Co/Au and YIG/Au nanostructures — •Ellen R. Wiedemann[1,3], Jochen Greser[1], Björn Heinz[1], Bert Lägel[2], Sandra Wolff[2], Gereon Niedner-Schatteburg[3], Burkard Hillebrands[1], and Evangelos Th. Papaioannou[1] — [1]Fachbereich Physik, TU Kaiserslautern, Germany — [2]Nano Structuring Center, TU Kaiserslautern, Germany — [3]Fachbereich Chemie, TU Kaiserslautern, Germany

Magnetoplasmonics is an emergent research field that aims to strongly modify the magneto-optic response in the presence of surface plasmons and to control plasmonic resonances with magnetic fields [1,2] In this work we show a new way to manipulate the magneto-optic response of magnetoplasmonic structures, taking advantage of the presence of the magnetic layer. We use patterned Ni, Co and YIG films covered with Au in the form of 2D (antidot lattices) and 1D (stripes) patterns. Different thicknesses and different geometries of the patterns generate a large enhancement of the polar and transverse magneto-optical signal close to SPP resonances. Furthermore we reveal that the choice of a ferrimagnetic dielectric (YIG) or ferrromagnetic metal leads to different enhancement factors of the magneto-plasmonic interaction. These magneto-plasmonic interactions will be shown by magnetical, optical and magnetooptical methods including magnetooptical Kerr-effect, ellipsometry, and Brillouin light scattering measurements.

[1] M. Rollinger et al. Nano Letters 16, 2432 (2016).

[2] E. Melander et al. http://arxiv.org/abs/1611.00078 (2016).

O 59.11 Tue 18:30 P2-OG1

Self-Organized Nanostructures as a Large Area Substrate for Plasmonic Surface-Enhanced IR-Spectroscopy — •Michael Tzschoppe[1], Jochen Vogt[1], Maria Caterina Giordano[2], Filippo Canepa[2], Carlo Mennucci[2], Francesco Buatier De Mongeot[2], and Annemarie Pucci[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Dipartimento di Fisica-Università di Genova, Genova, Italy

Large area arrays of self-organized plasmonic Au nanoantennas were fabricated on soda lime glass wafers over several cm^2. To this end, Au was deposited on glass substrates, patterned by an ion beam sputtering technique. In this way it was possible to fabricate nanoantennas with a controlled length distribution leading to highly dichroic plasmonic resonances in the mid-infrared. A self-assembled monolayer of octadecanthiol (ODT) was used to investigate the potential of these nanoantennas as a substrate for surface-enhanced infrared absorption (SEIRA) spectroscopy. Calculations lead to a lower limit of the enhancement factor in the order of 10^3. The homogeneity of the arrays, which allows measurements on a macroscopic scale with a standard FTIR spectrometer, prove this self-organizing technique to be promising for the synthesis of large area SEIRA substrates for sensing applications.

O 59.12 Tue 18:30 P2-OG1

Higher Harmonics Generation in tapered Plasmonic Waveguides — •Julian Obermeier and Markus Lippitz — Experimental Physics III, University of Bayreuth

Higher harmonics generation in single gold nanostructures is a commonly known effect. Many fascinating experiments showed that the nonlinear emission is strongly influenced and shaped by the particle plasmon resonance. However, when the structure dimension exceeds the diffraction limited excitation area, the higher order modes of the structure and even propagation of the fundamental field and waveguiding effects become important. In our experiments we investigate the local nonlinear response of single tapered plasmonic slab waveguides with finite width. After excitation with pulsed infrared light, the locally generated second and third harmonic field is emitted in the near ultraviolet and visible spectrum and collected by a high NA oil immersion objective. This configuration allows a high spatial resolution of the origin of the nonlinear emission far below the diffraction limit of the excitation wavelength. In addition power dependent measurements help to understand the nonlinear effects in the extended nanostructures but also show deviations from basic expectations. We present our measurement technique and experimental results to determine the local emission properties of extended gold nanostructures.

O 59.13 Tue 18:30 P2-OG1

Signatures of strong coupling on nanoparticles: Revealing absorption anticrossing by tuning the dielectric environment — •Felix Stete[1,2], Wouter Koopman[1], and Matias Bargheer[1,3] — [1]Institut für Physik & Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [2]Humboldt-Universität zu Berlin, School of Analytical Sciences Adlershof (SALSA), Unter den Linden 6, 10999 Berlin, Germany — [3]Helmholtz Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany

This contribution presents a method to unambiguously identify the strong coupling regime in plasmon-exciton core-shell systems via absortpion measurements. Two examples of core-shell nanoparticles were used, both with a shell of the J-aggregate forming cyanine dye TDBC and a gold core. In one case the core was formed by gold nanospheres, in the other by gold nanorods. The resonances were tuned by changing the particles' environment on a substrate by layer-by-layer deposition of thin polyelectrolyte films replacing air und thus shifting the plasmon resonance. The extinction spectra of both systems show an anticrossing indicating a regime of strong coupling. However true absorption spectra reveal that only the rods are strongly coupled whereas the spheres' absorption does not show an anticrossing indicating that the spheres are rather in a regime of induced transparency. The observations are discussed within a classical coupled oscillator model that reveals differences in contributions from excitons and plasmons.

O 59.14 Tue 18:30 P2-OG1

Optical microspectroscopy of DNA origami-assembled complex and dynamic plasmonic nanostructures — •Mo Lu[1], Markus Pfeiffer[1], Chao Zhou[2], Na Liu[2], and Klas Lindfors[1] — [1]Department of Chemistry, University of Cologne, Luxemburger Str. 116, D-50939 Köln, Germany — [2]Max-Planck-Institute for Intelligent Systems, Heisenbergstrasse 3, D-70569 Stuttgart, Germany

Metal nanoparticles can serve as optical antennas due to their capacity to support collective oscillations of conduction electrons, known as localized surface plasmons. This can be used to enhance the reception and emission of light from quantum emitters such as semiconductor quantum dots or dye molecules. In our work, we study active plasmonic systems based on DNA origami nanotechnology, where a gold nanorod acts as a nanoantenna and use a single organic fluorescent dye molecule as a quantum emitter. In this system, the plasmonic nanorods can execute progressive and reversible walking to the predefined destination with a stepwise of 7nm [1]. The interaction of the light-emitting molecules with the plasmonic particles is characterized in fluorescence microscopy experiments, where we observe a decrease in fluorescence lifetime and brightness as the distance between emitter and antenna is decreased. Furthermore, we also perform interferometric scattering microscopy to detect the plasmonic particles in this active system in order to track the dynamic process in real time. Our microspectroscopy results provide evidence of the promise of merging nano-optics and DNA technology.

References [1]. C. Zhou, et al., Nat. Commun. 6, 8102 (2015).

O 59.15 Tue 18:30 P2-OG1

Low-temperature scattering-type scanning near-field optical microscopy — •Denny Lang[1,2], Jonathan Döring[2], Susanne C. Kehr[2], Lukas M. Eng[2], Stephan Winnerl[1], Harald Schneider[1], and Manfred Helm[1,2] — [1]HZDR, 01328 Dresden, Germany. — [2]IAP, TU Dresden, 01062 Dresden, Germany.

We present a combination of a versatile low-temperature scattering-type near-field optical microscope (LT-s- SNOM [1]) with a tunable infrared free-electron laser (FEL [2]). Our s-SNOM operates over a broad temperature range from 15 - 300 K [1,3,4] and is unique in being tunable over a broad frequency range, thanks to the FEL. The overall LT-s-SNOM functionality down to lowest temperature was tested on both standard Au and structured Si-SiO$_2$ samples, revealing net near-field contrasts and no topography cross-talk. Secondly, we investigated several ferroelectric phase transitions in barium titanate single crystals at 273 K [1] and 193 K [5], allowing to associate clear near-field resonances to every phase and each ferroelectric domain; here, the clear benefit of our LT-s- SNOM pays off, being able to record s-SNOM, PFM, KPFM and topographic data with one and the same tip from every sample surface spot. Thirdly, we used these piezoelectrics to quantify the local temperature increase under the AFM tip upon IR irradiation. [1] Döring et al., Appl. Phys. Lett. 105, 053109 (2014). [2] Kuschewski et al., Appl. Phys. Lett. 108, 113102 (2016). [3] Yang et al., Rev. Sci. Instrum. 84, 023701 (2013). [4] McLeod et al., Nature Phys. (2016); DOI: 10.1038/NPHYS3882. [5] Döring et al., J. Appl. Phys. 120, 084103 (2016).

O 59.16 Tue 18:30 P2-OG1

Shaping of Femtosecond Laser Pulses for Plasmonics — •Moritz Heindl, Jonas Albert, and Markus Lippitz — Experimental Physics III, University of Bayreuth, Germany

Ultrashort and well defined laser pulses are used in a wide range of nonlinear optics experiments. In combination with plasmonic nanostructures, they allow to define the optical nearfield in time and space. The temporal degree of freedom is controlled by a pulse shaper using a spatial light modulator. It gives us control over the phase and amplitude in frequency space and thus the form of the pulse. Here we will present the design of our pulse shaper and experiments to check the functionality of the setup. Furthermore, we give an outlook on future experiments making use of spatial and temporal control of optical fields.

O 59.17 Tue 18:30 P2-OG1

Near-field imaging and spectroscopy of hybridized plasmonic nanocavities — •Anna-Katharina Mahro[1], Deirdre Kilbane[1,2], Michael Hartelt[1], Tobias Eul[1], Eva Prinz[1], Mirko Cinchetti[1,3], and Martin Aeschlimann[1] — [1]Physics Department and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]School of Physics, University College of Dublin, Ireland — [3]Experimentelle Physik VI, TU Dortmund, Germany

Knowledge of fundamental light-matter interactions such as the spectral response of nanostructures to incident light is necessary for designing plasmonic devices. This response is determined on the nanometer scale (below the diffraction limit of light). To achieve this high spatial resolution we use a photoemission electron microscope (PEEM). It images the near-field distribution of the photoelectrons in a parallel data acquisition scheme.

To gain information about the spectral response, we combine PEEM with a highly tunable femtosecond laser source, in our case an optical parametric oscillator (OPO). We demonstrate the potential of this experimental setup by investigating localized, propagating and hybridized surface plasmons in different arrangements of gold whispering gallery mode antennas (WGM) which are fabricated via focussed ion beam milling (FIB).

O 59.18 Tue 18:30 P2-OG1

Coupling of Quantum Emitters to Plasmonic Metamaterials — •Daniel Kuckla, Manuel Peter, and Stefan Linden — Physikalisches Institut, University of Bonn, Nußallee 12, D-53115 Bonn, Germany

Metamaterials consisting of sub-wavelength structures such as splitring resonators (SRRs) can give rise to unusual optical properties and allow the shaping of electromagnetic waves. In most experiments so far, the investigated metamaterials have been passive structures. However, active metamaterials are attracting more and more interest. For instance, the coupling of semiconductor quantum dots to the different modes of a SRR array has been investigated recently. Here, we focus on the effect of the electromagnetic interactions between the elements of an active metamaterial on its emission properties. For this purpose, we fabricate a series of rectangular SRR arrays with intentionally deposited quantum dots by electron beam lithography in combination with a process that allows us to chemically link nanoparticles from an aqueous solution to freely definable sites on the substrate. To study the influence of the interactions within the metamaterial, we vary within the series the lattice periods while keeping the unit cell size constant. Our SRRs are designed in such a way that the second and third plasmonic mode of the metamaterial with equal lattice periods overlap with the emission spectrum of the uncoupled quantum dots.

O 59.19 Tue 18:30 P2-OG1

Route to high-resolution scanning optical microscopy — •Daniel Friedrich, Heiko Gross, and Bert Hecht — Nano-Optics and Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany

Using confined photons for atomic-scale spectroscopic imaging offers new possibilities in high-resolution scanning optical microscopy and enhanced light-matter coupling. Recent investigations employ scanning probe microscopy to reveal strong coupling between single quantum dots and a single crystal broadband nanoresonator.(1)

By tuning the coupling strength between a plasmonic resonator and single quantum dots, (bio-)molecules or novel 2D-materials using scanning probe microscopy we expect new spectroscopic information with nanometer spatial resolution. Measuring photoluminescence and Raman scattering over the full visible range, in combination with state-of-the-art scanning probe technology with different optical accesses paves the way to novel spectroscopic imaging modalities and observation of a single-photon non-linearity.

(1) Groß, H., Hamm, J. M., Tufarelli, T., Hess, O. and Hecht, B., Strong coupling spectroscopy of single quantum dots at room temperature using a broadband nanoresonator. (submitted)

O 59.20 Tue 18:30 P2-OG1

Fourier Analysis of Overlapping Surface Plasmon Polaritons with Different Propagation Directions — •Pascal Dreher, Pierre Kirschbaum, David Janoschka, Amran Al-Ashouri, Martin Paul Geller, Michael Horn-von Hoegen, and Frank Meyer zu Heringdorf — Faculty of Physics and Center for Nanointegration (CENIDE), Duisburg, Germany

In the past, photoemission electron microscopy (PEEM) has been proven to be an excellent tool for studying surface plasmon polaritons (SPPs). Plasmonic contrast in the real space PEEM images is generated by two photon photoemission. Using femtosecond laser pulses in a pump-probe fashion, time resolution can be achieved. The combination of PEEM and time resolved techniques provides for the spatiotemporal observation of propagating SPPs. Using normal incidence geometry, the result is a direct conceptual visualization of the SPPs.

The estimation of ratios of electric field amplitudes of overlapping SPPs with different propagation directions is a cumbersome and erroneous task, if attempted from real space PEEM images. We present a novel approach based on an FFT analysis that allows the separation of several overlapping SPPs in Fourier space. Using this approach, it was possible to extract the coefficients of transmission and reflection of plasmonic Bragg reflectors as a function of the number of reflector grooves.

O 59.21 Tue 18:30 P2-OG1

Plasmon dispersion and dielectric funtion at a silver/porphyrin interface — •Klaus Stallberg and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstraße 4, 38678 Clausthal-Zellerfeld, Germany

Multi-photon photoelectron microscopy (nP-PEEM) is a valuable tool for the investigation of propagating surface plasmon polaritons (SPP). It has been demonstrated by other groups that nP-PEEM allows for a determination of the complex SPP wavevector. In our contribution we adapt this method to determine the SPP dispersion curve on a microscopic Ag(111) island. Our results are in good agreement with results from the literature which were obtained with all-optical methods on extended silver films. We further investigate the SPP dispersion at a silver/zinc-tetraphenylporphyrin interface, which can be regarded as a model system for SPP propagation in the presence of a dielectric with a strong optical absorption band. For excitation wavelengths near the porphyrin absorption (Soret-) band, the shape of the SPP dispersion curve signals an interaction of molecular and plasmonic excitations. In addition, we demonstrate that with nP-PEEM the complex dielectric constant of a thin organic film can be determined as a function of the film thickness during growth. Moreover, we investigate the frequency dispersion of the complex dielectric function of the porphyrin film.

O 59.22 Tue 18:30 P2-OG1

Long-Lived Electron Emission Reveals Ultra-localized Plasmon Modes in Gold Nanosponges — •Germann Hergert[1], Jan Vogelsang[1], Felix Schwarz[2], Dong Wang[2], Heiko Kollmann[1], Petra Gross[1], Erich Runge[2], Peter Schaaf[2] und Christoph Lienau[1] — [1]1Carl von Ossietzky Universität, Oldenburg, Germany — [2]2Technische Universität Ilmenau, Ilmenau, Germany

Materials with disorder on the nanometer scale are known to exhibit large field enhancement properties, making them viable for enhancing non-linear optical effects or for investigating quantum optical processes. Different 2D model systems have been used to study the role of disorder. Promising 3D models for this are nanoporous gold particles (”nanosponges”) which have recently attracted attention as templates for surface-enhanced Raman sensing due to their multiple plasmon resonances from the visible to the NIR spectral range, a high surface-to-volume ratio, and a high density of catalytic sites [1].

Here we report the observation of long-lived, spatially highly localized plasmon states on the surface of nanosponges. Using a 16-fs excitation pulse at 1600nm wavelength, we measure light-induced electron emission from single sponges with lifetimes of several tens of fs. We observe the long-lived electron emission, as a nonlinear process with the exponent n=5-7. This in combination with optical extinction measurements and FDTD calculations, points to a strong coupling of the localized modes with the delocalized dipolar plasmon mode, resulting in an extraordinary high excitation efficiency of the hot spot resonances.

[1] Wang, D.; Schaaf, P. J. Mater. Chem. 2012, 22, 5344-5348

O 59.23 Tue 18:30 P2-OG1

Polymer Orientation Sensitive Scanning Near-field Optical Microscopy — •Jinxin Zhan[1], Jens Brauer[1], Daniel Trefz[2], Sabine Ludwigs[2], Petra Gross[1], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]Institut für Polymerchemie, Stuttgart, Germany

Well aligned polymer fibers attract wide interest in film transistor, solar cell, and display applications etc. due to their excellent optical-to-electric transfer efficiency and their charge transport characteristics. Their latter performance is greatly influenced by the alignment of polymer chains on a nano- to microscopic scale. Hence, in order to study the relationship between their structure and propertity, especially the local fluctuations below the domain size of typically a few ten nanometers, an optical imaging method sensitive to polymer orientation with nanometer resolution is required. Here we use a Scanning Near-field Optical Microscope (SNOM) based on a backscattering geometry to investigate fiber alignment in a polymer P(NDI2OD-T2) film. Spectral absorption measurements reveal an optimum optical contrast of the polymer film near the resonance wavelength of P(NDI2OD-T2).

Changing the polarization direction of the linearly polarized excitation laser enables us to determine the molecular orientation with a resolution of about 10 nm. Extracting the polymer orientation from the SNOM optical signal is facilitated by adapting a well-established model that describes the tip as a dipole.[1]

O 59.24 Tue 18:30 P2-OG1

Relaxation dynamics of plasmonic hot-carriers in gold nanoparticles — •Emanuele Minutella[1,2], Florian Schulz[1], and Holger Lange[1,2] — [1]Physikalische Chemie, Universität Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, CUI

Using light to drive or control chemical or physical processes is a very interesting field of research. One problem is to guide the light's energy to the specific place where reaction takes place. Due to their plasmonic properties noble metal nanoparticles have the ability to collect very efficiency photons and convert them into hot-electron-hole-pairs. As a result of size and photon energy dependent transient absorption measurements we found a binary kinetic for the relaxation times of the hot electrons. Depending on the photon energy either interband or intraband excitations are possible. We found faster decay rates for the intraband relaxation than for the interband. These results can help to improve possible hot-carrier devices.

O 59.25 Tue 18:30 P2-OG1

Individual addressing and fine-tuning of mid-IR metallic and dielectric nanoantenna resonances by reversible optical switching of $Ge_3Sb_2Te_6$ thin-films — •Andreas F. Hessler, Ann-Katrin U. Michel, Julian Hanss, Martin Lewin, Tobias W.W. Mass, Peining Li, Xiaosheng Yang, Dmitry N. Chigrin, Thomas Kalix, Angela De Rose, Matthias Wuttig, and Thomas Taubner — Institute of Physics (IA) RWTH Aachen

Optically resonant thin film systems which are structured on the nanometer scale offer comprehensive control over light fields. Despite their nanometer thickness, these nano films can be used for the creation, detection and transformation of light. For optimal functionality, they need to be freely programmable and low optical losses.

By combining phase-change materials (PCMs) with a custom laser-setup, we addressed both issues. PCMs can have a high optical contrast between their amorphous and crystalline phases, while having low optical losses in the infrared. Moreover, they can be switched between phases with short high-energy laser pulses [1].

Here, we show two examples of metallic and dielectric nanostructures which can be addressed with our setup. We could directly and reversibly write arrays of dielectric resonators into a surface [2]. Additionally, we can address individual metallic nanoantennas, covered by a layer of $Ge_3Sb_2Te_6$, with ns-laser pulses to fine-tune their resonances.

[1] A.U.Michel et al., ACS Photonics 1, 833 (2014)
[2] P.Li et al., Nature Materials 15, 870 (2016)

O 59.26 Tue 18:30 P2-OG1

Surface-enhanced infrared spectroscopy with nanorod antenna arrays for investigating alkanethiols with different chain lengths — •Tobias W. W. Mass, Andreas F. Hessler, and Thomas Taubner — Institute of Physics (IA) RWTH Aachen

Metallic structures can efficiently couple light into a region of subwavelength size. In these regions, large local field enhancements can occur and enable an increased light absorption of molecules which are placed in these so called "hot spots". Arrays of nanorod antennas which are designed for surface-enhanced infrared absorption (SEIRA) spectroscopy enable the detection of molecular vibrations with high sensitivity [1,2].

Alkanethiol molecules of different chain length differ only in their number of CH_2-groups, while they all have one single CH_3-group. It has been shown with grazing incidence reflection spectroscopy that the absorption signals from the CH_2-groups depend linearly on the chain length, while those of the CH_3-groups stay constant [3].

In our work, we investigated how well we can distinguish small quantities of alkanethiol molecules by SEIRA spectroscopy. We calculated the quotient of the absorption signals of the CH_2- and CH_3-groups, which is largely independent of the specific nanoantenna geometries and observed a linearly rising trend.

[1] C.Huck et al., ACS Nano 8, 4908 (2014)
[2] T.W.W.Maß and T.Taubner., ACS Photonics 2, 1498 (2015)
[3] M.D.Porter et al., J. Am. Chem. Soc. 109, 3559 (1987)

O 59.27 Tue 18:30 P2-OG1

Local Field Enhancement in Nano-Slit Arrays for Nonlinear THz Studies — •Thomas Rittmann[1,2], Zhiren Zheng[1], Scott Dhuey[3], Stefano Cabrini[3], Jan Heye Buss[1], and Robert A. Kaindl[1] — [1]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA — [2]4th Physical Institute, Georg-August-University, Göttingen, Germany — [3]Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, USA

Nanoscale slit arrays in thin metal films act as strong field enhancers at terahertz (THz) frequencies while simultaneously retaining extraordinary optical transmission [1,2]. When driven with ultrashort THz pulses, this enables novel nonlinear THz studies of quantum materials [3]. We report time-domain THz spectroscopy of gold nano-slit arrays on single crystal quartz substrates for several slit widths down to 70 nm and for variable periodicities up to 50 um.

Besides confirming the general dependency of the field enhancement on inverse slit width and frequency, we observe its stagnation below a periodicity-dependent saturation frequency that results from spatio-temporal charge dynamics. The results are consistent with our numerical finite elements analysis and yield essential figures of merit for optimizing future nonlinear THz studies.

[1] M.A. Seo, *et al.* Nat. Photon. **22**, 152-156 (2009).
[2] M. Shalaby, *et al.* Appl. Phys. Lett. **99**, 041110 (2011).
[3] Z. J. Thompson, *et al.* Nano Lett. **15**, 5893 (2015).

O 59.28 Tue 18:30 P2-OG1

Constructing core/shell nanostructures with optimal structure and composition could maximize the solar light utilization. — •Max Sommerfeld, Rui Xu, and Yong Lei — TU Ilmenau, Ilmenau, Deutschland

Here, using an Au nanocone array as a substrate, a well-defined regular array of SnO2/TiO2 core/shell nanocones with uniformly dispersed Au nanoparticles (SnO2/TiO2/Au NCA) is successfully realized through atomic layer deposition, physical vapor deposition and annealing processes. By tuning the structural and compositional parameters, the advantages of light trapping and short carrier diffusion from the core/shell nanocone array, as well as the surface plasmon resonance and catalytic effects from the Au nanoparticles can be maximally utilized. Accordingly, a remarkable photoelectrochemical (PEC) performance can be acquired. The photocurrent density of the SnO2/TiO2/Au NCA electrode is four times that of a flat SnO2/TiO2 electrode at 1.23 V versus reversible hydrogen electrode (RHE) under simulated sunlight illumination. These results demonstrate a feasible route toward the scalable fabrication of well-modulated core/shell nanostructures and can be easily applied to other metal/semiconductor composites for high-performance PEC.

O 59.29 Tue 18:30 P2-OG1

Biosensing with plasmonic gold nanorod arrays — •Tino Uhlig[1], Stephanie Klinghammer[2], Larysa Baraban[2], Gianaurelio Cuniberti[2], and Lukas Eng[1] — [1]Institute of Applied Physics, Chair of Experimental Physics/ Photophysics, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Institute for Material Science, Chair of Material Science and Nanotechnology, Technische Universität Dresden, D-01062 Dresden, Germany

Label-free biosensing based on localized surface-plasmon resonances (LSPR) in noble-metal nanostructures has gained a lot of interest in past years. This is mostly due to the possibility of spectral tuning, miniaturization and flexible integration into nanobiotechnological architectures (e.g. microfluidics). Here we report on the fabrication of such a LSPR biosensor based on extended arrays of gold nano-antennas [1,2]. These nanorod carpets are prepared by electro-chemical filling of gold into nanometer-sized pores in an anodized aluminum oxide (AAO) template [3]. The chosen fabrication method [3] allows for a wide range of spectral tunability at visible wavelengths [2], hence facilitating optimized sensor-array performance at the highest sensitivity in the nanomolar range. We demonstrate the feasibility of our approach through monitoring the reproducible binding/unbinding of complementary single-stranded DNA molecules used here as a model system.

[1] R. Kullock et al., J. Opt. Soc. Am. B **27**, 1819 (2010).
[2] V. Fiehler et al., J. Phys. Chem. C **120**, 12178 (2016).
[3] F. Patrovsky et al., Thin Solid Films (2016) submitted.

O 59.30 Tue 18:30 P2-OG1

Photon Correlation Measurements on Quantum Dots —

•Lok-Yee Yan, Manuel Peter, and Stefan Linden — Physikalisches Institut, University of Bonn, Nußallee 12, D-53115 Bonn, Germany

Semiconductor quantum dots (QDs) can be used as single photon emitters in various applications. In our group we have developed a lithographic method that allows us to deposit colloidal semiconductor QDs on freely definable sites on the substrate. So far, we have used this method for the precise placement of small patches of QDs containing several emitters. The aim of this work is its improvement to reliable single QD placement. In order to show photon-antibunching of the fluorescence of a single QD we are performing a Hanbury-Brown-Twiss experiment (HBT). In the HBT the fluorescence is divided by a 50:50 beam splitter and detected by two avalanche photodiodes. By connecting the output signals of the photodiodes to a Time-Correlated Single Photon Counting unit, one signal serves as start and the other as stop signal. By measuring the histogram of the time difference between the two signals, we obtain the second-order correlation function $g^{(2)}(\tau)$. Since the excitation is done by a pulsed laser, we expect $g^{(2)}(\tau)$ to be periodic. To show photon-antibunching, we want to measure a significant decrease at $g^{(2)}(0)$.

O 59.31 Tue 18:30 P2-OG1

A time of flight delay line detector for characterization of electron emission from metal nanostructures — •Andreas Wöste, Jan Vogelsang, Thomas Quenzel, Petra Gross, and Christoph Lienau — Institut für Physik, Carl von Ossietzky Universität, 26129 Oldenburg, Germany

Strong-field photoemission from metallic nanostructures has recently been of considerable interest since e.g. electrons can be accelerated in large near field gradients or above threshold ionization may be induced from long-lived image potential states. A microscopic understanding of those processes requires detector systems capable to collect information about the emitted electron momentum distribution. One way to investigate this is via a hemispherical deflection analyzer. The recorded kinetic energy and the emission angle then enables extracting information about the local optical nearfields at the surface. However these kind of detectors lack the capability to measure the complete momentum distribution of the photoemitted electrons. To overcome those restrictions we implement a time of flight delay line detector (TOF-DLD) enabling simultaneous measurement of emission angles as well as the perpendicular and parallel momentum of each photoelectron individually. We test this by investigating the strong field electron emission from a sharply etched gold nanotip. With the TOF-DLD we are able to study the dependency of emission angle on the kinetic energy. To verify proper working of the new detector system we compare selected measurements with the results of a known hemispherical deflection analyzer.

O 59.32 Tue 18:30 P2-OG1

Large-area, low-cost, ultra-broad bandwidth Nickel-based plasmonic perfect absorber — •Ramon Walter[1], Matthias Zilk[2], Izzatjon Allayarov[1], Forian Sterl[1], Audrey Berrier[3], Thomas Pertsch[2], Thomas Weiss[1], and Harald Giessen[1] — [1]4th Physics Institute, University of Stuttgart — [2]Institute of Applied Physics, Friedrich-Schiller University Jena — [3]1st Physics Institute, University of Stuttgart

Plasmonic devices with a very high absorption over a wide wavelength range have the potential for many applications such as light trapping, photo catalysis, and as black background for novel displays. Perfect absorber devices are the first choice to achieve such applications. Such systems can show a very high absorption at their plasmonic resonance, just by optimizing their system impedance to vacuum values.

We present a way to realize such system, just by using the "bad" plasmonic material nickel for nanostructures, placed over an aluminum mirror and a magnesium fluoride spacer. By using a variation of the well-known nanosphere lithography, we present a way to create such devices on a large-area scale. Simply by drop coating deposited polystyrene nanospheres, we create a mask for a subsequent dry-etching process with an Argon ion beam. The resulting device shows a very high absorption over 90% nearly over the complete visible range, very high over a wide range of incident angles, nearly independently of the polarization.

We believe that our design has to potential for many applications where a large bandwidth of light absorption is preferable.

O 60: Solid-Liquid Interfaces: Structure, Spectroscopy, Reactions and Electrochemistry

Time: Tuesday 18:30–20:30 Location: P2-OG2

O 60.1 Tue 18:30 P2-OG2

The spin-resolved electronic structure of Au(110) — •Katharina T. Ritter, Fabian Schöttke, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster

Materials with strong spin-orbit coupling are known to exhibit Rashba-split electronic band structures. To understand the basic concepts, Au(111) is a widely used prototypical system for a spin-split surface state around the $\overline{\Gamma}$ point. As on Au(111), the surface state on Au(110) originates from the L-gap, but exists at the $\overline{\mathrm{Y}}$ point.

It is predicted that the Au(110) surface state around the $\overline{\mathrm{Y}}$ point shows a spin-dependent splitting in energy and momentum. Only the spin-integrated dispersion of the electronic states has been experimentally investigated so far. Here, we present spin-resolved data using spin- and angle-resolved (inverse) photoemission for the $\overline{\Gamma}\,\overline{\mathrm{Y}}$ direction to reveal the spin texture of the Au(110) surface state.

O 60.2 Tue 18:30 P2-OG2

Overcharging and charge reversal of surface charge in high electrolyte concentrations — •Christine Klinger, Markus Valtiner, and Christian Weber — Institut für physikalische Chemie, Fakultät für Chemie und Physik, Technische Universität Bergakademie, Freiberg, Deutschland

The structure of water and ions in the electric double layer influences adhesion and reactivity at solid/liquid interfaces. Previous investigation showed the suitability of atomic force microscopy (AFM) for the investigation of electric double layer structures, based on molecularly resolved force spectroscopy and imaging with atomic resolution. Using the AFM, we quantitatively measure the effect of overcharging and charge reversal of surface charge on mica due to the condensation of Cs-ions into the mica lattice. We examine the surface charge at mica applying different concentrations of aqueous CsCl solution with ionic strengths ranging from 10 mM to 100 mM. Thereby we can show that mica surfaces overcharging leading to a charge reversal in high electrolyte concentrations. In detail, our results provide an insight into the interaction forces and electric double layer structures depending on different environmental conditions.

O 60.3 Tue 18:30 P2-OG2

How accurate is the PBE functional for describing the properties of liquid sulfuric acid in ab-initio molecular dynamics simulations? — •Florian Wullschläger, Steffen Seiler, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

The structural properties of liquid sulfuric acid were investigated using the PBE functional in Car-Parrinello molecular dynamics (CPMD) simulations. The temperature and concentration dependency of the degree of H_2SO_4 dissociation was determined to gain insights into the accuracy of this common generalized-gradient functional in reproducing experimental data derived from Raman spectroscopy [1,2]. Furthermore, the structural features of the liquid were characterized by calculation of pair distribution functions and diffusion coefficients. Overall, we observed an overestimation of the degree of dissociation at low sulfuric acid concentrations, whereas in the high concentration limit the results of the PBE calculations are in good agreement with the experimental data.

[1] C.E. Lund Myhre, et al., *J. Phys. Chem. A* **107**, 1979 (2003).
[2] D.A. Knopf, et al., *J. Phys. Chem. A* **107**, 4322 (2003).

O 60.4 Tue 18:30 P2-OG2

Tuning oxygen reduction through interface engeneering — •Patrick Alexa[1], Doris Grumelli[1], Diana Hötger[1], Svetlana Klayatskaya[2], Mario Ruben[2], Rico Gutzler[1], and Klaus Kern[1,3] — [1]) Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Karlsruhe Institute of Technology, 76344

Eggenstein-Leopoldshafen, Germany — [3]Ecole Polytéchnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Electrocatalytical reactions, especially the oxygen reduction reaction (ORR) in alkaline media, are widely examined. They are of interest for the development of efficient fuel cells and metal-air batteries. Functionally designed catalysts at interfaces are crucial for the improvement of such reactions. The catalytic reactive sites can be metal centers (e.g. Co) incorpotated within organic molecules, e.g. phthalocyanines (Pcs). Here, we study the effect of side groups in Co-phthalocyanines (CoPcs) deposited on Au(111). Deposition of the CoPcs was followed by STM and XPS prior to oxygen reduction in 0.1M NaOH. By increasing the distance between Co atom and Au(111) surface through Pc functionalization with triisopropyl protection groups, the ORR activity is significantly diminished. Thus, a small distance between gold electrode and metal active site is essential for efficient ORR. The results highlight the importance of chemical tailoring of the catalyst interface for the rational design of efficient catalysts.

O 60.5 Tue 18:30 P2-OG2

First-Principles Studies of the Structural Properties of Nickel (Oxy)hydroxide as Oxygen Evolution Reaction Electrocatalysts — •Mohammad Javad Eslamibidgoli[1], Michael H. Eikerling[1], and Axel Gross[2] — [1]Department of Chemistry, Simon Fraser University, 8888 University Drive, Burnaby, V5A 1S6, BC, Canada — [2]Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Nickel oxide (NiO$_x$)-based electrocatalysts are among the most promising materials for oxygen/hydrogen evolution reactions in alkaline conditions. In the late 1960s, X-ray diffraction studies revealed four main phases for Ni (oxy)hydroxide electrodes [1]: It involves two phases of nickel hydroxide, α- and β-Ni(OH)$_2$, and two phases for the oxidized materials, β- and γ-NiOOH. In this contribution, we report first-principles calculations of bulk properties, surface configuration, electronic structure, charging effects and catalytic properties of various phases and surface terminations of Ni (oxy)hydroxide. Using a spin polarized DFT-D + U approach, we first focus on understanding the structure and orientational order of interfacial water on the (001) surfaces. This is followed by investigations of the mechanisms of the oxygen evolution reaction at the surface accounting for implicit and explicit solvent.

[1] H. Bode *et al.*, Electrochim. Acta **11**, 1079 (1966).

O 60.6 Tue 18:30 P2-OG2

Electrochemical etching of GaAs, InP and InSb after ion irradiation — •Alrik Stegmaier, Ulrich Vetter, and Hans Hofsäss — 2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Microelectromechanical systems (MEMS) combine electrical and mechanical features on the micrometer scale and are used for an increasing number of applications, including energy harvesters, accelerometers and pressure sensors [1]. With Proton Beam writing (PBW) it is possible to produce these three dimensional MEMS structures by varying only the fluence of the proton irradiation on a III-V semiconductor sample, followed by electrochemical etching [2,3].

As such, the electrochemical etching of the sample is of large importance for producing high quality final structures. Here we extend the reported electrochemical models [4] to both InSb and the highly irradiated case, typically ecountered during PBW. With this, we can show significant improvements of both the etching time and quality over our previous findings [5].

[1] V. Cimalla et al., J. Phys. D: Appl. Phys., 40(20), 6386, 2007
[2] J.A. van Kan et al., Appl. Phys. Lett., 83(8), 1629, 2003
[3] P. Mistry et al., Nucl. Instr. Meth. Phys. Res. B, 237, 188, 2005
[4] P. Allongue et al., J. Electroanal. Chem., 317, 77-99, 1991
[5] M. Schulte-Borchers et al., J. Micromech. Microeng., 22, 025011, 2012

O 60.7 Tue 18:30 P2-OG2

***In situ* X-ray reflectivity studies of electrochemical Cu deposition on industrial Ru covered Si wafers** — •Timo Fuchs, Jonathan Laufer, Finn Reikowski, Jochim Stettner, and Olaf Magnussen — Institut für Experimentelle und Angewandte Physik, Universität Kiel, Olshausenstr. 40, 24098 Kiel, Germany

Further decrease in size of Cu semiconductor interconnects is of special interest for the ongoing improvements in computing capacity. An interconnect consist of trenches and vias, which are typically coated with a Cu seed layer on top of a Ta/TaN diffusion barrier layer, that allows homoepitaxial growth of the electrochemically applied Cu. However, the fabrication of reliable devices on the base of Cu seed layers becomes increasingly difficult, when typical feature sizes are below 20 nanometers and the homogeneity and roughness of the layers become crucial. Consequently, current efforts focus on the development of substrates for seedless Cu electroplating, using ultrathin Ru adhesion layers of high conductivity on a TaN diffusion barrier.

For the successful control of structural properties of the Cu layer, an in-deep understanding of early Cu growth processes on an atomic level, i.e. nucleation and coalescence of Cu islands on Ru, is indispensable. We are presenting first structural data, gained by *in situ* X-ray reflectivity measurements at a lab source of the bare Ru/TaN/SiO2/Si substrate as well as *in operando* studies of the growing Cu layer. The results of this investigation will serve as a base for future grazing incidence small angle x-ray scattering (GISAXS) studies using synchrotron radiation.

O 60.8 Tue 18:30 P2-OG2

DFT study of the diffusion of S on a Br-precovered Cu(100) surface — •Lukas Deuchler[1], Eckhard Pehlke[1], Björn Rahn[2], and Olaf Magnussen[2] — [1]Institut für Theoretische Physik und Astrophysik, CAU Kiel. Germany — [2]Institut für Experimentelle und Angewandte Physik, CAU Kiel. Germany.

Diffusion at electrochemical interfaces is a decisive factor for, e.g., metal electrodeposition using halide ion containing electrolytes [1]. The modification of surface diffusion energy barriers due to an applied sample potential has been ascribed to the interaction of the electric dipole moment of the system with the electric field at the surface [1,2]. The diffusion of Sulfuric tracer adatoms on Cu(100) surfaces has been investigated using video-STM. On the c(2x2)Cl/Cu(100) [3] and on the c(2x2)Br/Cu(100) surface, S-adatoms respond qualitatively differently to the applied sample potential, i.e. by a decrease or an increase of the hopping rate of the S adatom. Density-functional total-energy calculations with VASP [4] for the diffusion path suggest a possible explanation to this unexpected experimental observation. We note that our theoretical analysis is based on former theoretical research on S/c(2x2)Cl/Cu(100) diffusion by J. Stremme and A. Franke [5,6].

[1] M. Ruge *et al.* , Phys. Rev. Lett. 112, 055503 (2014).
[2] M. Giesen *et al.*, Surf. Sci. 595, 127 (2005).
[3] T. Tansel, O. Magnussen, Phys. Rev. Lett. 96, 026101 (2006).
[4] See //www.vasp.at.
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[6] J. Stremme, Diplomarbeit 2009, Universität Kiel.

O 60.9 Tue 18:30 P2-OG2

DFT-study of adsorption and diffusion including electric field effect for halogen atoms on the (001) surfaces of Cu, Ag, Au and an AgAu-alloy — •Alexandra Davila, Jan Thiel, Nico Reimann, and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, CAU Kiel, Germany

The growth dynamics in metal electrodeposition experiments depend on the electric potential of the sample electrode [1]. This has been ascribed to the dependence of the activation energy for surface diffusion of the metal adatoms on the sample potential. The composition of the electrolyte, especially halides, e.g. Cl$^-$ ions, will also play an important role on the surface mobility [1]. Motivated by these results, we present a DFT based analysis [2,3] of activation energies under homogeneous electric field, which simulates the effect of the sample potential, for halogen (Cl, Br, I) adatoms on the (001) surfaces of Cu, Ag, and Au. The effect of electric field on the energy differences between hollow and brigde sites follow the linear relation derived by Giesen *et* al. [4], with deviations from linearity less than 10 meV for electric field ranging from -0.6 V/Å to 0.6 V/Å. In case of I/Au(001) we observe a qualitative change of the PES as a function of electric field. Furthermore, we show changes of the topology of the PES for the case of an adsorbed Cl-atom on an AgAu alloy.

[1]T. Tansel and O. Magnussen, Phys. Rev. Lett. 96 (2006).
[2]//www.vasp.at.
[3]P. Giannozzi *et* al., J. Phys. Condens. Matter 21, 395502 (2009).
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O 60.10 Tue 18:30 P2-OG2

The Ag$_x$Pt$_{1-x}$/Pt(111) surface alloy system as model catalyst for the ORR - Studies on the effect of structure and corrosion on the electrocatalytic activit — •Stephan Beckord, Sylvain Brimaud, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, 89069 Ulm, Germany

Bimetallic surface alloys often exhibit catalytic and electrochemical properties which significantly differ from those of the respective pure metals. AgPt electrode surfaces were predicted to exceed the activity of Pt on the oxygen reduction reaction [1], where the latter is known to be the best mono metallic catalyst for this reaction. The increased activity of AgPt was also confirmed by experimental studies in our institute. In this work we present results on the effect of restructuring and corrosion of the model electrode surfaces under reaction conditions on the electrocatalytic characteristics and activity of well-defined $Ag_xPt_{1-x}/Pt(111)$ surface alloys. The surface alloys were prepared and structurally characterized by scanning tunneling microscopy (STM) under ultra high vacuum (UHV) conditions before and after electrochemical investigation. The electrochemical behavior of the model electrodes was studied before and after electrochemical dissolution of Ag atoms in a flow-cell setup by cyclic voltammetry (CV), the activity by measurements on the ORR, respectively. Correlation between structural changes in the corroded surfaces and the oxygen reduction reaction activity are discussed. [1] J. Greeley and J.K. Norskov, J. Phys. Chem. 113 (2009) 4932.

O 60.11 Tue 18:30 P2-OG2

Influence of Mg^{2+} und Li^{+} Ions on the electrochemical decomposition of BMP TFSI on Au electrodes — •Gülsah Yetis[1], Dorothea Alwast[1], Johannes Schnaidt[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-89081 Ulm, Germany

Many ionic liquids (ILs) are known for their high electrochemical stabilities and therefore, in combination with Li^{+} and Mg^{2+} salts, are regarded as promising electrolytes for lithium-ion or magnesium batteries, respectively. In order to improve these batteries, a fundamental understanding of the interaction between the IL and said metal salts is necessary which determines the stability of the electrolyte. The influence of Li^{+} and Mg^{2+} cations on the decomposition of the IL N-butyl-N-methylpyrrolidinium-bis(trifluoromethanesulfonyl)imide (BMP TFSI) is studied by differential electrochemical mass spectrometry (DEMS). Thus, volatile decomposition products can be detected during cyclovoltammetric measurements. We show that the addition of LiTFSI and $MgTFSI_2$ diminishes the stability window of the IL at both positive and negative potentials. In the presence of the metal cations, products of the TFSI anion decomposition are detected during the negative potential scan, whereas no BMP reduction is observed. Further effects of the metal salts on the IL degradation in comparison to the behavior of the pure IL will be discussed.

O 61: Heterogeneous Catalysis

Time: Tuesday 18:30–20:30 Location: P2-OG2

O 61.1 Tue 18:30 P2-OG2

Simulation of gas-phase mediated sintering — •Elisabeth Dietze[1,2] and Philipp Plessow[1,2] — [1]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Institute of Catalysis Research and Technology (IKFT), Karlsruhe, Germany Institute of Catalysis Research and Technology (IKFT), Karlsruhe, Germany

It is a longstanding question whether sintering of Pt under oxidizing conditions is mediated by surface migration of Pt species or through the gas phase, by PtO_2. Simulations have shown that ripening through the gas phase is relevant [1]. In addition, experiments have shown how sintering depends on the gas flow and the geometrical setup of the reactor for the sintering of Pt particles in an oxidizing atmosphere [2]. Accurate prediction of gas-phase mediated sintering requires to go beyond continuum approximations and to model mass transport in the gas phase. The transport is modeled through an explicit simulation of single-particle scattering events in the gas phase, using a kinetic Monte Carlo (kMC) model that describes the collision of an explicit molecule within an uniform background of ideal gas that is characterized by its temperature as well as its mass distribution, collision cross section and collective gas-flow. Since Argon is often used as a gas in experiments it is an appropriate model system. First results are promising. The diffusion constant of an Ar^{40} molecule in Ar^{40} could be reproduced.

[1] P. Plessow, F. Abild-Pedersen, ACS Catal. 2016, 6 (10), 7098-7108. [2] T.W. Hansen, A.T. Delariva, S.R. Challa, A.K. Datye, Acc. Chem. Res. 2013, 46 (8), 1720-30.

O 61.2 Tue 18:30 P2-OG2

Ab-initio Study of Photocatalytic Water Splitting on $LiNbO_3$ — •Christof Dues, Wolf Gero Schmidt, and Simone Sanna — Theoretische Physik, Universität Paderborn, D-33095 Paderborn

Photocatalytic water-splitting for hydrogen production promises to offer a way for clean, low-cost and environmentally friendly production of hydrogen by solar energy. Besides titanium dioxide also ferroelectric lithium niobate has been studied as a possible photocatalyst in this context [1]. The internal polarisation in this material is expected to lead to a long lifetime of photo-induced carriers as well as reaction pathways that involve both the positively and negatively charged surface.

In the present work the water splitting at $LiNbO_3$ Z-Cut surfaces is studied within density functional theory (DFT). Thereby the approach of Nørskov et al. [2] for estimating the free energy profil of the reactions is followed. Saddle points in the potential energy hypersurface are determined using the nudged elastic band method [3] and constrained DFT is used to model the excited configurations.

[1] B. Zielińska et al., J. Phys. Chem. Solids **69**, 236 (2008).
[2] J. K. Nørskov et al., J. Phys. Chem. B **108**, 17886 (2004).
[3] G. Henkelman et al., J. Chem. Phys. **113**, 9901 (2000).

O 61.3 Tue 18:30 P2-OG2

Theoretical Investigation of the Role of CO Adsorption on the Properties of 55-Atom PtCo Nanoalloys — •Diego Guedes-Sobrinho[1], Anderson S. Chaves[2], Rafael L. H. Freire[1], and Juarez L. F. Da Silva[1] — [1]University of São Paulo, São Carlos, Brazil — [2]University of Campinas, Campinas, SP, Brazil

The understanding of composition dependent properties of PtCo nanoalloys is crucial for several potential applications, such as catalytic and anti-corrosive capacities. However, our current comprehension of these systems in an atomistic level is far from satisfactory. In this work, we report a density functional theory investigation of the structural, energetic, and electronic properties of PtCo 55-atoms nanoalloys by using $Pt_nCo_{(55-n)}$ (n = 0, 6, 13, 20, 28, 35, 42, 49, and 55) models, in which the CO ligands saturation properties were investigated including van der Waals (vdW) corrections.[A. Tkatchenko *et al.*, JCP **138**, 074106 (2013)] We found that in gas-phase the maximum stability was obtained for icosahedron (ICO-like) structures at all the compositions with both transition metals.[D. Guedes-Sobrinho *et al.* **119** (27), 15669 (2015)] The adsorption of CO ligands on the nanoalloys surface affect drastically the alloy stability, which decrease for high amounts of Pt, in which the effective charge distribution in the CO molecules correlates directly with the nanoalloys composition. The most of compositions remain ICO-like, except for perfect core−shell when the vdW correction are not added, in which the CO ligands pull out all the inner Co atoms, by yielding a disordered structure.

O 61.4 Tue 18:30 P2-OG2

Hydrogenation reactions on Pd nanoparticles studied under UHV conditions — •Marian Rötzer, Maximilian Krause, Florian Schweinberger, and Ueli Heiz — Technische Universität München, Lehrstuhl für Physikalische Chemie, München

Hydrogenation reactions of unsaturated hydrocarbons are of major importance for chemical industry. Therefore we investigated the hydrogenation of ethylene and acetylene on supported palladium nanoparticles consisting of 20-40 atoms under ultra-high vacuum conditions (UHV). In order to evaluate the influence of support material on the nanoparticles, two different amorphous silica films are synthesized either on a Mo(211) or a Pt(111) single crystal. The presence of different types of hydrogen species on the particles and how they can be effectively tuned by the support material are tested by temperature-programmed desorption (TPD). A pulsed molecular beam technique is used to study the hydrogenation of ethylene and acetylene under isothermal conditions. A special focus is put on the available reaction pathways for these two reactions on both support systems. Important differences are discussed and how they can be tuned by proper choice of support material based on a mechanistic level.

O 61.5 Tue 18:30 P2-OG2

Ethylene hydrogenation on supported Ni, Pd and Pt nanoparticles: Catalyst activity, deactivation and the d-band model — Andrew S. Crampton[1], Marian D. Rötzer[1], •Maximilian Krause[1], Florian F. Schweinberger[1], Bokwon Yoon[2], Uzi Landman[2], and Ueli Heiz[1] — [1]Technische Universität München, Lehrstuhl für Physikalische Chemie, Zentralinstitut für Katalyseforschung und Fakultät für Chemie, Lichtenbergstr. 4, 85748 Garching, Germany — [2]School of Physics, Georgia Institute of Technology, Atlanta, GA 30332-0430, USA

Ethylene was hydrogenated over cluster-ensembles with narrow size distributions. Ni, Pd and Pt particles (1-1.5 nm) were softlanded on an MgO(100)-thin film on Mo(100) (X_n/MgO(100)/Mo(100); X=Ni, Pd, Pt). The pulsed molecular beam reactive scattering (p-MBRS) technique was employed at 300 and 400 K to test the catalytic activity and deactivation of the particles.

While Pt particles showed the highest hydrogenation activity, they were also the most stable particles upon heating to 400 K. A trend within the group of the periodic table was found: Pd particles were less stable and active than Pt, Ni particles the least.

ϵ_c, the position of the d-band centroid taken from density functional theory calculations, correlates with the trend in activity and stability: for Pt ϵ_c lies the farthest away from the Fermi edge, for Ni the nearest.

For further characterization the particles were adsorbed with CO before and after reaction and examined with infrared reflection absorption spectroscopy.

O 61.6 Tue 18:30 P2-OG2

Size dependence of supported Rh nanoclusters in the decomposition of methanol — •Ting-Chieh Hung[1], Ting-Wei Liao[1], Zhen-He Liao[1], Po-Wei Hsu[1], Pei-Yang Cai[1], Hsuan Lee[1], Yu-Ling Lai[2], Yao-Jane Hsu[2], Hui-Yu Chen[3], Jeng-Han Wang[3], and Meng-Fan Luo[1] — [1]Department of Physics, National Central University, Taiwan — [2]National Synchrotron Radiation Research Center, Taiwan — [3]Department of Chemistry, National Taiwan Normal University, Taiwan

Catalyzed methanol decomposition has been extensively studied as a principal reaction in direct methanol fuel cells. The process provides not only an efficient transformation from chemical energy to electricity but also a convenient source of hydrogen. To shed light on the reaction, we perform experiments on a realistic model system, oxide-supported Rh nanoclusters. We present the study of adsorption and decomposition of methanol on Rh clusters grown on an ordered thin film of θ-Al_2O_3/NiAl(100) by combining infrared absorption spectroscopy (IRAS), temperature programmed desorption (TPD) and synchrotron-based photoemission spectroscopy (PES). The investigation shows that methanol adsorbs at 100 K and the formation of CO begins at about 200 K. The quantities of CO and H_2 (D_2) produced per Rh surface site remain unaltered on clusters of diameter $>$1.5 nm and height $>$0.6 nm. In contrast, on clusters with diameter $<$1.5 nm and height $<$0.6 nm, the production per Rh surface site increases with decreasing size.

In this presentation, we will discuss the size dependence of oxide supported Rh clusters in the decomposition of methanol.

O 61.7 Tue 18:30 P2-OG2

CO-Adsorption on Pt/h-BN nanocluster arrays — Fabian Düll, Florian Späth, Johann Steinhauer, Philipp Bachmann, Udo Bauer, Hans-Peter Steinrück, and •Christian Papp — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen

Nanocluster arrays supported on two-dimensional templates are intriguing systems for the investigation of catalytic processes. We report on the reactivity of Pt nanoparticles deposited on h-BN/Rh(111). In our model study we employ high-resolution XPS to investigate the interaction of such nanoclusters with CO. Three CO-induced species are observed in the C 1s core level spectra. These are assigned to CO adsorbed in on-top and bridge terrace sites and step sites in comparison with single crystal data. The step sites are occupied first during adsorption and show the highest desorption temperature, indicating that these are the most stable adsorption sites for CO. Also a temperature induced site change of CO from terrace to step sites is observed. The first adsorption/desorption cycle differs from later cycles, due to sintering. This behavior is explained by a change of the shape of the nanoparticles during the first adsorption/desorption cycle. Furthermore, we will discuss similarities and differences to platinum nanoclusters supported on graphene.

O 61.8 Tue 18:30 P2-OG2

Surface assisted synthesis of a porphyrin fragment on Cu(111) and its FM-AFM characterization — •Felix Bischoff, Jacob Ducke, Alexander Riss, Johannes V. Barth, and Willi Auwärter — Physik-Department E20, TUM, James-Franck-Str. 1, 85748 Garching

In-vacuo heterogeneous nano-chemistry bares the potential for creating compounds not achievable with other approaches due to the reactivity of intermediate or final products. For example, the thermal instability of porphyrin fragments such as oligopyrroles often renders them inapplicable for standard UHV preparation techniques. Therefore di- or tripyrrins and related species are scarce in vacuum based surface science and these classes of molecules remain nearly unstudied despite their promising properties as metal-complexing agents in functional organo-metallic compounds or as fluorescent sensors. In this combined low-temperature scanning tunneling microscopy (LT-STM) and frequency modulated atomic force microscopy (FM-AFM) study we will demonstrate the formation of a hitherto unreported porphyrin fragment synthesized through pyrrole cleaving from free-base tetraphenylporphyrins (2H-TPP) on Cu(111). The novel copper metalated tripyrrin derivative is structurally characterized by visualizing its chemical structure via FM-AFM with CO-functionalized tips and via tip manipulations. We will furthermore suggest a possible reaction pathway by identifying reaction intermediates. Additionally, the products of the thermally activated flattening reaction of 2H-TPP on Cu(111) will be structurally determined by FM-AFM.

O 62: Surface Dynamics

Time: Tuesday 18:30–20:30 Location: P2-OG2

O 62.1 Tue 18:30 P2-OG2

Photon-induced desorption from interstellar ices using XUV free-electron laser pulses — •John Thrower, Tushar Suhasaria, Robert Frigge, Sebastian Roling, and Helmut Zacharias — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany

Solid state processes occurring on grain surfaces play an important role in the chemistry of the interstellar medium. In dense molecular clouds, the low temperature (ca. 10 K) grains are coated with a layer of H_2O dominated ice doped with additional species such as CO, CO_2, CH_4 and NH_3. In photon-dominated regions, as well as in accretion disks, these ices are bathed in a flux of UV photons which can lead to the formation of more complex species as well as promoting desorption.

We have used the XUV pulses (40.8 eV) from the FLASH facility to promote photon-induced desorption from such ice films, namely CO and D_2O:CH_4, adsorbed at 18 K on a graphite substrate. Desorbing CO molecules were state-selectively detected, revealing that desorbing neutral CO molecules display a relatively low degree of rotational excitation (T_{rot} = 160 K) but are vibrationally hot ($T_{vib} \sim 1500$ K), suggesting desorption via a CO^- intermediate.

Irradiation of D_2O:CH_4 ice resulted in the desorption of simple ionic fragments from the deposited species, methane recombination products up to $C_3H_x^+$, and carbon clusters, C_n, up to n=11. The latter display a highly non-linear (m=5) dependence on the incident laser intensity, permitting investigation of the underlying ultrafast dynamics using two-pulse time-correlated desorption.

O 62.2 Tue 18:30 P2-OG2

Energy dissipation at metal surfaces: The surprisingly high non-adiabaticity of Na diffusion on Cu(111) — •Simon P. Rittmeyer and Karsten Reuter — Technische Universität München

The role of electron-hole pair excitations during dynamical surface processes on metal substrates has been controversially discussed. With high-level non-adiabatic calculations still intractable for extended metal surfaces, the concept of electronic friction within the local density friction approximation (LDFA) offers approximate, but numerically highly efficient insight.

We have recently shown this approach to yield reasonable results for the vibrational damping of high-frequency adsorbate vibrations on various metal surfaces [1]. With this confidence we now apply it to thermal surface diffusion, where non-adiabatic energy losses are expected to clearly compete with energy losses due to phononic coupling. In order to quantitatively disentangle these dissipation channels, we compare LDFA-based Langevin molecular dynamics simulations for Na on Cu(111) to experimental signatures obtained from state-of-the-art ^{3}He spin echo measurements [2]. Despite the minimal electronic friction coefficient of Na and the relatively small mass mismatch to Cu promoting efficient phononic dissipation, we find that a surprisingly high amount of about 20% of the total energy loss is attributable to electronic friction.

[1] S.P. Rittmeyer *et al.*, Phys. Rev. Lett. **115**, 046102 (2015).
[2] S.P. Rittmeyer *et al.*, Phys. Rev. Lett. **117**, 196001 (2016).

O 62.3 Tue 18:30 P2-OG2

A test experiment to determine the long term behaviour of work function and quantum efficiency of gold surfaces — •Kerstin Schönung and KATRIN Collaboration — Max-Planck-Institut für Kernphysik, Postfach 10 39 80, 69029 Heidelberg

The KArlsruhe TRItium Neutrino experiment KATRIN will perform a model-independent measurement of the effective neutrino mass by examining the β-electron energy spectrum of a gaseous molecular tritium source (WGTS). To achieve the desired sensitivity of $0.2\,\mathrm{eV/c^2}$ (90 % C.L.) the plasma potential of the tritium gas must be temporally and spatially stable within 20 meV. In order to achieve this stringent stability requirement the work function of the so called Rear Wall, which terminates the tritium volume at its rear end and defines the plasma potential therein, must be known even more precisely. The temporal fluctuations must be investigated. In addition to the work function fluctuations, the charge of the plasma in the tritium source could increase over time by the remaining positive ions produced by the tritium decays. In order to prevent this charging and the subsequent inhomogeneity of the plasma potential, the gold surface of the Rear Wall will be used to emanate electrons by the photoelectric effect. For a proper design of the required light source the quantum efficiency of the Rear Wall surface and its stability has to be determined.

A new experiment which investigates both, the in-situ work function and the quantum efficiency of the Rear Wall surface, is currently built up at KIT. In addition to the setup, first results will be presented. We acknowledge the support of the BMBF (05A14VK2).

O 62.4 Tue 18:30 P2-OG2

Charge density wave domain growth in 1T-TaS2 mapped by ultrafast LEED — •Theo Diekmann[1], Simon Vogelgesang[1], Gero Storeck[1], Sebastian Schramm[1], Max Gulde[1], Gerrit Horstmann[1], Kai Rossnagel[2], Sascha Schäfer[1], and Claus Ropers[1] — [1]IV. Physical Institute - Solids and Nanostructures, University of Göttingen, Germany — [2]Institute for Experimental and Applied Physics, University of Kiel, Germany

We developed an ultrafast low-energy electron diffraction (ULEED) setup for the study of time-resolved structural dynamics at surfaces, extending our previous ULEED-experiments operating on ultrathin films in transmission [1]. To this end, a nanoscopic needle emitter is utilized in a miniaturized electrostatic lens geometry as a high-brightness source providing well-collimated electron pulses with a minimal duration of 16 picoseconds at the sample and electron energies in the range of 50-200 eV.

In a first application of this setup, we study the structural phase transition from the room-temperature nearly commensurate (NC) to the incommensurate (IC) charge density wave phase at the surface of 1T-TaS2 [2]. Following intense optical excitation, we observe the formation and consecutive growth of IC domains by a thorough analysis of time-dependent diffraction spot profiles. Our results demonstrate the potential of ULEED for the study of complex ultrafast structural and electronic processes at surfaces.

[1] M. Gulde et al., Science 345, 200 (2014)
[2] K. Haupt et al., Phys. Rev. Lett. 116, 016402 (2016)

O 63: Focus Session: Charge Transport at Surfaces and Nanostructures with Multi-probe Techniques

Time: Tuesday 18:30–20:30 Location: P2-OG3

O 63.1 Tue 18:30 P2-OG3

Multiprobe measurements on a stepped Bi_2Se_3 surface — •Sebastian Bauer, Mandana Soleimani-Esfahani, Stephanie Hoepken, and Christian A. Bobisch — Faculty of Physics, Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstraße 1-21, 47057 Duisburg

Bi_2Se_3 is a well-known representative of the new material class of 3D topological insulators (TI). TIs have a spinpolarized surface state for which direct backscattering of electrons is forbidden. Therefore, they are discussed for future spintronic devices [1]. We present a detailed multiprobe analysis of a 15 QL thick stepped Bi_2Se_3 film which was grown in situ on an inclined Si(111) surface. Scanning tunneling potentiometry [2] gives us a direct view into the nanoscale electron transport on the Bi_2Se_3 surface. While a lateral current flows along the surface, an STM tip records simultaneously the local electrochemical potential and the topography on the Bi_2Se_3 surface. We found that beside surface steps [3], also grain boundaries scatter the conducting electrons in the film. An additional rotational four point probe measurement shows an electronic anisotropy of the sheet conductivity due to the anisotropic arrangement of the Bi_2Se_3 steps on the surface. The computed step conductivity of about 1000 S/cm confirms former STP results [4] and reveals the contribution of step edges as electron scatterer.

[1] M. Z. Hasan, C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010). [2] C. A. Bobisch and R. Möller, CHIMIA 66, 23-30 (2012). [3] S. Bauer, C. A. Bobisch, Nat. Com. 7, 11381 (2016). [4] T. Kanagawa et al., Phys. Rev. Lett. 91, 036805 (2003).

O 63.2 Tue 18:30 P2-OG3

Molecular manipulation of acetylbiphenyl with a four-probe-STM — •Frank Eisenhut[1], Corentin Durand[2], Francesca Moresco[1], Jean Pierre Launay[2], and Christian Joachim[2,3] — [1]Institute for Materials Science, Max Bergmann Center of Biomaterials, and Center for Advancing Electronics Dresden, TU Dresden, Dresden, Germany — [2]GNS & MANA Satellite, CEMES, CNRS, Toulouse, France — [3]International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Namiki Tsukuba, Ibaraki, Japan

A low temperature ultrahigh vacuum four-probe scanning tunneling microscope has been used to study acetylbiphenyl (ABP) molecules on Au(111). Supramolecular assemblies of ABP interacting via hydrogen bonds were investigated and the tetrameric structure were controllably moved several nanometers by voltage pulses along the fcc domain of the Au(111) herringbone reconstruction. Meanwhile, scanning with another tip was possible without influencing the manipulation. The investigation is an important step towards the preparation of the first international nano-car race [1].

[1] F. Eisenhut et. al., Training for the 1st international nano-car race: the Dresden molecule-vehicle. Eur. Phys. J. Appl. Phys. (2016) 76: 10001.

O 63.3 Tue 18:30 P2-OG3

Polycyclic aromatic hydrocarbon-based nanocars equiped with triptycene wheels — Henri-Pierre Jacquot de Rouville[1,2,4], Claire Kammerer[1,2], Corentin Durand[1,2], •Christian Joachim[1,2,3], and Gwénaël Rapenne[1,2] — [1]Université Paul Sabatier, Toulouse, France — [2]GNS, CEMES-CNRS, Toulouse, France — [3]International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Namiki Tsukuba, Ibaraki, Japan — [4]Present adress : ITODYS-CNRS, Université Paris Diderot, Paris, France

Technomimetic molecules[1] are molecules designed to imitate macroscopic objects at the molecular level, also transposing the motions that these objects are able to undergo. We designed and synthesized two nanocars including triptycene wheels in an extended aromatic platform as a cargo zone[3].

However, the manipulation of the planar one on metallic surfaces proved to be difficult due to a strong molecule-surface interaction, the curved nanocar adress this problem by decreasing the interaction between the aromatic system and the surface. STM experiments are currently underway to test the molecule before the nanocar race organized next spring in Toulouse, France.

[1] G. Rapenne, Org. Biomol. Chem. 2005, 3, 1165. [2] (a) H.P. Jacquot de Rouville, R. Garbage, R.E. Cook, A.R. Pujol, A.M. Sirven, G. Rapenne, Chem. Eur. J. 2012, 18, 3023; (b) C. Joachim, G. Rapenne, ACS Nano, 2013, 7, 11.

O 63.4 Tue 18:30 P2-OG3

Disentangling *in situ* top and bottom conductance of a topological insulator thin film — •Felix Lüpke, Markus Eschbach, Tristan Heider, Martin Lanius, Peter Schüffelgen, Daniel Rosenbach, Nils von den Driesch, Vasily Cherepanov, Gregor Mussler, Lukasz Plucinski, Detlev Grützmacher, Claus M. Schneider, and Bert Voigtländer — Peter Grünberg Institute and JARA-FIT, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Charge transport in thin films of 3D topological insulator materials can be through the top and the bottom topological surface state as well as through the interior of the film. The latter undesirable conductivity can be minimized by the use of thin films (10 nm) and the use of MBE grown ternary material systems with reduced bulk conductivity. However, it is still difficult to separate the contributions of the three channels to the conduction. Using a multi-tip STM we performed *in situ* gate-dependent four-probe conductivity measurements of $(Bi_{0.53}Sb_{0.47})_2Te_3$ thin films. Combining the information from these measurements with the band structure obtained from subsequent ARPES measurements, we determine the carrier densities as well as the mobilities in the top and bottom topological surface state channels.

O 63.5 Tue 18:30 P2-OG3

Quasi-free-standing bilayer graphene nanoribbons probed by electronic transport — •Johannes Aprojanz[1], Ilio Miccoli[1], Jens Baringhaus[1], Timo Lichtenstein[1], Lauren A. Galves[2], Joao Marcelo J. Lopes[2], and Christoph Tegenkamp[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Graphene nanoribbons (GNR), directly grown on insulating SiC-templates, have attracted much intention due to their unique electronic properties. The growth of armchair and zig-zag orientated GNR with tunable band gaps and topologically protected metallic edge states was recently demonstrated [1,2]. Here, we present a detailed study of the structural and electronic transport properties of novel oxygen-intercalated bilayer graphene nanoribbons grown along step edges of SiC(0001) substrates [3]. The local transport properties as well as the microscopic structure have been investigated using a 4-tip STM/SEM system. Probe spacing dependent measurements combined with spectroscopic analyses reveal a hole concentration of $1 \times 10^{13}\mathrm{cm}^{-2}$ and mobilities up to 700 cm^2/Vs of as-grown GNR at room temperature, which we attribute to an interlayer charge hopping mechanism.

[1] Baringhaus et al., Nature **506**, 349 (2014)
[2] Palacio et al., Nano Letters **15**, 182 (2015)
[3] Oliveira et al., Nat. Comm. **6**, 7632 (2015)

O 63.6 Tue 18:30 P2-OG3

Electronic Transport Measurements of 2-Dimensional Systems with a 4-Probe STM — •Tim Flatten[1], Sven Borghardt[2], Frank Matthes[1], Beata Kardynal[2], Daniel E. Bürgler[1], and Claus M. Schneider[1] — [1]Peter Grünberg Institut, Electronic Properties (PGI-6), Forschungszentrum Jülich — [2]Peter Grünberg Institut, Semiconductor Nanoelectronics (PGI-9), Forschungszentrum Jülich

The recent emergence of 2-dimensional materials such as the transition metal dichalcogenides (TMD) requires new measurement techniques for exploring their physical properties. TMDs are interesting due to their large variety of electric properties ranging from insulating and semiconducting with direct or indirect band gap to metallic behavior depending on their composition and thickness. We employ a 4-probe scanning tunneling microscope (4-probe STM) operating in ultra-high vacuum (UHV) and at temperatures down to 5 K to combine STM with lateral 4-probe transport measurements. A top-mounted scanning electron microscope (SEM) enables positioning of the 4 independently driven STM tips on a sub-micrometer scale. We investigate the influence of ex-situ sample preparation and in-situ treatment on the surface morphology and cleanness by STM imaging and measure their effect on the electronic transport properties of single TMD flakes. In first steps, we perform scanning tunneling spectroscopy (STS) on single monolayer $MoSe_2$ flakes adsorbed on various insulating substrates to measure the dependence of their electronic band gap on the substrate properties.

O 63.7 Tue 18:30 P2-OG3

Imaging the local voltage landscape of a Bi_2Te_3 surface — •Mandana Soleimani Esfahani, Stephanie Hoepken, Sebastian Bauer, and Christian A. Bobisch — Faculty of Physics, Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstraße 1-21, 47057 Duisburg, Germany.

Bi_2Te_3 is a prominent prototype system for the new material class of topological insulators (TI) [1]. Compared to other TI materials like Bi_2Se_3 the bulk conductivity in Bi_2Te_3 is lower and the electron transport through the surface state should be enhanced. For Bi_2Se_3 we have already shown that surface defects like step edges and grain boundaries have an impact on the local transport field [2]. Now, we study the local electron transport on a Bi_2Te_3 surface by scanning tunneling potentiometry (STP, [3]). During the STP measurement a lateral current flows along the Bi_2Te_3 surface, resulting in a lateral variation of the electrochemical potential. The latter is probed by a STM tip simultaneously mapping the potential as well as the topography of the Bi_2Te_3 surface with nanometer lateral resolution. This allows for a detailed study of the electron transport field on the surface of Bi_2Te_3 on the atomic scale.

[1] M. Z. Hasan, C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
[2] S. Bauer, C. A. Bobisch, Nat. Com. 7, 11381 (2016).
[3] C. A. Bobisch and R. Möller, CHIMIA 66, 23-30 (2012).

O 63.8 Tue 18:30 P2-OG3

A six-tip AFM - SEM combination for semiconductor chip failure analysis — •Stefan Korte, Vasily Cherepanov, Richard Spiegelberg, Peter Coenen, and Bert Voigtländer — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

The structure size of modern semiconductor electronics is shrinking to dimensions where the electrical failure analysis of single components like transistors on a chip is hard to conduct. We developed a six-tip AFM combined with an SEM to contact single transistors on a chip with multiple tips. Its compact size reduces probe drifts to below 0.1 nm/min. This is necessary to create contacts stable enough for electrical measurements even on state-of-the-art semiconductor chips. Fast AFM scanning with FM-AFM using needle sensors and home-built fast PLL detection electronics is used to position the tips exactly on the contacts. In first trials we contacted single transistors of an SRAM cell on a chip built with 65 nm structure size for electrical characterization.

O 63.9 Tue 18:30 P2-OG3

Manipulation of tolyl-terpy molecules along the Au(111) reconstruction — •Rémy Pawlak[1], Tobias Meier[1], Marcin Kisiel[1], Antoine Hinaut[1], Thilo Glatzel[1], Catherine Housecroft[2], and Ernst Meyer[1] — [1]University of Basel, Department of Physics, Klingelbergstr. 82, CH-4056, Basel, Switzerland — [2]University of Basel, Department of Chemistry, Spitalstrasse 51, CH-4056, Basel, Switzerland

In spring 2017, the first international ”NanoCar Race” will be held in Toulouse (France) in a unique low-temperature ultra high vacuum four-probe scanning tunneling microscope. During the competition, the participants will have to simultaneously drive their vehicles over 100 nm along the Au(111) herringbone structure, only using electron injections from one of the STM tips. Here, we report on the adsorption characteristics and first driving experiences of the 4’-(4-Tolyl)-2,2’:6’,2”-terpyridine, so-called Swiss Nano Dragster on gold [1]. We show that our molecule is translated in a controlled way and high directionality through appropriate electrical excitation. We also find that peculiarities of the gold reconstruction can irremediably trap the molecules and reached a maximum speed of about 20 nm/hour.

[1] R. Pawlak, T Meier et al. Driving experiences on the gold racetrack with the Swiss Nano-Dragster. In preparation.

O 63.10 Tue 18:30 P2-OG3

Scanning tunneling potentiometry using a triangular geometry of the electric contacts — •Hüseyin Azazoglu, Sebastian Bauer, Rolf Möller, and Christian A. Bobisch — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Scanning tunneling potentiometry (STP) [1] is used to study the microscopic resistivity in an electric conductor. The direction of the electric current is varied on the nanometer scale by applying three point contacts in an equilateral triangle using different relative voltages at the tips. Thereby, we can rotate the global current direction by any angle up to 360° during the STP measurements. The Si(111)-$\sqrt{3}\times\sqrt{3}$:Ag surface reconstruction [2] was studied. We find that the measured local potential varies as a function of the global current direction. This demonstrates the ability to manipulate the electric transport on the nanoscale with the help of the three-point-geometry, e.g., this technique can be used to study scattering at an individual defect as a function of the angle of incidence.

[1] P. Muralt et. al., Appl. Phys. Lett. 48, p. 514, (1986). [2] J. Homoth et al, Nano Letters 9,1589, (2009).

O 63.11 Tue 18:30 P2-OG3

Transport on Si(553)-Au and Si(557)-Au atomic chains: The effect of oxygen adsorption — Frederik Edler[1], Ilio Miccoli[1], •Jan P. Stöckmann[1], Herbert Pfnür[1], Christian Braun[2], Simone Sanna[2], Wolf G. Schmidt[2], and Christoph Tegenkamp[1] — [1]Universität Hannover, 30167 Hannover — [2]Universität Paderborn, 33098 Paderborn

Atomic chain ensembles grown by self-assembly are prototype 1D systems with partly outstanding electronic properties such as Peierls instabilities or dimensional crossover from Fermi to Luttinger liquid behavior. Recently [1], the Au-induced atomic chain structures on Si(hhk) attracted a lot of attention. The strong spin-orbit coupling gives rise to spin polarized surface bands and in case of Si(553)-Au even quantum spin liquid behavior. However, such properties can strongly be altered by imperfections, e.g. defects induced by adsorbates. In this contribution, we present a systematic study of the transport properties of Si(553)-Au and Si(557)-Au system by means of a 4-tip STM system in combination with SPALEED tuned by adsorption of molecular oxygen. Our DFT calculations show that the origin of metallic surface bands along the wires of similar Si(hhk)-Au surfaces are strongly dependent on the structure of Au chains, Si-adatom chains and Si edges. Here we see an inert behavior for the Si(553)-Au surface while a strong decrease in the conduction along the chains is present for the Si(557)-Au.

[1] B. Hafke et al., Phys. Rev. B **94** (2016) p. 161403

O 63.12 Tue 18:30 P2-OG3

Metal-to-insulator transition in a quantum spin system — •Ilio Miccoli[1], Frederik Edler[1], Jan P. Stöckmann[1], Bernd Hafke[3], Michael Horn-von Hoegen[3], Herbert Pfnür[1,2], and Christoph Tegenkamp[1,2] — [1]Institut für Festkörperphysik, Hannover Uni., 30167-DE — [2]Laboratory of Nano Quantum Engineering, Hannover, 30167-DE — [3]CENIDE, Duisburg-Essen Uni., 47048-DE

Atomic wires on surfaces are prototype 1D systems for studying fundamental aspects, e.g. charge density waves (CDW) or dimensional crossover from a Fermi to a Luttinger liquid behavior. Among others, Au-induced wire structures on Si(553) substrates revealed a lot of attention because of their quasi-1D metallic structures with a pronounced magnetic order, which mimics a 2D quantum spin liquid state.[1] By means of low energy electron diffraction (LEED) and 4-tip STM, we investigated the surface structure and transport properties of Si(553)-Au as a function of temperature. LEED revealed an isotropic order-disorder transition at 90 K, i.e. both the ×3 periodicity along and the magnetic ordering in between the wires vanishes simultaneously. In transport the system undergoes a metal-insulator transition (MIT). Thereby, while heating the resistance across the wires decreases sharply at 90K by 2-3 order of magnitude. Interestingly, we found also a MIT along the wires, which occurs at the same temperature. This combined study gives direct evidence also for a CDW formation along the wires. Moreover, the magnetic ordering stemming from localized electrons fed back to the 1D electronic states at Fermi energy.

[1] B. Hafke et al., Phys. Rev. B **94** (2016) p. 161403

O 63.13 Tue 18:30 P2-OG3

A frame suspended into four Cucurbituril wheels: meet the Ohio Bobcat Nanowagon — •Eric Masson[1] and Saw Wai Hla[1,2] — [1]Dept of Chemistry and Biochemistry and Dept of Physics and Astronomy, Ohio University, Athens, OH 45701, USA — [2]Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439 USA

We present the design, synthesis and characterization of the Ohio Bobcat Nanowagon, a [5]pseudorotaxane assembly bearing an H-shaped frame threaded into four Cucurbit[7]uril (CB[7]) wheels. The key motifs in the frame are two benzimidazolium groups, which link a terphenyl drive shaft (the horizontal bar of the ”H” frame) to the axle shafts (the vertical bars of the ”H” frame). Four pyridinium units terminate the latter. Positive charges at the pyridinium and benzimidazolium units allow the frame and the CB[7] wheels to assemble into the final nanowagon in water. The white solid obtained upon freeze-drying was used for STM analysis.

O 63.14 Tue 18:30 P2-OG3

Conformation manipulation of binaphthyl-dimer with a low temperature STM — •We-Hyo Soe[1], Marek Kolmer[2], Xavier Bouju[1], Yasuhiro Shirai[3], Kosuke Minami[3], Katsuhiko Ariga[3], and Waka Nakanishi[3] — [1]GNS & MANA Satellite, CEMES, CNRS, Toulouse, France — [2]Centre for Nanometer-Scale Science and Advanced Materials (NANOSAM), Jagiellonian University, Krakow, Poland — [3]International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan

One of the low temperature ultrahigh vacuum scanning tunneling microscope (STM) of the LT-UHV 4-STM has been used to study binaphthyl-dimer molecules on Au(111) [1],[2]. The molecule has three C2 symmetry conformations energetically possible, namely, cis, trans, and planar-like conformations. Right after the molecules deposition on a clean gold surface, only cis conformation molecules forming small 2D islands have been observed. Using a STM tip single molecule mechanical manipulation protocol, single planar conformation molecules have been produced one by one corresponding to our registered nanocar. This confirms that on an Au(111) surface, single and isolated binaphthyl-dimer molecules equipped with 2 paddles are ready to compete for the first international nano-car race in Toulouse, spring 2017.

[1] Y. Shirai, K. Minami, W. Nakanishi, Y. Yonamine, C. Joachim and K. Ariga, Jap. Journ. Appl. Phys., 55 (2016) 1102A2. [2] S. Fujiyoshi, S. Takeuchi, T. Tahara, J. Phys. Chem. A, 108 (2004) 5938.

O 63.15 Tue 18:30 P2-OG3

Koala TetraProbe Multi-Tip STM - Charge Transport Measured at the Nanoscale by a Multi-Tip STM — •Bert Voigtländer, Vasily Cherepanov, and Peter Coenen — mProbes GmbH Jülich, Germany

The ultra-compact Koala TetraProbe STM integrates four independent STM units within a diameter of 50 mm resulting in an unsurpassed mechanical stability, enabling atomic resolution imaging with each tip [1,2]. Each tip and the sample can be positioned independently under control of an optical microscope or an SEM. Software controlled switching between current probe and voltage probe for each tip allows virtually any possible ”concerted” spectroscopic measurements involving the four tips and the sample. A four tip STM/AFM combination and a low temperature version are available. Applications include: Local potential measurements on the nanoscale [3], controlled nondestructive measurements in spectroscopy mode, four point measurements with free positionable local probes on structured samples [4], and measurements of the surface conductivity [5].

[1] www.mprobes.com; [2] V. Cherepanov, E. Zubkov, H. Junker, S. Korte, M. Blab, P. Coenen, B. Voigtländer, Rev. Sci. Instrum. 83 (2012) 033707; [3] F. Lüpke, S. Korte, V. Cherepanov, B. Voigtländer, Rev. Sci. Instrum. 86 (2015) 123701; [4] S. Korte, M. Steidl, W. Prost, V. Cherepanov, B. Voigtländer, W. Zhao, P. Kleinschmidt, .T. Hannappel, Appl. Phys. Lett. 103 (2013) 143104; [5] S. Just, M. Blab, S. Korte, V. Cherepanov, H. Soltner, B. Voigtländer, Phys. Rev. Lett. 115 (2015) 066801.

O 63.16 Tue 18:30 P2-OG3

Recent technology advancements in SPM based electrical probing at low temperatures — •Markus Maier, J Köbele, R Thiel, A. Priou, D. Stahl, M. Fenner, and T. Roth — Scienta Omicron GmbH, Limburger Straße 75, 65232 Taunusstein, Germany

A major challenge in the development of novel devices in nano- and molecular electronics is their interconnection with larger scaled electrical circuits. Local electrical transport measurements by multiple atomic scale precision probes can significantly improve the analysis of individual nano-scaled structures without the need of a full electrical integration. The LT NANOPROBE is a sophisticated instrument that merges the requirements of a 4-probe system, efficiently and precisely navigated by a scanning electron microscope (SEM) and at the same time satisfies the needs for high performance SPM. The excellent stability in the pm range allows for atomic resolution in STM and nc-AFM (QPlus) and expands applications from electrical nano-probing towards tunnelling and force spectroscopy and even the creation of atomically precise structures. The system is operated at temperatures below 5K, specifically also during SEM operation. The microscope stage works at very low thermal drift in the range of 100pm/h. We will present measurements that prove the instrument's performance level, specifically thermal drift, stability and QPlus AFM measurements. We will also show the newest technology improvements, such as high frequency capabilities and optical access for pumped probe experiment. Future challenges as well as applications and scientific drivers for this type of scientific instrumentation will be discussed.

O 63.17 Tue 18:30 P2-OG3

4-Point Nano Probing: Comparison of Single-Chip 4-Point Micro Probes as exposed to Multi Probe STM Heads — •T. Berghaus[1], T. Richter[1], and Y. Miyatake[2] — [1]nanoscore gmbh, Maisebachstr. 3, 61479 Glashütten, Germany — [2]UNISOKU Co. Ltd., 2-4-3 Kasugano Hirakata, OSAKA 573-0131, Japan

STM-based nano probing has become of increasing interest as tool for characterising the properties of layered tructures, 2D materials like graphene, one-dimensional conductors, as well as for the investigation of topological insulators. Two fundamentally different instrumental implementations have evolved:(i) 2-Probe or 4-probe STMs using conventional macro-fabricated STM tips and having independent positioning, scan, and imaging means for each of the tips as proposed by Aono et al.[1]. (ii) STMs with single channel means for positioning, scan, and imaging, but using micro fabricated multi-tip chips - such as micro 4-point probe chips (micro 4PP)[2]. Here we compare the two approaches. The multi STM approach appears to be more flexible because of the independent tip positioning. On the other hand it is more expensive and difficult to control. Whereas the micro 4-PP approach offers many more possibilities for integration into demanding environments such as ultra low temperature or high magnetic fields as recently presented by Jian-Feng Ge et al. [3]. Further throughput and reproducibility can be enhanced by using commercially available micro-4PP chips [4].

[1] M.Aono et al.Oyo Buturi 67, 1361 (1998) [2] S. Hasegawa et al.Surf. Sci. 500, 84 (2002) [3] Jian-Feng Ge et al. Rev. Sci. Inst. 86, 053903 (2015). [4] Capres A/S, DK-2800 Kgs. Lyngby

O 64: Scanning Probe Techniques: Method development

Time: Tuesday 18:30–20:30 Location: P2-OG3

O 64.1 Tue 18:30 P2-OG3

A convenient method for large scale STM mapping of freestanding atomically thin membranes — •Bernd Uder and Uwe Hartmann — Institute of Experimental Physics, Saarland University, Germany

Two-dimensional sheets atomically flat and with high flexibility are very attractive to be used as ultrathin membranes but inherently challenging for microscopic investigations. We report a method using Scanning Tunnelling Microscopy (STM) under ultrahigh vacuum conditions for large scale mapping of graphene membranes. This is achieved by operating the STM with unusual parameters. We found that large scale scanning on atomically thin graphene membranes delivers viable results using very high tip scan speeds combined with high feedback loop and low tunnelling current settings. This is successful due to a different behaviour of the freestanding membrane in STM compared to a solid substrate. The contrast on a thin membrane is ruled by tip membrane force interactions and the interplay with the integral distance regulator working at high gain. For low tunnelling currents the force interaction is tunable by changing the bias between tip and sample. We applied our method to map differences of membrane quality of commercial available single layer graphene covering 2 micrometer sized holes and multi-layered graphene covering a TEM 2000 mesh.

O 64.2 Tue 18:30 P2-OG3

Electromechanical contact resonance in band excitation piezoresponse force microscopy — •Sebastian Badur, Thomas Göddenhenrich, and André Schirmeisen — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, D-35392

Contact resonance atomic force microscopy is a key analyzation method for local piezoresponse or electrochemical strain effects. A drawback of this technique are the various parasitic contributions affecting the signal contrast formation, e.g. a topographical crosstalk, an overall distributed electrostatic force or the stiffness of the mechanical tip-to-sample coupling. In order to investigate and minimize these influences we present an approach using the band excitation method around different cantilever eigenmodes combined with a switching between the electrical cantilever and mechanical sample excitation. Measurements are performed on $BaTiO_3$ under UHV conditions.

O 64.3 Tue 18:30 P2-OG3

A dilution refrigerator based UHV spin-polarized STM operating at 30 mK in a vector magnetic field — Henning von Allwörden[1], Andreas Eich[1], Jan Hermenau[2], Andreas Sonntag[2], Jan Gerritsen[1], Daniel Wegner[1], and •Alexander Ako Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Department of Physics, Hamburg University, Hamburg, Germany

Spin-resolved scanning tunnelling microscopy (STM) has advanced as a leading technique to probe the behaviour of single spins down to the level of individual atoms. Nevertheless, a severe limitation in probing spin-dependent phenomena in materials of interest, such as quantum magnets and topological superconductors, is the extremely high energy resolution needed to resolve fine features and minute variations in spectroscopy resulting from interactions. To this end, we advance spin-resolved STM toward the lowest temperatures today, by constructing a microscope that operates in a UHV-based dilution refrigerator capable of a vector magnetic field. Moreover, this new microscope is situated in the new SPIN laboratory, located at the IMM in Nijmegen, which is optimized for ultra-low noise measurements. We present the design of this laboratory, and we illustrate our first benchmark tests at base temperature, as well as the noise characteristics.

O 64.4 Tue 18:30 P2-OG3

Scanning Tunneling Microscopy with a JFET-sensor — •Stephanie Hoepken, Sebastian Bauer, Hermann Nienhaus, Christian A. Bobisch, and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

We examined a new working mode for scanning tunneling microscopy (STM). It is an STM in which a junction-field-effect-transistor (JFET) serves as a sensor for the tunnelling current. The tunnelling tip is directly connected to the gate of the JFET, which is operated in an open-gate mode with no other electric connection to the gate. The drain current provides a corresponding signal at low impedance which is used for the electronic control of the tip sample distance. The technique allows us to work at very low currents in the range of about 100 to 200 fA. First of all the JFET was characterised to evaluate its operating point. At stable operation the tunnelling current is matched by the gate leakage current. By choosing the bias voltage applied to the sample, the tunnelling conductance can be set. In the recorded STM-pictures this voltage is about -1 to -2 V. Furthermore, an essential point in operating a JFET-STM is the control of the tip sample distance. The drain current's reaction to a changing tunnelling current is low pass filtered by the gate capacity, but it was found that a sufficient scanning speed can be accomplished by optimised control parameters mainly by using the proportional part of the feedback loop. With these parameters detailed pictures of an Au(111)-sample could be recorded.

O 64.5 Tue 18:30 P2-OG3

Combined pump probe experiments with scanning tunneling microscopy — •Kira Kolpatzeck, Philip Kapitza, Ebru Ekici, Rolf Möller, and Christian A. Bobisch — Faculty of Physics, Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

We will employ two experimental strategies to analyze charge carrier dynamics and luminescence with atomic scale lateral resolution by pump-probe spectroscopy. For timescales down to 1 ns, all electronic pump-probe measurements with a scanning tunneling microscope (STM) [1] are performed. Here, our first results show, that the luminescence that stems from inelastic tunneling processes can be used to quantitative map fast voltage pulses in the tunnel junctions [2]. This is achieved by performing time correlated counting of the emitted photons during the voltage pulse. In parallel, we develop and build an experiment in which THz radiation is coupled into the tunneling junction of a new build STM to allow for pump-probe experiments in the ps range [3]. The concept of the experimental setup will be presented.

[1] S. Loth et al., Science 329, 1628 (2010).
[2] C. Grosse et al., Appl. Phys. Lett. 103, 183108 (2013).
[3] T. L. Cocker et al., Nature Photonics 7, 620 (2013).

O 64.6 Tue 18:30 P2-OG3

Comparison of the signal-to-noise ratio of the first two flexural modes for qPlus AFM sensors — •Dominik Kirpal and Franz Giessibl — Universität Regensburg

Higher flexural modes are used due to their higher eigenfrequencies and spring constants. In this work we calculated theoretically and determined experimentally the sensitivity for the first two flexural modes of qPlus sensor [1,2]. We found that the sensitivity of the second mode is about 3 times higher than of the first mode. This affects the detector, oscillator and thermal noise [3]. At low temperatures the detector noise is dominant, in ambient conditions and liquid environments thermal and oscillator noise are substantial [4]. The influences of these noise contributions are discussed depending on the experimental setup.

[1] Giessibl, Applied Physics Letters, 76, 1470 (2000).
[2] Ooe et al., arXiv preprint:1605.06584 (2016).
[3] Giessibl et al., Physical Review B, 84, 125409 (2011).
[4] Wutscher, and Franz J. Giessibl, Review of Scientific Instruments 82.9 (2011): 093703.

O 64.7 Tue 18:30 P2-OG3

Fast and Reliable Pre-Approach for Scanning Probe Microscopes based on Tip-Sample Capacitance — Marc de Voogd[1], Matthijs van Spronsen[1], Floris Kalff[2], Ben Bryant[2], Oliver Ostojic[1], Arthur den Haan[1], Irene Groot[1,3], Tjerk Oosterkamp[1], Sander Otte[2], and •Marcel Rost[1] — [1]Leiden Institute of Physics, Leiden University, P.O. Box 9504, 2300 RA Leiden, the Netherlands — [2]Department of Quantum Nanoscience, Kavli Institute of Nanoscience,Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands — [3]Leiden Institute of Chemistry, Leiden University,P.O. Box 9502, 2300 RA Leiden, the Netherlands

Within the last three decades Scanning Probe Microscopy has been developed to a powerful tool for measuring surfaces and their properties. However, despite continuous improvements, the time required for a safe approach can still be very time consuming, especially if the microscope is not equipped or suited for the observation of the tip-sample distance with an additional optical microscope. Here we show that the measurement of the tip-sample capacitance provides an ideal solution for a fast and reliable pre-approach. The tip-sample capacitance shows a generic behavior as a function of the distance, even though we measured it on several completely different setups. Insight into this behavior is gained via an analytical and computational analysis, from which two additional advantages arise: the capacitance measurement can be applied for observing, analyzing, and re-tuning of the approach motor, as well as for the determination of the (effective) tip radius.

O 64.8 Tue 18:30 P2-OG3

Tuning the functionality of a junction field effect transistor at cryogenic temperatures: new prospects and possible applications — •Meike Flebbe, Paul Graf, Christian A. Bobisch, Hermann Nienhaus, and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

By cooling a conventional junction field-effect transistor (JFET) to 80 K an electrometer with extremely high impedance can be realized. It may be used as a detector for ultimately low currents or charges, e.g. for low temperature scanning probe microscopy (SPM). The characteristics of the JFET at room temperature and in the cooled state were recorded and compared. While the gate leakage current at about 300 K is in order of magnitude of a few pA, it becomes very low when the JFET is cooled to 80 K. A careful measurement provides an estimate of the leakage current of 4×10^{-20} A [1]. The electrometer can be used from DC up to a frequency of 10 kHz. Without reduction of the bandwidth signal of a few μV can be detected. Working at low frequencies currents as low as a few attoampere can be detected. Despite the high sensitivity the sensor is fairly robust. If the input voltage is out of the operational range the forward current or the Zener current of the gate junction protects the transistor against destructive charging. Finally, different schemes have been developed to apply the sensor for scanning tunneling microscopy and potentiometry.

[1] R. Möller and H. Nienhaus, patent pending, Open FET Sensor, Provendis Ref.-Nr: 4817

O 64.9 Tue 18:30 P2-OG3

Advances in scanning field-emission microscopy — •Danilo A. Zanin, Hugo Cabrera, Gabriele Bertolini, Lorenzo G. De Pietro, Alessandro Vindigni, Thomas Bähler, Oguzhan Gürlü, Mehmet Erbudak, Urs Ramsperger, and Danilo Pescia — ETH Zurich, Zurich, Switzerland

The impact of Scanning Tunneling Microscopy (STM) to nanotechnology continues to be undisputed, but this does not prevent the search for new methods with the aim of revealing aspects complementary to those highlighted by STM. Inspired by the Russel Young topografiner we designed the Scanning Field-emission Microscopy (SFM) to analyze secondary electron escaping a tip-target nano-sized junction. On one side, SFM detects "non-geometrical" aspects of the surface, which are not straightforwardly revealed by STM. On the other side, those very same electrons used to build a one-nanometer-resolved image of a surface are ultimately made available to a macroscopic environment for further processing. We report on the latest result of this technique.

O 64.10 Tue 18:30 P2-OG3

Lateral manipulation of single iron-adatoms with CO terminated tips by combined STM/AFM — •Julian Berwanger, Ferdinand Huber, and Franz Josef Giessibl — Institute for Experimental an Applied Physics, University of Regensburg, 93040 Regensburg

By positioning single iron adatoms with a scanning probe microscope on a Cu(111) surface, spin-based logical operators and quantum bits can be built on the atomic scale [1,2]. Building these devices requires a precise, controlled and reproducible mechanism for positioning single adatoms. CO terminated tips allows to image metal clusters with atomic resolution [3]. We performed lateral manipulation of single iron adatoms with a combination of scanning tunneling and atomic force microscopy using monoatomic Cu- and CO-terminated tips. For both types of tips we find that the force responsible for the manipulation is purely attractive and the predicted diffusion barrier of 28.5meV [4] is lowered due to the presence of the tips [5] by about 70%. Moreover, this work demonstrates the feasibility of using the high resolution capability of a CO tip [6] and simultaneously manipulating adatoms laterally without the need of changing the tip before.

[1] A. A. Khajetoorians et al. Science 332, 1062 (2011)
[2] S. Loth et al. Science 335, 196 (2012)
[3] M. Emmrich et al. Science 348, 6232 (2015)
[4] N. N. Negulyaev et al. PRB 79, 195411 (2009)
[5] M. Emmrich et al. PRL 114, 146101 (2015)
[6] L. Gross et al. Science 325, 110 (2009)

O 64.11 Tue 18:30 P2-OG3

Cantilever dynamics induced by light — •Sven Kraft, Heinrich Behle, Kai Wardelmann, Mohammedreza Bahrami, Dieter Schick, Semjon Köhnke, Boris Hage, Ingo Barke, and Sylvia Speller — University of Rostock, Institute of Physics, 18051 Rostock, Germany

Atomic Force Microscopy methods have been advanced to image a variety of properties on the nanoscale. In this work we discuss the interaction of light fields with the cantilever [1]. On the one hand a temporally controlled illumination of the cantilever leads to bending and oscillation due to radiation pressure and photothermal effects. The light-driven cantilever actuation can replace the dither piezo actuation. In liquids this leads to reduced dynamics in the medium and thereby to better defined resonances. On the other hand light itself, e.g. in form of spatially modulated light landscapes can give rise to additional forces which may serve as an observable to map nearfield interactions [2].

[1] D. Ramos, J. Tamayo, J. Mertens, and M. Calleja, J Appl Phys 99, 124904 (2006)

[2] D.C. Kohlgraf-Owens, S. Sukhov, and A. Dogariu, Phys Rev A 84, 011807(R) (2011)

O 64.12 Tue 18:30 P2-OG3

A Scanning Tunneling Microscope with femtosecond optical near-field excitation — •Benjamin Schröder, Katharina Kaiser, Steffen Bornemann, Claus Ropers, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Photochemical reactions on metal oxide surfaces are governed by the site-specific surface structure, including defect concentration and distribution. To investigate these highly-localized optical excitation mechanisms, we implemented a low-temperature Scanning Tunneling Microscope operating under ultra high vacuum conditions. Our setup features stable imaging conditions with atomic resolution under pulsed optical excitation of the tip-sample gap at peak intensities up to 1 GW/cm^2.

Using this setup, we are able to desorb hydrogen adatoms and move oxygen vacancies from TiO$_2$ surfaces by applying current or voltage pulses [1,2]. Currently, we are investigating the possibility of stimulated desorption and diffusion processes by optical near-field excitation.

This project is financially supported by the DFG in the SFB 1073 (project C4).

[1] Acharya et al., J. Phys. Chem. C 114, 21510 (2010)

[2] Minato et al., ACS Nano 9, 6837 (2015)

O 64.13 Tue 18:30 P2-OG3

Low Vibration Laboratory with a Single-Stage Vibration Isolation for Microscopy Applications — Bert Voigtländer[1,2], Peter Coenen[1,2], Vasily Cherepanov[1,2], •Peter Borgens[1,2], Thomas Duden[3], and F. Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA) Fundamentals of Future Information Technology, 52425 Jülich, Germany — [3]Konstruktionsbüro Duden, Borgsenallee 35, 33649 Bielefeld, Germany

Vibrational isolation and electromagnetic shielding are crucial for every high-precision scanning probe microscope. In many cases, multistage vibration isolation stages are used, which add considerably to the complexity (and cost) of a SPM system. For this reason, recent approaches tend towards single-stage vibrational systems which can provide similar results while requiring much lower expenditure.

In this contribution, we report on the construction and the vibrational performance of a low vibration laboratory for microscopy applications comprising a 100 ton floating foundation supported by passive pneumatic isolators (air springs), which rest on a 200 ton solid base plate. Careful optimization of the air spring system results in a vibration level of the laboratory floor well below the one induced by acceleration of 10ng for most frequencies. Additional accoustic and electromagnetic isolation is accomplished by a room-in-room concept.

O 65: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond

Time: Tuesday 18:30–20:30 Location: P2-OG4

O 65.1 Tue 18:30 P2-OG4

Angular projection potentials for density functional calculations — •Rudolf Zeller — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Development of advanced 21st century applications benefits from a quantum-mechanical understanding of material properties by density-functional theory. However, because the Kohn-Sham-Schrödinger equation must be solved numerically, for all but the smallest systems considerable computer resources are needed which makes very precise calculations difficult. In order to overcome this problem numerous techniques have been developed in the past to make the calculations affordable.

It is my aim to present a novel approach based on non-local potentials which act as projection potentials in the space of spherical harmonics. I will explain the unconventional mathematical techniques that can be used to prove that the Kohn-Sham-Schrödinger equation for these potentials can be solved exactly in the angular variables and, in view of the present computing capabilities, practically exactly in the radial variables. I will discuss the advantage of the use of angular projection potentials for precise total-energy calculations. The advantage arises from the fact that, as a consequence of the practically exact calculable density, the stationarity property of the total-energy functional with respect to the potential can be exploited to full extent.

O 65.2 Tue 18:30 P2-OG4

DFPT within the All-Electron FLAPW Method: Application to Phonons — •Christian-Roman Gerhorst, Markus Betzinger, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In all-electron methods based on Density Functional Theory, typically the Finite Displacement approach is employed when describing the effect of a phonon perturbation on an electronic many-particle system. In difference to this common procedure, we implement the considerably more effective Density Functional Perturbation Theory (DFPT) into our full-potential linearized augmented plane-wave (FLAPW) code `FLEUR`; i.e. an all-electron code avoiding any approximation to the shape of the potential including the $1/r$ singularity. This is a nontrivial problem, because we have to tackle a position-dependent basis set generating additional Pulay and surface terms beyond the contributions known for force calculations when atoms are displaced. In this contribution, we report about the key challenge to the realization of the DFPT, which is the self-consistent solution of the Sternheimer equation providing the linear response of the electron density to a phonon perturbation. In a next step, we will use these results to construct the Dynamical Matrix encoding all relevant phonon information to shed light on the phonon-related properties of electronic many-particle systems.

O 65.3 Tue 18:30 P2-OG4

Conceptual problemsof self-interaction corrections — •Charlotte Vogelbusch, Ronald Starke, and Lenz Fiedler — TU Freiberg, Institute for Theoretical Physics, Germany

Electronic structure calculations with density functional theory usually include the so-called self-interaction error which occurs due to the approximation of the exchange-correlation functional.

A corresponding self-interaction correction has first been introduced by J. P. Perdew and A. Zunger. This poster deals with the main aspects and problems of their method. In particular, we discuss the recent modification of the Perdew-Zunger self-interaction correction proposed by M. R. Pederson [2].

[1] J. P. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)

[2] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)

O 65.4 Tue 18:30 P2-OG4

Numerical improvements of Fermi-Löwdin orbital self-interaction correction — •Lenz Fiedler, Torsten Hahn, Charlotte Vogelbusch, and Jens Kortus — TU Freiberg, Institute for Theoretical Physics, Germany

Electronic structure theory calculations based on density functional theory (DFT) using semilocal approximations for exchange and correlation are subjected to the self-interaction error. The recently proposed Fermi-Löwdin orbital method for self-interaction correction (FLOSIC) is based on sets of localized orbitals, that are a unitary invariant transformation of the Kohn-Sham orbitals [1,2]. The practical application of this method is however still numerically costly because one needs to determine the Fermi orbital descriptors that minimize the total energy. Numerical improvements to this optimization will drastically improve the performance of the whole FLOSIC DFT method.

We present the implementation of a preconditioned conjugate gradient [3] and a quasi-Newton L-BFGS algorithm [4] that draw on approximations of the analytical Hessian of the energy function. For a set of small molecules, benchmarks are done for different approximated Hessians. We here discuss the influence of different methods to approximate the Hessian and the usage of off-diagonal Hessian elements on the optimization performance.

[1] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
[2] J. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)
[3] D. Liu, J. Nocedal, Math. Prog. B 45, 503 (1989)
[4] W. Hager, H. Zhang, SIAM J. Optim., 16-1, 170 (2005)

O 65.5 Tue 18:30 P2-OG4

Electronic and Magnetism Properties of Vacancy-Defected, Fluorine Doped and Adsorption upon MO3 (M= Cr, Mo, W) Surface: a first-principles study — •Masoud Mansouri[1,2] and Tahereh Mahmoodi[1] — [1]Department of Physics, Mashhad Branch, Islamic Azad University, Mashhad 9187147578, Iran — [2]Computational Science Unit, Research Center for Applied Biology, Mashhad Branch, Islamic Azad University, Mashhad, Iran

In this work, a systematic DFT calculation was carried out to investigate the effects of various kinds of dopants on the electronic structure of MO3 (M= Cr, Mo, W) Surface. The possibility to obtain magnetic phase from native defects in pure bulk is investigated. We found that vacancies can induce a magnetic phase of *2 μB with a local magnetic moment, whereas corresponding M vacancies (VM) provides the transition of the insulating MO3 into a metallic-like phase and changes the electronic transport. Moreover, We find that Fluorine (F) doping improves the metallic phase MO3*x Fx (x= 0.04, 0.08, 0.16), where the near Fermi states are formed mostly from M d-orbital and admixture of O-2p orbitals. Next, we present results on the influence of the common gas molecules (Ch4, H2S and NO2) on the electrical resistivity. The most stable configurations, magnetism, adsorption energies, Fermi surface and electronic properties are thoroughly discussed.

O 65.6 Tue 18:30 P2-OG4

An Investigation of Group V dopants in Silicon using Linear Scaling DFT — •Jack Poulton and David Bowler — London Centre for Nanotechnology, 19 Gordon St, London, WC1H 0AH

The aim of our work is to model the incorporation and properties of group V element dopants in silicon using linear scaling density functional theory. In doing so we hope to learn how to incorporate new impurities and make predictions as to how the behaviour of these impurities for comparison with experimental data. This will then allow us to determine the suitability of certain dopants for usage as qubits in a silicon based solid state quantum computer.

O 65.7 Tue 18:30 P2-OG4

Deciphering chemical bonding with Fermi-Löwdin orbitals — •Torsten Hahn[1], Sebastian Schwalbe[1], Jens Kortus[1], and Mark Pederson[2] — [1]Institute for Theoretical Physics, TU Freiberg, Germany — [2]Department of Chemistry, Johns Hopkins University, Baltimore Maryland (MD), US

The recently developed Fermi-Löwdin orbital based method for the correction of the self-interaction error within Density Functional Theory (FLO-SIC) [1,2] does provide improved orbital eigenvalues and more realistic level ordering [3]. We demonstrate the versatility of this method to provide details of chemical bonding by applying it to several systems featuring both localized and delocalized multi-center chemical bonding.

We present results on systems with varying structural complexity: Boron clusters, compounds containing planar tetra-coordinated carbon as well as several aromatic and anti-aromatic molecules. The FLO-SIC method yields an inherently 'chemical' representation of bonding in terms of Lewis-type lone and binding electron pairs as well as delocalized multi-center, many-electron bonds. We anticipate that this parameter free methodology becomes a reliable tool to obtain insights into fundamental bonding details especially in situations where standard DFT fails.

[1] M. R. Pederson et.al, JCP 140, 121103 (2014).
[2] M. R. Pederson, JCP 142, 064112 (2015).
[3] T. Hahn et al., JCP 143, 224104 (2015).

O 65.8 Tue 18:30 P2-OG4

Binding energy curves for diatomic molecules obtained by FLO-SIC DFT — •Simon Liebing[1], Sebastian Schwalbe[1], Torsten Hahn[1], Jens Kortus[1], and Mark Roger Pederson[2] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany — [2]Department of Chemistry, Johns Hopkins University, Baltimore, USA

The recently developed Fermi-Löwdin orbital method to correct the self-interaction error within DFT (FLO-SIC) [1,2] is used to study bond dissociation of diatomic molecules (e.g. N_2, O_2 and LiF). Binding energy curves are derived within this FLO-SIC methodology and the obtained results are compared to quantum chemical methods (RHF, UHF and ROHF in combination with CCSD/CCSD(T)). Due to the fact that FLO-SIC DFT recovers the correct -1/r behaviour of the potential, the obtained energies for large (infinite) separations agree well with the quantum chemical results. Further, changing Fermi orbital configurations as a function of the separation distance are observed. These distinct configurations could be interpreted as step-wise breaking of multiple bonds during the stretching of the considered molecule and corresponding alterations of spins within its electronic structure.

[1] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)
[2] T. Hahn et al., JCP, vol. 143, 224104 (2015)

O 65.9 Tue 18:30 P2-OG4

Groundstates of the ternary clathrate $Ba_8Ni_xGe_{46-x-y}\Box_y$ obtained with an iterative cluster expansion approach — •Martin Kuban, Santiago Rigamonti, Maria Troppenz, and Claudia Draxl — Humboldt-Universität zu Berlin

Intermetallic clathrates are promising candidates for the construction of thermoelectric (TE) devices. These rely on a junction between n- and p-type semiconductors. The clathrate compound $Ba_8Ni_xGe_{46-x-y}\Box_y$ is of special interest, as it presents a crossover from p-type to n-type conductivity around $x = 4.0$ [1]. Thus, a junction on the same base material could be tailored. In this work, we perform an *ab-initio* study of the structural stability and electronic properties of this compound in the composition range $0 \leq x \leq 6$ and $0 \leq y \leq 4$. Both the substitutional species (Ni) and vacancies ($\Box$) are treated on the same footing, through a cluster expansion (CE) in the quasi-ternary Ge/Ni/$\Box$ sublattice. The large size of this sublattice (46 sites) leads to a combinatorial explosion of the number of configurations, i.e. the possible arrangements of the substitutional atoms and vacancies in the lattice. As this prevents the use of standard CE methodology, we make use of an iterative CE technique (iCE) as implemented in the code `CELL` [2]. The iCE is based on efficient samplings of the configurational space. The structural properties (lattice constants, bond distances, etc.) as well as the electronic bandstructure of the stable structures are analyzed.

[1] U. Aydemir *et al.*; Dalton Trans **44**, 7524 (2015).
[2] S. Rigamonti *et al.*, in preparation.

O 65.10 Tue 18:30 P2-OG4

The inapplicability of exact constraints, and a minimal two-parameter DFT+U generalisation, for self-interaction error correction — •Glenn Moynihan[1], Gilberto Teobaldi[2,3], and David D. O'Regan[1] — [1]School of Physics, CRANN and AMBER, Trinity College Dublin, Ireland. — [2]Stephenson Institute for Renewable Energy and Department of Chemistry, The University of Liverpool, U.K. — [3]Beijing Computational Science Research Center, China.

In approximate DFT, the self-interaction error (SIE) is a ubiquitous systematic inaccuracy responsible for underestimated insulating gaps, inaccurate dielectric properties and reaction barriers. It hinders the predictive applicability of DFT to spectroscopy, photochemistry, electrochemistry, and crystal-structure stability. It is, however, amenable to approximate correction using efficient methods such as DFT+U [1]. A calculation scheme for the Hubbard U parameters by variationally extremising a suitable functional might be desirable. but we show here that such an approach is not readily viable. Specifically, we prove that self-consistent constrained DFT [3] cannot be generalised for the non-linear constraints needed to target SIE [2]. We circumvent this using a generalised DFT+U functional, enabling the simultaneous correction of total-energies and ionization potentials, or either together with Koopmans' condition. For the latter, we outline a practical, approximate first-principles scheme by which the required Hubbard parameter pair, U_1 and U_2, may be estimated. [1] H. J. Kulik, et al., Phys. Rev. Lett. **97**, 103001 (2006). [2] Phys. Rev. B Rapid Comms., Accepted (2016), arXiv:1608.07320. [1] Phys. Rev. B **94**, 035159 (2016).

O 65.11 Tue 18:30 P2-OG4

A Hubbard U based correction method for exciton binding in neutral excitations: TDDFT+U — •Okan K. Orhan and David D. O'Regan — School of Physics, Trinity College Dublin, Ireland.

The DFT+U (density-functional theory + Hubbard U) method is widely used to improve the approximate DFT description of the ground state properties of solids and molecules comprising transition-metal ions. We introduce its generalisation to the time domain in the guise of TDDFT+U (time-dependent DFT+U), intended to extend these improvements to the calculation of neutral excitations. Related methods have been previously discussed [1,2], and here we offer a detailed treatment emphasising single-particle excitations and absorption spectra. Our software implementation is a combination of the linear-scaling DFT+U [3] and linear-response TDDFT [4] functionalities available in the ONETEP code [5]. In a study of small nickel-comprising molecules, we find that the Hubbard U correction to the exchange-correlation kernel acts to partially cancel the effects of the DFT+U term of the underlying ground-state potential, enhancing the exciton binding.
[1] C.-C. Lee, H. C. Hsueh, and W. Ku, Phys. Rev. B **82**, 081106(R) (2010). [2] D. Shin, G. Lee, Y. Miyamoto, and N. Park, J. Chem. Theory Comput., **12** (1), pp 201-208 (2016). [3] D. D. O'Regan, N. D. M. Hine, M. C. Payne, and A. A. Mostofi, Phys. Rev. B **85**, 085107 (2012). [4] T. J. Zuehlsdorff, N. D. M. Hine, M. C. Payne, and P. D. Haynes, J. Chem. Phys. **143**, 204107 (2015). [5] C. K. Skylaris, P. D. Haynes, A. A. Mostofi, and M. C. Payne, J. Chem. Phys., **122** (8), 084119 (2005). For the ONETEP code, see http://www.onetep.org

O 65.12 Tue 18:30 P2-OG4

Implementation of Electron-Phonon Coupling in the KKR Formalism and its Applications to Simple Metals — Carsten Eberhard Mahr, •Michael Czerner, Christian Franz, and Christian Heiliger — Justus-Liebig-University, 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 density functional theory (DFT) based Korringa-Kohn-Rostocker (KKR) Green's function formalism code.

By approximating the Fröhlich-type interaction with a self-energy $\Sigma_{\rm eph} = -i\frac{\hbar}{2\tau}$ we are able to compute the dressed propagator G by solving Dyson's equation $G = G_{\rm ref} + G_{\rm ref} \cdot \left(\Delta V + \Sigma_{\rm eph}\right) \cdot G$, where $G_{\rm ref}$ is the Green's Function of an arbitrary (though typically repulsive) reference system. The corresponding electron-phonon scattering time τ is extracted from electron linewidth calculations.

We demonstrate the physical validity of the beforementioned calculational scheme for non-equilibrium properties by comparing evaluated temperature dependent resistivity characteristics of transport systems consisting of copper, aluminum and other simple metals to experiment. Further, technical details of the implementation in the KKR basis set are presented.

O 66: Overview Talk: Anders Nilsson

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

Invited Talk O 66.1 Wed 9:30 TRE Phy
Probing catalytic surface reactions in real time — •Anders Nilsson — Department of Physics, Stockholm University, Sweden

In heterogeneous catalysis, reactants adsorbed on surfaces are converted to products, which eventually desorb via various intermediates. The transition state separates reactants and intermediates from products and the free energy required to reach it determines the kinetics of an elementary chemical reaction. Many surface reaction intermediates are, however, transient species with a short residence time and the population of species in the transition state region is near-zero making their observation a challenge during steady state conditions. Ultrafast pump-probe techniques have, however, opened up opportunities by promoting a sufficient population of molecules in transient states to allow detection on short time scales. Here recent results on probing chemical reactions on surfaces using X-ray free-electron lasers LCLS (Linac Coherent Light Source) at SLAC National Accelerator Laboratory) will be presented. Four examples will be shown CO desorption, Oxygen activation, CO oxidation and CO hydrogenation on Ru(0001). We demonstrate that both transient intermediates and the transition state region can be detected in surface chemical reactions.

O 67: SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - defects, structure and thermodynamics

Time: Wednesday 10:15–11:30 Location: IFW A

O 67.1 Wed 10:15 IFW A
Structure, thermodynamics and Li storage of and in amorphous siliconoxycarbides: insights from first-principle calculations — •Jochen Rohrer and Karsten Albe — FG Materialmodellierung, FB Material- und Geowissenschaften, Technische Universität Darmstadt

Precursor-derived amorphous siliconoxycarbides (SiOC) are attracting increased attention as potential anode material for Li-ion batteries. Capacities of 600 mAh/g and above have been achieved. Furthermore, SiOCs have been reported to be thermodynamically stable relative to the crystalline boundary phases cristobalite, SiC and graphite. On the microscale, SiOCs are well characterized and can be described by regions consisting of amorphous SiO_2, graphitic free carbon and mixed ternary regions. The details of the atomic structure within the ternary regions are, however, still under debate.

In this contribution we present strategies to model and determine local atomic characteristics of SiOC using density functional theory calculations. Using cluster models, we systematically investigate the bonding environment of carbon in ternary Si-O-C regions. Thereby we consider various coordinations and the possibility of hydrogen incorporation into the amorphous network [1]. Based on the predicted local C environment, we then design periodic supercell models with variable carbon content, compute thermodynamic stability and investigate Li storage in a way similar to our previous work on Si anodes [2].

[1] J. Rohrer et al., *submitted to Int. J. Mater. Res.* (Nov 2016).
[2] J. Rohrer and K. Albe, *J. Phys. Chem.* C **117**, 18796 (2013).

O 67.2 Wed 10:30 IFW A
Oxygen Defects in LTO – Structural Models and Adapted DFT Treatments — •Markus Schuderer, Karsten Reuter, and Christoph Scheurer — Technische Universität München, Germany

$Li_4Ti_5O_{12}$ (LTO) receives increasing interest as a zero-strain anode material for lithium ion batteries. One route pursued to improve its limited electronic conductivity is via the deliberate introduction of oxygen defects during synthesis. Little is presently known though, whether these defects enrich at the electrode-electrolyte interface and concomitantly contribute to structural or charge transfer limitations. Aiming to contribute to this context from the perspective of first-principles electronic structure calculations, we assess differing setups in terms of reliability and computational efficiency. This comprises a comparison of periodic supercell and solid-state embedded cluster approaches, as well as treatments on the semi-local or screened hybrid level of density-functional theory. While semi-local functionals delocalize the excess charge density associated with the defect and lead to metallic systems, the hybrid functional recovers the experimentally observed band gap and localizes the charge density on titanium ions directly coordinating the defect. We show that this localization can already be appropriately captured with small embedded clusters, rendering this approach numerically far more efficient in particular for studies of surface or interface defects.

O 67.3 Wed 10:45 IFW A
Ion channelling contrast to reveal structure and growth behaviour of $LiNi_{0.5}Mn_{1.5}O_4$ battery materials — •Manuel

Mundszinger[1], Tobias Wälde[1], Jörg Bernhard[1], Michael Kinyanjui[1], Marilena Mancini[2], Peter Axmann[2], Margret Wohlfahrt-Mehrens[2], Ute Golla-Schindler[1], and Ute Kaiser[1] — [1]Ulm University, Central Facility for Electron Microscopy, Group of Electron Microscopy of Materials Science, Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), Helmholtzstrasse 8, 89081 Ulm

Ion channelling contrast [1] was utilized to characterize the crystallinity and crystalline architecture of $LiNi_{1.5}Mn_{0.5}O_4$ particles [2] for battery cells. The $LiNi_{0.5}Mn_{1.5}O_4$ particles were cut by the focused ion beam (FIB) machine; then the FIB was used to produce channelling contrast revealing the polycrystallinity of the material, allowing to determine grain size distribution and architecture. For systematic investigations, differently sized particles (10-30 micrometre in diameter) were examined. We found that with increasing particle size the number and the average size of the grains increases. This allows to conclude that during growth new grains are formed as well as existing grains grow. SAED and HRTEM reveal that the structure is cubic. Ion channelling contrast and EBSD contrast were compared showing very similar results. This work was done in the LiEcoSafe project funded by the BMBF (03X4636C).
[1] C. A. Volkert et al, MRS Bulletin, 32:389-399, 5, 2007.
[2] P. Axmann et al, Journal of Power Sources 301 (2016) 151-159.

O 67.4 Wed 11:00 IFW A

Modeling occupational disorder in $Li_4Ti_5O_{12}$ battery materials: Intrinsic complexity and its effect on ion mobility — •Hendrik H. Heenen, Christoph Scheurer, and Karsten Reuter — Technische Universität München, Germany

Lithium-titanium-oxide ($Li_4Ti_5O_{12}$, LTO) is unique among battery materials due to its exceptional cyclability and high rate capability. This performance is assumed to derive at least partly from the occupational disorder introduced via mixed Li/Ti occupancy in the LTO spinel-like structure. Notwithstanding, the exact atomic-scale influence of this disorder on Li ion mobility remains an open question.

We explore the vast configuration space accessible during high-temperature LTO synthesis by Wang-Landau sampling. Use of a numerically efficient, density-functional theory validated interatomic potential [1] allows for extensive sampling in simulation cells large enough to appropriately capture the long-range disorder. The determined configurational ensemble is indeed characterized by a large degree of microscopic inhomogeneity. Subsequent room-temperature molecular dynamics simulations reveal the dominant fraction of Li ions in this ensemble to be immobile on nanosecond timescales. However, certain disorder motifs give rise to a novel correlated ion diffusion mechanism. We discuss this mechanism in the context of the evolution and morphology of the so-called two-phase reaction appearing during Li intercalation [2].
[1] M. Vijayakumar *et al.*, J. Power Sources **196**, 2211 (2011)
[2] M. G. Verde *et al.*, ACS Nano **10**, 4312 (2016)

O 67.5 Wed 11:15 IFW A

Ab initio modeling of Li-rich transition metal oxyfluorides — •Holger Euchner[1] and Axel Gross[1,2] — [1]Helmholtz Institute for Electrochemical Energy Storage, Helmholtzstraße 11, 89081 Ulm — [2]Institute of Theoretical Chemistry, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm

Recently, Li-rich transition metal (TM) oxyfluorides, were identified as promising electrode materials in Li-ion batteries [1,2]. Due to the evidenced robustness of the underlying framework – a disordered rock salt structure (DRS), consisting of two disordered fcc sublattices, exhibiting TM/Li and O/F disorder, respectively – this class of materials is a potential candidate for future application in Li-ion technology.

To provide insight into underlying mechanisms and potential for improvement, we have conducted a computational study of a number of $Li_xTM_{1-x}O_yF_{1-y}$ compounds. Using periodic density functional theory calculations, the impact of different TMs as well as different O/F concentrations on structural stability, (de-)lithiation behavior and Li diffusion is investigated. Apart from predicting open circuit voltage and energy density, we present an analysis of Li-diffusion pathways and corresponding barriers, which we relate to local environment and bonding characteristics of Li atoms.
[1] R. Chen et al., Adv. Energy Mater. **5**, 9 (2015).
[2] S. Ren et al., Adv. Sci. **2**, 10 (2015).

O 68: Focus Session: Non-equilibrium Dynamics in Light-driven Materials: Theory Meets Experiment

Time: Wednesday 10:30–13:00 Location: TRE Phy

Invited Talk O 68.1 Wed 10:30 TRE Phy

Electronic orders in light-driven materials — •Philipp Werner[1], Yuta Murakami[1], Hugo Strand[1], Shintaro Hoshino[2], and Martin Eckstein[3] — [1]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — [2]RIKEN Center for Emergent Matter Science, Wako, 351-0198 Saitama, Japan — [3]Max Planck Research Department for Structural Dynamics, University of Hamburg-CFEL, 22761 Hamburg, Germany

The prospect of nonequilibrium control of material properties has caught the interest of the condensed matter community. In particular, recent experiments demonstrating a light-enhanced superconducting-like state in cuprates and fulleride compounds has triggered a number of theoretical studies on order parameter dynamics in lattice systems perturbed by periodic driving or strong quasi-static fields.

Here, we use the nonequilibrium dynamical mean field theory in a Kadanoff-Baym and Floquet implementation to address some relevant issues which have been ignored in previous studies. In particular, we will consider parametric phonon driving in the Holstein model, and show that the nonthermal energy distribution in the driven state generically leads to a weakening of the superconducting order.

As a second example, we will discuss order parameter switching by quasi-static electric fields in fulleride compounds. Here, we will focus on the Jahn-Teller metal phase, which has recently been identified as an orbital-selective Mott state. Electric field pulses can switch this composite ordered state between physically distinct realizations, which may be potentially exploited in ultrafast persistent memory devices.

Invited Talk O 68.2 Wed 11:00 TRE Phy

Pump/probe photoemission spectroscopy in charge density wave insulators — •James Freericks — Department of Physics, Georgetown University, Washington, DC 20057

In this talk, I will discuss time-resolved photoemission spectroscopy in charge-density-wave (CDW) insulators that form due to an electronic nesting instability. A strongly correlated electronic CDW has a number of interesting features. As the temperature is raised, the gap in the spectrum remains unchanged all the way up to Tc, while the gap fills with subgap states, which eventually metallize the system. There is a critical interaction strength where the metallization occurs the instant the temperature is increased from 0. The system also displays Mott-like physics at strong interaction strength. We illustrate that these systems have an interesting response to the pump. In some cases, the gap region fills in due to the pump, implying the disappearance of the spectral gap, but in the presence of a well formed spatial charge-density-wave order parameter. At the critical interaction strength, the system is exceedingly difficult to pump. Whatever energy is pumped in on the leading edge of the electric field, is pumped out on the trailing edge. These calculations result from the exact solution of the nonequilibrium Falicov-Kimball model via dynamical mean-field theory. We also discuss experimental implications for these results.

Invited Talk O 68.3 Wed 11:30 TRE Phy

Controlling magnetism and pairing in a periodically driven Hubbard model — •Stephen Clark[1,2], Jonathan Coulthard[3], Juan Jose Mendoza-Arenas[4], Martin Eckstein[2], Dieter Jaksch[3], and Andrea Cavalleri[2,3] — [1]Department of Physics, University of Bath, UK — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [3]Department of Physics, University of Oxford, UK — [4]Departamento de Fisica, Universidad de los Andes, Colombia

In this talk I will describe theory work illustrating striking effects of periodic driving for three different regimes: (i) high frequency $\omega \gg U, t$, (ii) resonant $\omega = nU$ and (iii) in-gap $U \gg \omega \gg t$. Floquet theory when $U \gg t$ predicts renormalisation of t for (i), substantial modifications of both t and U for (ii) and a suppression of t with super-exchange J essentially unchanged for (iii). To demonstrate this physics I will outline non-equilibrium DMFT results showing how the mechanism governing the magnetic melting of an initial classical Neel state can be controlled and switched in the half-filled Hubbard model in infinite dimensions. I will also describe how attaining dominant super-exchange interactions in regime (iii) leads to the emergence of strong singlet-pairing correlations in the driven state. This is demonstrated in the one-dimensional Hubbard model below half-filling in the thermodynamic limit using time-dependent DMRG calculations. By spanning different fillings, dimensions and driving regimes these results show how periodic driving leads to compelling new pathways for controlling magnetism and potentially engineering light-induced superconductivity.

Invited Talk O 68.4 Wed 12:00 TRE Phy

Ultrafast Terahertz and XUV ARPES Probes of Quantum Materials Dynamics — •Robert A. Kaindl — Materials Sciences Division, E. O. Lawrence Berkeley National Laboratory, Berkeley, USA

In this talk I will discuss the application of ultrashort light pulses - from THz to Extreme-UV - to the study of vibrational coupling and emergent correlations in quantum materials. Transition-metal oxides, in particular, exhibit an intriguing self-organization of charges into nanoscale "stripes", whose driving forces and role in high-Tc superconductivity remain unresolved. We will first present transient multi-THz and mid-IR experiments that capture the initial steps of vibrational symmetry breaking and charge ordering in stripe-phase nickelates, indicating the precursor role of charge localization and exposing the electronic and structural coupling dynamics [1]. In the second part, I will discuss our development of ultrafast angle-resolved photoemission spectroscopy (ARPES) with extreme-ultraviolet (XUV) pulses at 50-kHz repetition rate, and its application to sensitively access electronic dynamics of quantum materials across momentum space [2]. Studies of semiconducting and correlated dichalcogenides access the crossover of light-induced perturbation and melting of charge density waves and provide evidence for excitonic signatures in ARPES spectra. [1] G. Coslovich, et al. Nature Comm. 4, 2643 (2013); arXiv:1603.07819 (2016). [2] H. Wang, et al. Nature Comm. 6, 7459 (2015); J. H. Buss, et al. in preparation (2016).

Invited Talk O 68.5 Wed 12:30 TRE Phy

Ultrafast spin interactions revealed with terahertz radiation — •Tobias Kampfrath — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The terahertz (THz) frequency range is attracting increasing interest for both applied and fundamental reasons. First, bit rates in current information technology may soon approach the THz range. Second, its low photon energy (4.1 meV at 1 THz) makes THz radiation an excellent probe and stimulus of many fundamental excitations of solids, for instance phonons and Cooper pairs. This talk considers experiments showing that THz pulses are also a very useful and versatile tool to reveal spin interactions on the time scales of elementary relaxation processes. Examples include (i) the ultrafast transfer of energy and angular momentum between phonons and the ordered electron spins of the textbook ferrimagnet yttrium iron garnet (YIG) as well as (ii) the femtosecond transport of magnons across the interface of the spin Seebeck bilayer system YIG/Pt.

O 69: Plasmonics and Nanooptics VI: Light-Matter Interactions and Characterisation

Time: Wednesday 10:30–12:30 Location: TRE Ma

O 69.1 Wed 10:30 TRE Ma

Remote excitation and detection of surface-enhanced Raman scattering from graphene — •Nicolas Coca Lopez, Nina Gordon, Tobia Mancabelli, Nicolai Hartmann, and Achim Hartschuh — Department of Chemistry and Center for Nanoscience, Ludwig-Maximilian-University Munich

In this contribution, we show the remote excitation and detection of surface enhanced Raman scattering (SERS) from graphene. Surface plasmon polaritons (SPPs) were launched by focused laser illumination at the termination of a metallic nanowire (NW) which served as a plasmonic waveguide. An SPP excited by the laser travels to the other end of the waveguide that is placed on top of single layer graphene, resulting in the remote excitation of Raman scattering. In the reversed direction, locally excited Raman scattering from graphene is coupled to an SPP traveling along the NW and scattering out at its end. By projecting the sample scattered light onto a CCD camera mounted on a spectrometer we quantified the SPP contributions at different wavelengths in combination with polarization dependent measurements.

O 69.2 Wed 10:45 TRE Ma

Helicity Sorting of Photons: A Spin Optical Device — •Enno Krauss[1], Gary Razinskas[1], Dominik Koeck[1], Swen Grossmann[1], and Bert Hecht[1,2] — [1]NanoOptics & Biophotonics Group, Experimentelle Physik 5, Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Röntgen Research Center for Complex Material Systems (RCCM), Am Hubland, 97074 Würzburg, Germany

Spin optics adds an additional degree of freedom and therefore promises new functionalities in optical nanocircuits in analogy to spintronics. Here we study experimentally and theoretically spin-optical devices, so-called photon helicity sorters, based on "birefractive" propagation in a plasmonic two-wire transmission line. We study the mechanism that leads to spin-orbit coupling in these devices including the role of a geometrical phase.

O 69.3 Wed 11:00 TRE Ma

Optical properties of hybrid chiral plasmonic systems — •Martin Schäferling, Maxim L. Nesterov, Xinghui Yin, Harald Giessen, and Thomas Weiss — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Chiroptical spectroscopy is a vital technique in the life sciences. The combination of chiral media with plasmonic nanostructures offers a possibility to enhance the tiny chiroptical responses. Theoretical studies of such hybrid systems are necessary to understand the occurring interactions. A well-established method to investigate the potential interaction strength between plasmonic nanostructures and a chiral molecule is the analysis of chiral near-fields [1]. This method works for the presence of a few molecules in the limit of weak coupling. However, in systems where a sizeable amount of a chiral medium is present, additional effects beyond the capabilities of this model can occur.

In this contribution, we analyze the full hybrid system combining plasmonic nanostructures with chiral media. In one approach, we use numerical full-wave simulations where we introduced an effective chiral medium via its constitutive equations. Our results reveal the importance of coplanarity of the incident field with the generated near-field in addition to strong field enhancement [2]. Additionally, we show first results of a semi-analytical approach using perturbation theory [3] to analyze the influence of a chiral medium on plasmonic resonances.

[1] M. Schäferling et al., Phys. Rev. X **2**, 031010 (2012).
[2] M. L. Nesterov et al., ACS Photonics **3**, 578 (2016).
[3] T. Weiss et al., Phys. Rev. Lett **116**, 237401 (2016).

O 69.4 Wed 11:15 TRE Ma

Colloid-defined Scattering Interfaces with Tailored Disorder for PV Applications — Peter Michael Piechulla[1], •Lutz Mühlenbein[1], Alexander Sprafke[1], Ralf B. Wehrspohn[1], Stefan Nanz[2], Aimi Abass[2], and Carsten Rockstuhl[2] — [1]FG Mikrostrukturbasiertes Materialdesign, MLU Halle-Wittenberg — [2]Institut für Theoretische Festkörperphysik, KIT, Karlruhe

Optical interfaces with tailored scattering properties are of interest for numerous applications, such as light management in photonic devices. In particular, thin film solar cell absorber materials exhibit long absorption lengths in the long wavelength range compared to the absorber thickness, which makes effective light trapping structures indispensable. Numerical studies reveal that interfaces with a certain degree of disorder outperform strictly periodic structures due to their improved broadband response. However, the proposed design in these studies are mostly either hypothetical in nature or rely on expensive top down fabrication methods. In our approach, we deposite a monolayer of colloidal particles onto a substrate using self-organization effects. Colloidal size distribution and manipulation of interaction potentials between particles and substrate provide effective levers to obtain desired surface profiles. The structure is then stabilized by conformal coating using atomic layer deposition and can be used as back side structure for solar cells. In this contribution, we will identify relevant fabrication parameters of these structures and present experimental data for their scattering properties. The presented experimental work is motivated by optical simulations that are specific to colloidal structures.

O 69.5 Wed 11:30 TRE Ma

Characterization of thin-load polymethyl-methacrylate plasmonic waveguides using PEEM — •Malte Grossmann[1], Martin Thomaschewski[1], Alwin Klick[1], Elzbieta Sobolewska[2], Arkadiusz Jaroslaw Goszczak[2], Till Leissner[2], Jacek Fiutowski[2], Horst-Günter Rubahn[2], and Michael Bauer[1] — [1]Institute of Experimental and Applied Physics, University of Kiel, Leibnizstraße 19, D-24118 Kiel, Germany — [2]Mads-Clausen-Institute, NanoSYD, University of Southern Denmark, Alsion 2, DK-6400 Sønderborg, Denmark

Surface plasmon-polaritons (SPPs) are promising candidates for future signal transport applications due to their capability of bypassing the diffraction limit of light. However, for applications such as onchip communications SPPs have to be confined laterally. This can be achieved using plasmonic waveguides. Here we present work on dielectric-loaded SPP waveguides (DLSPPW) using a thin load (30 to 50 nm) of polymethyl-methacrylate (PMMA).

PMMA DLSPPW of variable width are fabricated on gold substrates using electron-beam lithography. We investigate the waveguides using photoemission electron microscopy supported by a wavelength-tunable near-infrared laser. The dispersive characteristics of the waveguides are compared to finite-element-method calculations. We are able to determine waveguide mode effective index with quantitative agreement and mode confinement with qualitative agreement to expectations set by the finite-element-method calculations for both singlemode and multimode waveguiding.

O 69.6 Wed 11:45 TRE Ma

Design and fabrication of metasurfaces with high polarization sensitivity on top of crystalline gold plates — •Manuel Gonçalves[1], Vaishnavi Rao[1], Gregor Neusser[2], Christine Kranz[2], Boris Mizaikoff[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Institute of Analytical and Bioanalytical Chemistry, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany

Metasurfaces emerged in the last 10 years as one of the most successful realizations of plasmonic metamaterials. The two-dimensional geometrical arrangement of sub-wavelength plasmonic and dielectric nanostructures permits to use metasurfaces in a variety of ways: transformation of the polarization of light beams, beam focusing, holography, generation of structural colors. The units constituting plasmonic metasurfaces are tailored based on the plasmonic properties of single, or coupled particles. Among the several lithography techniques used for fabrication, focused ion-beam (FIB) is best indicated for milling crystalline films and particles, due to the accuracy achieved.

We have investigated the optical properties of grooves milled in crystalline gold plates and have designed a metasurface to be used in reflection using several groove elements. Due to the large sensitivity of the plasmonic absorption on the polarization of the light irradiating the grooves, the metasurface can be used as a polarization sensitive optical filter for specific bands in the visible and NIR spectrum.

O 69.7 Wed 12:00 TRE Ma

Imaging with SNOM and EELS in plasmonics — •Vlastimil Křápek[1,2], Petr Dvořák[1,2], Ai Leen Koh[3], Zoltán Édes[1,2], Michal Horák[1,2], Michal Kvapil[1,2], Lukáš Břínek[1,2], Tomáš Šamořil[1,2], Martin Hrtoň[1,2], and Tomáš Šikola[1,2] — [1]Central European Institute of Technology, Brno University of Technology, Purkyňova 123, CZ-612 00 Brno, Czech Republic — [2]Institute of Physical Engineering, Brno University of Technology, Technická 2, CZ-616 69 Brno, Czech Republic — [3]Stanford Nano Shared Facilities, Stanford University, Stanford, California 94305, USA

Scanning near-field optical microscopy (SNOM) is a powerful tool for imaging and analysis of surface plasmon polaritons (SPPs) [1]. However, the correct interpretation of SNOM images requires profound understanding of principles behind their formation. To study fundamental principles of SNOM imaging in detail, we performed spectroscopic measurements of plasmon interference patterns by an aperture-type SNOM setup equipped with a supercontinuum laser and a polarizer. The series of wavelength- and polarization-resolved measurements, together with results of numerical simulations, then allowed us to identify the role of individual near-field components in formation of SNOM images.

Electron energy loss spectroscopy (EELS) is a technique for imaging of localized plasmon resonances with unprecedented spatial resolution. We present our EELS imaging of gold plasmonic particles suitable for the enhancement of optical processes [2].

[1] P. Dvořák *et al.*, Nano Lett **13**, 2558 (2013).
[2] V. Křápek *et al.*, Opt. Express **23**, 11855 (2015).

O 69.8 Wed 12:15 TRE Ma

Multimodal Tip-Enhanced Microscopy — Kai Braun, •Otto Hauler, Dai Zhang, and Alfred J. Meixner — Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen

Electromagnetic coupling between plasmonic resonances of two closely spaced metal particles can lead to a strongly enhanced optical near field in the gap between. It is the leading amplification mechanism for surface- and tip-enhanced Raman scattering (SERS/TERS) or enhanced molecular luminescence and has widespread applications in nanoplasmonics. Collecting correlated signals of photoluminescence (PL) and Raman as well as topography, tip-enhanced hyperspectral imaging is able to provide a thorough map of the chemical and morphology-related optical properties in multi-component material systems. Introducing new microscope functions offer us insights into various aspects, such as morphology related photophysical and photochemical processes. Despite its attractive capabilities, developing a tip-enhanced near-field microscope providing reliable and reproducible performance is demanding. In the last years great efforts have been made in our lab to develop stable, reproducible and reliable near-field optical microscopes, which largely meet the above requirements. They successfully demonstrated their capability in high-resolution optical imaging and spectral mapping, or using the tip as local probe for enhanced coupled fields. Furthermore we demonstrate the direct manipulation and measurement of surface properties via electrical charging or injection of charge carriers

O 70: 2D Materials Beyond Graphene III

Time: Wednesday 10:30–13:00 Location: WIL A317

O 70.1 Wed 10:30 WIL A317

Band structure and excitons of monolayer and bulk ReSe$_2$: A many-body view — •Jonathan Noky[1], Matthias Drüppel[1], Philipp Eickholt[2], Thorsten Deilmann[3], Koji Miyamoto[4], Peter Krüger[1], Markus Donath[2], and Michael Rohlfing[1] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Physikalisches Institut, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [3]Center for Atomic-Scale Materials Design (CAMD), Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark — [4]Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan

Transition metal dichalcogenides (TMDCs) are a fascinating new class of semiconductors, which attracted a lot of interest in the past few years. They are promising materials for new optical and electronic devices on the nanoscale. Here, we focus on one of the less studied members of this group: ReSe$_2$. In contrast to other TMDCs, it grows in a distorted $1T$ structure, which leads to new anisotropic properties.

We present electronic and excitonic spectra for both monolayer and bulk ReSe$_2$ within many-body perturbation theory (MBPT). For this, we apply the GW-BSE (Bethe-Salpeter equation) approach within the efficient LDA+GdW approximation [1]. Our results on the quasiparticle band structure are complemented with experimental ARPES data. Based on the band structure we investigate the excitons. The lowest four states show distinct dipolar characteristics, which is in contrast to many other TMDCs.

[1] M. Rohlfing, Phys. Rev. B. **82**, 205127 (2010)

O 70.2 Wed 10:45 WIL A317

Fabrication and characterization of coupled TMDC heterostructures — •Borja V. Pano[1,2], Bastian Miller[1,2], Alexander W. Holleitner[1,2], and Ursula Wurstbauer[1,2] — [1]Walter Schottky Institute and Physics-Department, Technical University Munich, Am Coulombwall 4a, 85748 Garching — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 Munich, Germany

Atomically thin transition metal dichalcogenides (TMDC) have emerged as an exciting class of two-dimensional (2D) semiconductors with unique electronic and optoelectronic properties, and are of interest for both fundamental research and novel device applications.

We investigate heterostructures of four different TMDC monolayers (MoS$_2$, WS$_2$, MoSe$_2$, WSe$_2$). Due to the formation of a type II band alignment between the layers and the strong Coulomb binding energy in 2D TMDC, these devices open a promising path for studying long-lived interlayer excitons, where bound electrons and holes are localized in different layers.

A polymer-based dry transfer technique is used to vertically stack micromechanical cleaved monolayers with angle alignment of the crystal axes. We characterize the heterostructures through optical and atomic force microscopy, Raman and photoluminescence spectroscopy. We observe strong signatures of interlayer coupling.

We acknowledge the financial support by the DFG and the excellence cluster Nanosystems Initiative Munich (NIM).

O 70.3 Wed 11:00 WIL A317

Switchable white graphene: electrochemical surface science of the boron nitride nanomesh — •Stijn Mertens — TU Wien, Institut für Angewandte Physik, Wiedner Hauptstraße 8-10/134, 1040 Vienna, Austria — KU Leuven, Chemistry Department, Celestijnenlaan 200F, 3001 Leuven, Belgium

On Rh(111), a monolayer of hexagonal boron nitride (h-BN) forms a so-called nanomesh superstructure [1] with a 3.2-nm lattice constant and strong electronic corrugation, useful for trapping atoms and molecules [2,3].

We show by electrolyte-to-vacuum transfer experiments and thermal desorption spectroscopy that hydrogen underpotential deposition (H upd) [4] leads to submonolayer quantities of hydrogen intercalated between the h-BN overlayer and Rh(111). In situ STM reveals that this lifts the corrugation of the nanomesh and is fully reversible under potential control. Copper upd is used to quantify the defect density in the nanomesh, and to determine the electrochemical window where the nanomesh is stable. Dynamic contact angles of an electrolyte drop show that the microscopic change within the 2-dimensional material leads to a macroscopic effect related to a 10% change in adsorption energy [4]. The static friction on the other hand, which can be extracted by extending the Young equation for non-equilibrium effects, remains unchanged for the surface in the two states.

[1] Corso et al., Science 303 (2004) 217. [2] Berner et al. Angew. Chem., Int. Ed. 46 (2007) 5115. [3] Dil et al. Science 319 (2008) 1824. [4] Mertens, Greber et al. Nature 534 (2016) 676.

O 70.4 Wed 11:15 WIL A317

In-situ LEEM investigation of the growth of hexagonal boron nitride on metal surfaces — •Janina Felter, Markus Franke, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and Jülich Aachen Research Alliance (JARA)-Fundamentals of Future Information Technology, Germany

Hexagonal boron nitride (hBN) is a prominent and frequently studied member of the family of two-dimensional (2D) materials. Due to its structural and electronic properties, in particular its insulating nature, it is of highest interest as part of hetero-epitaxial systems in conjunction with other 2D materials or organic thin films. However, the production of high quality hBN monolayers and organic thin films on hBN necessitates a deep understanding of nucleation and growth of these materials. Here, we present a detailed in-situ and real-time study of the growth of hBN monolayers on Cu(111) using Low-Energy Electron Microscopy (LEEM). We correlate the results with structural information obtained by μLEED and discuss the influence of substrate temperature, growth rate and movement of step edges.

O 70.5 Wed 11:30 WIL A317

Time-of-Flight Secondary Ion and Neutral Mass spectrometry of particles ejected from 3D and 2D materials during irradiation with highly charged and swift heavy ions — •Philipp Ernst[1], Florian Meinerzhagen[1], Matthias Herder[2], Stephan Sleziona[1], Andreas Wucher[2], and Marika Schleberger[1] — [1]University Duisburg-Essen, AG Schleberger, Germany — [2]University Duisburg-Essen, AG Wucher, Germany

We have studied the ionization probability for strontium titanate bombarded by energetic ions, i.e. swift heavy ions (SHI) and highly charged ions (HCI). Strontium titanate is a dielectric and as such is known to be very sensitive to both, SHI and HCI irradiation, which result in characteristic surface modifications [1,2]. Therefore, it has been postulated that both projectile types trigger similar mechanisms leading to these modifications. To test this hypothesis, we compare time-of-flight mass spectra taken during irradiation with SHI at different electronic stopping powers (dE/dx) and with HCI with varying potential energy (^{129}Xe ions with a potential energy from E_{pot} 4.5 up to 59 keV by constant kinetic energy E_{kin}), respectively. Both, emitted secondary ions (SIMS) and secondary neutrals (SNMS), were detected in order to determine differences of the ionization probability. To further test if the spatial distribution of the energy deposition (HCI a few nm, SHI up to tens of microns) does play a role, exemplary measurements with a 2D dielectric have been performed.

[1] F. Meinerzhagen, et al. Rev. Sci. Instr, 87 (2016) 013903.

[2] F. Aumayr, et al. J. Phys. Condens. Matter, 23 (39) (2011).

O 70.6 Wed 11:45 WIL A317

A monolayer of MoS$_2$ on Au(111) as a decoupling layer for single molecules — •Christian Lotze, Nils Krane, Robert Steyrleuthner, Robert Bittl, Jan Behrends, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin

Thiophene based molecules are commonly used for semiconducting devices like solar cells or light emitting diodes. In order to optimize these, a detailed understanding of the molecules electronic structure and the environmental influence on the latter is of great interest.

Scanning tunneling spectroscopy (STS) allows to address individual molecules in a precisely known surrounding. However, it bears the drawback that it requires a conductive substrate. Deposition of organic molecules on a metal substrate leads to strong hybridization of the electronic states. Preservation of the molecular character requires the inclusion of thin band-gapped materials.

Here, we present STS experiments performed on 2,5-bis(3-dodecylthiophen-2-yl)thieno[3,2-b]thiophene-n (BTTT-n; n=1,2) molecules adsorbed on a single layer molybdenum disulfide (MoS$_2$) on

Au(111). We show that it acts as an effective decoupling layer. Differential conductance spectra of the molecules exhibit a multitude of sharp characteristic peaks, that are connected to the highest occupied molecular orbital. We propose that these originate from a surprisingly effective excitation of vibronic resonances by the tunneling electrons.

O 70.7 Wed 12:00 WIL A317

Surface-confined Mott transition in the strongly correlated compound 1*T*-TaSe$_2$ — •Florian Diekmann, Christian Sohrt, Kerstin Hanff, Lars-Philip Oloff, Arndt Quer, Matthias Kalläne, and Kai Rossnagel — Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany

The surface associated modification of the electronic structure of 1*T*-TaSe$_2$ in the commensurate charge density-wave (CDW) state is examined by utilising photon energy dependent X-Ray photoemission spectroscopy. In particular, the CDW-induced splitting of the Ta 4*f* core levels is probed over a wide range of photon energies from 80 eV to 6 keV corresponding to a variation of the information depth from extreme surface to effective bulk sensitivity. The measured depth-dependent core-level splitting corroborates the idea of a surface-confined Mott transition due to a modified CDW at the surface [1,2].

[1] L. Perfetti *et al.*, Phys. Rev. Lett. **90**, 166401 (2003).

[2] C. Sohrt *et al.*, Faraday Discuss. **171**, 243 (2014).

O 70.8 Wed 12:15 WIL A317

Insights into structure and binding of micron-sized hexagonal boron nitride islands on Ir(111) — •Marin Petrović, Michael Horn-von Hoegen, and Frank-J. Meyer zu Heringdorf — Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany

Single-layer hexagonal boron nitride (hBN) islands have been synthesized on Ir(111) via chemical vapor deposition (CVD) of borazine at various temperatures. By using low-energy electron microscopy (LEEM) as the main experimental tool, two types of hBN islands were identified which differ in their shape (triangular and trapezoidal) and in their rotational registry with respect to the iridium. Moreover, photoemission electron microscopy (PEEM) and IV-LEEM spectroscopy measurements show that the two island types exhibit different work functions and interaction strengths with iridium, which is proposed to be the origin of their divergence in shape and growth modes. In addition, it is found that for CVD synthesis above ≈950 °C additional boron islands are formed on the iridium surface, which is a result of increased decomposition of hBN and significant solubility of boron in iridium at high temperatures.

O 70.9 Wed 12:30 WIL A317

Intervalley scattering dynamics in MoS$_2$ imaged by two-photon photoemission with a high-harmonic probe — •Robert Wallauer, Johannes Reimann, Nico Armbrust, Jens Guedde, and Ulrich Hoefer — Fachbereich Physik und Zentrum für Materialwissenschaften Philipps-Universität, 35032 Marburg, Germany

We will report on the application of time- and angle-resolved two-photon photoemission (2PPE) with a high-harmonic probe for the investigation of the electron dynamics of MoS$_2$ in momentum space. For this purpose, we combined a high-repetition rate high-harmonic source with tunable femtosecond pump pulses and a 3D (k$_x$, k$_y$, E) electrostatic electron spectrometer. At our high-harmonic photon energy of 23.5 eV we essentially probe only the first layer, which is not necessarily equal to a bulk sample.

We used this setup to study the electron dynamics in the conduction band of MoS$_2$ after optical excitation with different pump photon energies. Thereby we showed that optical excitation above the A exciton resonance at 1.8 eV with 2.05 eV pump pulses results in an immediate occupation of the conduction band at K followed by an ultrafast transfer to the conduction band minimum at Σ [1]. Subsequently, the occupation at both high-symmetry points decays slowly on a ps timescale. We will present new data for pump photon energies in the range of 1.8 - 2.1 eV and show how the dynamics of this transfer depend on the excess energy above the exciton resonance.

[1] R. Wallauer et al., Appl. Phys. Lett. 109, 162102 (2016).

O 70.10 Wed 12:45 WIL A317

Theoretical aspects in the investigation of intrinsic magnetic order in monolayer FePS3 — •Pilkwang Kim[1], Jae-Ung Lee[2], Sungmin Lee[1,3], Ji Hoon Ryoo[1], Soonmin Kang[1,3], Tae Yun Kim[1], Cheol-Hwan Park[1,4], Je-Geun Park[1,3], and Hyeonsik Cheong[2] — [1]Department of Physics and Astronomy, Seoul National University (SNU), Seoul 08826, Korea — [2]Department of Physics, Sogang University, Seoul 04107, Korea — [3]Center for Correlated Electron Systems, Institute for Basic Science (IBS), Seoul 08826, Korea — [4]Center for Theoretical Physics, Seoul National University (SNU), Seoul 08826, Korea

It has been a while since Onsager established that there can be a phase transition at a finite temperature in the two-dimensional (2D) Ising system. However, experimental verification of such long-range magnetic order has been mostly limited to the magnetism arising from extrinsic effects such as defects and chemical dopants. Bulk iron phosphorus trisulfide (FePS3) is a van der Waals material with an Ising-type antiferromagnetic order. In this presentation, we discuss the results of our first-principle calculations on the electronic structure and vibrational spectrum of monolayer FePS3. The calculations are compared with the experimental Raman spectra that exhibit several new peaks emerging below the Néel temperature. We demonstrate that the drastic changes in the Raman spectra can be understood in terms of the zone-folding effects, which suggests that monolayer FePS3 exhibits intrinsic anti-ferromagnetic order.

O 71: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - IV

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

Invited Talk O 71.1 Wed 10:30 GER 38

Electronic excitations in 2D materials and heterostructures — •Kristian Sommer Thygesen — Technical University of Denmark, Lyngby, Denmark

Atomically thin two-dimensional (2D) materials have recently emerged as a new class of materials with unique and highly tunable optoelectronic properties. Different 2D crystals can be stacked to form van der Waals heterostructures (vdWH) where the individual 2D layers are held together by weak van der Waals forces leading to atomically well-defined interfaces. This fascinating scenario opens up the possibility of designing heterostructures with tailored electronic or optical properties. I will give a general introduction to the electronic properties of 2D materials, including characteristic features of their dielectric screening and collective excitations with special emphasis on the challenges related to their ab-initio description. I will show how the dielectric function of a given 2D material can be controlled by embedding it into a vdWH, and how this in turn can be used to control the band structure, exciton binding energies or the plasmon dispersion in 2D materials.

O 71.2 Wed 11:00 GER 38

Charge and energy transport at the nanoscale: A DFT perspective — •Florian G. Eich, Fabio Covito, and Angel Rubio — Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, D-22761 Hamburg, Germany

Understanding the interplay between charge and energy transport at the nanoscale paves the way for novel thermoelectric devices, which may prove useful for the development for sustainable energy sources. However, concepts, such as heat flow, temperature and entropy are only well-established at the macroscopic level for slow dynamics. This raises the question about whether these concepts can be employed for small length and short time scales. We will present our recent efforts to use a time-dependent density-functional theory framework, dubbed nonequilibrium thermal DFT, in order to generalize temperature and heat or energy flow to the microscopic regime. To this end we will highlight the analogy of the formally exact microscopic equations of motion for charge density and energy density in thermal DFT to the macroscopic equations of motion of hydrodynamics. Furthermore, we will present first result using our approach to compute transient energy energy currents induced by a temperature gradient and show that in the steady-state limit persistent temperature oscillations develop.

O 71.3 Wed 11:15 GER 38

Conductance of aromatic and antiaromatic molecular circuits — Narendra P. Arasu and •Héctor Vázquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

Molecular structures with delocalized conjugated orbitals play an essential role in molecular transport due to their high conductance and small attenuation factors. While much work has been done on aromatic molecules, some studies have shown that conductance actually decreases with aromaticity [1].

In this talk I will discuss the effect of (anti)aromaticity on conductance. I will show results of first-principles transport calculations for an aromatic-antiaromatic pair of molecules and compare with experiment. Conductance is calculated using DFT and NEGF including corrections to the DFT level positions. The corrected conductance values are in very good agreement with experiment. We find that the conductance of the antiaromatic molecule is much higher than that of its aromatic counterpart. Calculations show this to be a consequence of the smaller HOMO-LUMO gap of the antiaromatic complex as well as on the molecular level alignment at the junction [2].

[1] W. Chen, H. Li, J.R. Widawsky, C. Appayee, L. Venkataraman, and R. Breslow, J. Am. Chem. Soc. 136 918 (2014).

[2] S. Marqués-González, S. Fujii, J.-Y. Shin, H. Shinokubo, N.P. Arasu, H. Vázquez and M. Kiguchi, (to be submitted).

O 71.4 Wed 11:30 GER 38

Current-induced cooling of Carbene-based molecular junctions: role of electrodes structure — •Giuseppe Foti and Héctor Vázquez — Institute of Physics, Czech Academy of Sciences Cukrovarnicka 10, Prague 6

In this talk I will present our first principles calculations based on density functional theory (DFT) plus Nonequilibrium Green's functions (NEGF) of the current-induced heating and cooling dynamics of a series of Carbene-based molecular junctions [1]. I will show how the atomistic details of electrode terminations have a strong impact on the heating dynamics of the junctions and how they can maximize the cooling of the system. In the cases where the molecule is attached to blunt leads and the electronic coupling to bulk states is strong the cooling efficiency of the most active vibrational modes decreases monotonically as bias increases. This results in the heating of the junction. On the other hand, when the molecule is connected to sharp electrode terminations such as chain-like structures, which can be formed experimentally when the metal-molecule bond is mechanically strong, and the electronic coupling to electrode states is weak, the cooling efficiency shows a non-monotonic behavior. It first decreases as a function of voltage but then increases at relatively high biases, effectively cooling down the junction [2]. These results reveal the important role of the atomistic structure of metal-molecule interface in the current-induced damping of localized molecular vibrations.

[1] Foti, G.; Vázquez, H. Nanotechnology 2016, 27, 125702.

[2] Foti, G.; Vázquez, H. submitted

O 71.5 Wed 11:45 GER 38

DFTB-based recursive Green's function algorithms for electron transport in quasi-1D systems — •Fabian Teichert[1,2,4], Andreas Zienert[3,4], Jörg Schuster[4], and Michael Schreiber[2] — [1]Dresden Center for Computational Materials Science (DCMS), Dresden, Germany — [2]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [3]Center for Microtechnologies (ZfM), Technische Universität Chemnitz, Chemnitz, Germany — [4]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Within the last decades, quantum transport theory and density functional theory have become very important for predicting the electronic properties of new materials and future electronic devices.

We focus on the problem of improving quantum transport algorithms for large quasi-1D systems which are enormously time-consuming today. We combine the density functional tight binding (DFTB) approach with the recursive Green's function formalism (RGF), which is very effective for such systems. First, we show how to improve the RGF for the case of randomly distributed real defects. For this, we use the steps of the renormalization decimation algorithm (RDA), which is part of the electrode calculation. Second, we show how to improve the calculation of the surface Green's functions of electrodes which have a long unit cell. Here, we employ the decimation technique to reduce the dimensionality of the periodic Hamiltonian matrix, leading to effective matrices, which are treated by the RDA. Finally, we apply these algorithms to carbon nanotubes and present our results.

O 71.6 Wed 12:00 GER 38

Conditions for formation of two-dimensional electron gas at the LaFeO$_3$/SrTiO$_3$ — •Igor Maznichenko[1], Sergey Ostanin[1], Arthur Ernst[2], Ingrid Mertig[1,2], Katayoon Mohseni[2], Holger L. Meyerheim[2], Eberhard K.U. Gross[2], Pengfa Xu[3], Wei Han[3], Philip M. Rice[3], Jaewoo Jeong[3], Mahesh G. Samant[3], and Stuart S.P. Parkin[2,3] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [3]IBM Almaden Research Center, 650 Harry Road, San Jose, California 95120, USA

The formation of a conducting two dimensional electron gas (2DEG) at the interface between two insulating oxide layers was explained theoretically for atomically and chemically abrupt interfaces via polar discontinuity.

Here we show that a 2DEG is formed at the interface between thin layers of lanthanum ferrite, LaFeO$_3$ (LFO), that are more than 3 unit cells thick, when grown epitaxially on SrTiO$_3$ (STO) (001). The interface property highly depends on the surface property of TiO$_2$ terminated STO. The interface is conducting if the STO is not annealed in an oxygen environment prior to the LFO growth, while insulating if the STO is annealed.

First principles calculations reveal that a 2DEG should be realized for an ideal interface but that modest chemical intermixing suppresses it. These calculations also show that the presence of oxygen vacancies supports 2DEG formation due to electronic doping.

O 71.7 Wed 12:15 GER 38

Thermal Renormalization of the Electronic Structure: Trends across Chemical and Structural Space — •Honghui Shang[1], Christian Carbogno[1], Patrick Rinke[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Aalto University, Helsinki, Finland

Advances in electronic structure theory now allow us to compute the renormalization of the electronic structure due to thermal nuclear motion from first principles [1]. In this work, we present a systematic computational assessment of this renormalization for 82 octet binaries in both the zincblende and the rocksalt structure. After validating our computational approach that is based on finite-differences [2] and Fröhlich-type corrections [3] for polar materials, we discuss and analyze the observed trends: For instance, we find that most materials exhibit the expected band-gap reduction upon temperature increase; however, some materials (e.g. CuCl and CdO) do not follow this trend and exhibit the opposite behavior. We discuss the underlying electronic mechanism as well as its dependence on the chemical composition and structure of the material. In this context, also the sensitivity of such calculations with respect to the chosen basis set and exchange-correlation functional (LDA, PBE, HSE06) are critically investigated.

[1] F. Giustino, arXiv:1603.06965 (2016).

[2] G. Antonius, *et al. Phys. Rev. Lett.* **112**, 215501 (2014).

[3] J. P. Nery and P. B. Allen, *Phys. Rev. B* **94**, 115135 (2016).

O 71.8 Wed 12:30 GER 38

Spin-wave excitations and electron-magnon scattering from many-body perturbation theory — •Mathias C.T.D. Müller, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We study the spin excitations and the electron-magnon scattering in bulk Fe, Co, and Ni within the framework of many-body perturbation theory as implemented in the full-potential linearized augmented-plane-wave method. Starting from the *GW* approximation we obtain a Bethe-Salpeter equation for the magnetic susceptibility treating single-particle Stoner excitations and magnons on the same footing. Due to approximations used in the numerical scheme, the acoustic magnon dispersion exhibits a small but finite gap at Γ. We analyze this violation of the Goldstone theorem and present an approach that implements the magnetic susceptibility using a renormalized Green function instead of the non-interacting one, leading to a substantial improvement of the Goldstone-mode condition [1]. Finally, we employ the solution of the Bethe-Salpeter equation to construct a self-energy that describes the scattering of electrons and magnons. The resulting renormalized band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy. We also see kinks in the electronic bands, which we

attribute to electron scattering with spatially extended spin waves.
[1] Müller *et al.*, Phys. Rev. B **94**, 064433 (2016).

O 71.9 Wed 12:45 GER 38

Charged supercells revised: Small Polarons in Oxides with proper account for long-range polarization — •Sebastian Kokott, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, DE

Formation of small polarons (excess charges localized within one unit cell) often determines charge mobility and optical absorption in oxide materials. In this work, we address two important challenges in the DFT description of small polarons: sensitivity to the errors in exchange-correlation (XC) treatment and finite-size effects in supercell calculations. The polaron properties are obtained using a modified neutral potential-energy surface (PES) [1]. Using the hybrid HSE functional and considering the whole range $0 \leq \alpha \leq 1$ of exact exchange, we show that the modified PES model significantly reduces the dependence of the polaron level and binding energy in MgO and TiO$_2$ on the XC treatment. It does not eliminate the dependence on supercell size. Based on Pekar's model [2], we derive the proper long-range behavior of the polaron and a correction that allows to obtain the polaron properties in the dilute limit (tested for supercells containing up to 1,000 atoms). The developed approach reduces drastically the computational time for exploring the polaron PES, and gives a consistent description of polarons for the whole range of α. It allows us to find a self-trapped hole in MgO that is noticeably more stable than reported previously.—[1] B. Sadigh *et al.*, PRB **92**, 075202 (2015); [2] S.I. Pekar, ZETF **16**, 335 (1946). This work received funding from the Leibniz ScienceCampus "GraFOx".

O 72: Oxide and Insulator Surfaces: Adsorption I

Time: Wednesday 10:30–12:45 Location: WIL C107

O 72.1 Wed 10:30 WIL C107

Detection of Protons on Atomically Defined Cobalt Oxide Thin Films on Ir(100). An Infrared Reflection Absorption Spectroscopy Study of D2O and Deuterated Benzoic Acid on Co3O4(111), CoO(111), CoO(100) on Ir(100) — •Matthias Schwarz, Susanne Mohr, Chantal Hohner, Kristin Werner, Tao Xu, and Jörg Libuda — Lehrstuhl für Physikalische Chemie II Friedrich-Alexander-Universität Erlangen-Nürnberg

We applied infrared reflection adsorption spectroscopy (IRAS) in a comparative surface science model study under ultra-high vacuum (UHV) conditions to investigate the interaction of D2O and deuterated benzoic acid (D-BA) with well-ordered Co3O4(111), CoO(111) and CoO(100) thin films on Ir(100) For both, water and D-BA, nature and thermal stability of the formed surface species are strongly depend on the surface structure. On Co3O4(111), water forms partially dissociated clusters with strongly temperature dependent size and structure. On the oxygen-terminated CoO(111) surface, water can dissociate and bind to defect sites only. On CoO(100) only coordination of molecular water at 200 K is observed. For higher temperatures no protons were found. D-BA forms benzoates on all three surfaces and we could identify the surface OD groups formed in this process. On Co3O4(111) and CoO(111) the protons and the benzoates show a broad distribution of chemical states. In sharp contrast, a well-defined coadsorbate layer consisting of carboxylates and protons is found on CoO(100).

O 72.2 Wed 10:45 WIL C107

Hungry Porphyrins: Protonation and Self-Metalation of Tetraphenylporphrin on TiO$_2$(110) - 1 × 1 — •Julia Köbl[1], Tao Wang[2], Cici Wang[2], Martin Drost[1], Fan Tu[1], Qian Xu[2], Huanxin Ju[2], Daniel Wechsler[1], Matthias Franke[1], Haibin Pan[2], Hubertus Marbach[1], Hans-Peter Steinrück[1], Junfa Zhu[2], and Ole Lytken[1] — [1]Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 — [2]National Synchrotron Radiation Laboratory, 42 S Hezuohua Road, Hefei, 230029, China

In order to obtain a detailed understanding of organic electronic devices such as dye-sensitized solar cells, one has to characterize the interactions of organic molecules with oxide substrates at the atomic level. Thus, we have studied the adsorption and self-metalation of tetraphenylporphyrin (2HTPP) on TiO$_2$(110) - 1 × 1 with X-ray Photoelectron Spectroscopy (XPS) and Scanning Tunneling Microscopy (STM). Upon adsorption at room temperature, the first monolayer of 2HTPP is protonated, forming porphyrin diacid (4HTPP^{2+}). As the surface is heated to 400 K, all unprotonated 2HTPP molecules in the second layer metalate, forming titanyl tetraphenylporphyrin (TiOTPP), but the protonated molecules in the first layer stay intact. As the surface is heated further to 550 K even the protonated 4HTPP^{2+} molecules metalate and only TiOTPP remain on the surface[a]. Supported by the DFG through FOR 1878 (funCOS), the Chinese Scholarship Council and BayCHINA.

[a] Köbl et al., Chemistry Select, 2016, 1, 6103 - 6105.

O 72.3 Wed 11:00 WIL C107

Insights into the adsorption of SO$_2$ on the rutile (110) surface from first principles — •Thomas Teusch and Thorsten Klüner — Carl-von-Ossietzky-Universität, Oldenburg, Germany

Titanium dioxide is well known for its photocatalytic activity. One example for an industrial applied reaction is the synthesis of sulfonic acids [1].

In order to simulate this reaction systematically with state-of-the-art calculations, the interaction between SO$_2$ and the rutile surface needs to be investigated in detail.

Therefore, we modelled the rutile (110) surface with respect to the surface energy and investigated preferred adsorption sites of SO$_2$ in the ground and excited state.

In this work we present first results of the adsorbate-rutile interaction within density functional theory (DFT) using the Crystal14 [2] program package.

[1] Parrino, F., Ramakrishnan, A., Kisch, H. Angew. Chem. 2008, 47, 7107 - 7109

[2] Dovesi, R., Saunders, V. R., Roetti, C., Orlando, R., Zicovich-Wilson, C. M., Pascale, F., Civalleri, B., Doll, K., Harrison, N. M., Bush, I. J., D'Arco, Ph., Llunell, M., Causà, M., Noël, Y. Crystal14, University of Torino, 2014

O 72.4 Wed 11:15 WIL C107

Diffusion barriers block defect occupation on reduced CeO2(111) — P. G. Lustemberg[1], Y. Pan[2], R. Pérez[3], M. V. Ganduglia-Pirovano[3], and •N. Nilius[4] — [1]Instituto de Física Rosario, 2000 Rosario, Argentina — [2]Institute of Physics, Chinese Academy of Sciences, 100190 Beijing , China — [3]Instituto de Catálisis y Petroleoquímica, 28049 Madrid, Spain — [4]Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg, Germany

Surface defects are believed to control the adsorption behavior of reducible oxides. We challenge this perception on the basis of a combined STM/DFT study that explores the mechanisms of Au adsorption on reduced CeO2(111). While theory predicts a clear binding preference to O-vacancies, Au atoms were found to populate mostly regular surface sites. Even at elevated temperature, no defect decoration is observed and gold rather aggregates at oxide step edges. Our findings are explained with the polaronic nature of the Au-ceria system, which results in a strongly diabatic diffusion of adatoms. The associated barriers are higher than in the adiabatic regime, in particular if the hopping step couples to an electron transfer between Ce3+ ions in the oxide and ad-gold. As population of O vacancies always requires such a charge exchange, adatom diffusion into the defect is kinetically hindered. Our study thus demonstrates that polaronic effects strongly govern the adsorption behavior, hence the chemistry of reducible oxides.

O 72.5 Wed 11:30 WIL C107

STM study of water adsorption on crystalline Cu2O films — •Christoph Möller and Niklas Nilius — Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg, Germany

A direct band gap of 2.1 eV makes cuprous oxide a promising material for the photocatalytic splitting of water. To explore elementary processes associated with this reaction, we have prepared Cu2O(111) thin films on an Au(111) support and investigated them by low-temperature STM. Water exposure below 100 K gives rise to a weakly-bound, physisorbed state of water that cannot be imaged with STM. After annealing to 200 K, a chemisorbed state is reached and small, magic H2O clusters as well as extended, flat islands appear on the surface at dosages below and above 0.1 ML, respectively. Although water islands seem to be amorphous at first glance, protrusions resolved in the STM exhibit a smeared, hexagonal pair-correlation function. Its periodicity of 6 Å matches the Cu2O(111) lattice parameter, suggesting that the molecules populate characteristic sites on the oxide surface, e.g. low-coordinated Cu ions. Further insight into water binding comes from TDS measurements performed on the same system.

O 72.6 Wed 11:45 WIL C107

In-situ Spectro-electrochemical Infrared Investigations at Atomically-Defined Pt/Co3O4(111) Model Catalysts — •Firas Faisal, Olaf Brummel, Manon Bertram, Corinna Stumm, and Jörg Libuda — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

We prepared in ultra-high-vacuum (UHV) highly ordered thin films of Co3O4(111) on Ir(100) and deposited Pt nanoparticles to obtain model catalysts for electrochemical investigations. The model systems were directly transferred from UHV into the spectro-electrochemical cell and back without contact to ambient conditions. As a probe reaction we used the electrooxidation of CO, monitored by electrochemical infrared-reflection absorption spectroscopy (EC-IRRAS) in thin film configuration. All samples were characterized by low-energy electron diffraction (LEED) and Auger electron spectroscopy (AES) before and after the electrochemical treatment. We identified a pH and potential window in which the Co3O4(111) film is perfectly stable in the electrochemical environment. This allowed us to explore potential-dependent differences in the CO site occupation on the UHV-prepared supported model catalyst in comparison to a Pt(111) reference sample prepared by flame annealing. Specifically, we observed strong suppression of bridging CO on Pt facets and identify additional strongly bound CO at low coordinated Pt atoms which persists at the electrode up to high electrode potentials.

O 72.7 Wed 12:00 WIL C107

The effect of Ni substitutional defects on the structure and chemical properties of MgO surfaces — •Aliaksei Mazheika and Sergey V. Levchenko — Fritz-Haber-Institut der MPG

Ni-MgO solid solutions are promising materials for catalytic reduction of CO_2 and dry reforming of CH_4. To explain the catalytic activity, an *ab initio* study of Ni-substitutional defects in MgO (Ni_{Mg}) has been performed. At first, the validation of the theory level was done. We compared results of CCSD(T) embedded-cluster calculations of Ni_{Mg} formation energies and adsorption energies of CO, CO_2 and H_2 on them to the HSE(α) hybrid DFT functional with the fraction of the exact exchange α varied between 0 and 1 [1]. HSE(0.3) was found to be the best compromise in this study. Our periodic HSE(0.3) calculations show that Ni_{Mg} defects are most stable at corner sites, followed by steps, and are least stable at (001) terraces. Thus, Ni-doping stabilizes stepped MgO surfaces. The dissociative adsorption of H_2 on the terrace is found to be endothermic (+1.1 eV), whereas on (110) surface with Ni_{Mg} it is highly exothermic (−1.6 eV). Adsorbed CO_2 is also significantly stabilized (−0.6 vs. −2.2 eV). These findings explain recent microcalorimetry measurements of H_2 and CO_2 adsorption at doped Ni-MgO samples [2].—[1] A. Mazheika and S.V. Levchenko, DOI: 10.1021/acs.jpcc.6b09505; [2] A. Mazheika, M.-M. Millet, S. Wrabetz, A. Tarasov, E. Frei, S.V. Levchenko, A. Trunschke and R. Schlögl, manuscript in preparation.

This work was funded by the UNICAT cluster of excellence.

O 72.8 Wed 12:15 WIL C107

Enhanced photocatalytic activities of net-like hematite nanoparticle/graphene oxide composite and mechanism study — •Huanming Zhang[1], Min Zhou[1], Yang Xu[1], Fanna Meng[2], Lihong Qi[2], Yujin Chen[2], and Yong Lei[1] — [1]Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, Prof-Schemidt-Strasse 26, 98693 Ilmenau, Germany — [2]Key Laboratory of In-Fiber Integrated Optics, Ministry of Education, College of Science, Harbin Engineering University, 150001 Harbin, China

In photocatalytic water oxidation, hematite possesses many attractive features, for instance favorable optical band gap (approximately 2.1 eV), chemical stability, natural abundance, nontoxicity and low cost. However, its surface reaction kinetics is sluggish. Herein, a facile strategy was developed to fabricate net-like hematite nanoparticle/graphene oxide (GO) composite (NHG), in which the degree of oxidization of GO could be controlled by simply changing annealing time, and GO replaces part of α-Fe2O3 as the reaction interface to speed up the oxygen evolution rate. NHG with GO of appropriate oxidization degree and content exhibited much higher photocatalytic activities than α-Fe2O3 nanorods and commercial α-Fe2O3. The strategy presented here could be expanded as a general method to synthesize other types of photocatalysts modified with GO for applications in photocatalysis.

O 72.9 Wed 12:30 WIL C107

Structure determination of the $(7x\sqrt{3})$rect phase on Ag(111) — •Regina Wyrwich[1], Travis Jones[2], Wolfgang Moritz[1], Sebastian Günther[3], Martin Ehrensperger[1], Sebastian Böcklein[1], Tevfik Menteş[4], Andrea Locatelli[4], Miguel Niño[4], Simone Piccinin[5], Axel Knop-Gericke[2], Robert Schlögl[2], and Joost Wintterlin[1] — [1]Ludwig-Maximilians-Universität München, Germany — [2]Fritz-Haber-Institut Berlin, Germany — [3]Technische Universität München, Germany — [4]Sincrotrone Trieste S.C.p.A., Italy — [5]CNR-IOM Demicritos Trieste, Italy

The so-called ‘electrophilic oxygen’, characterized in XPS by an O 1s energy of 530.7 eV, is considered to be responsible for the Ag-catalyzed epoxidation of ethylene, a large-scale industrial process. The chemical nature of this oxygen species has remained unclear, but is certainly different from the known oxygen-induced reconstructions on the silver surface. A $(7x\sqrt{3})$rect phase on Ag(111) incorporates this oxygen species, but all attempts to find a structure model have failed for a long time. Recent DFT calculations revealed that only covalently bound oxygen species exhibit O 1s energies in this region, which led to the consideration of oxygen bound to sulfur, a common contamination in ethylene. Based on a model proposed by DFT we have now solved the structure by a LEED I(V) analysis. The structure involves a reconstruction consisting of alternating rows of Ag triangles and SO_4 units along the $\sqrt{3}$ direction of Ag(111). The Ag atoms are found in three different geometries, on hcp, fcc, and bridge position. The findings shed new light on the already complex Ag/O system.

O 73: Nanostructures at Surfaces: Metals, Oxides and Semiconductors III

Time: Wednesday 10:30–13:00 Location: REC/PHY C213

O 73.1 Wed 10:30 REC/PHY C213

Formation of GaP rotational twins at the interface to Si(111) — •Lars Winterfeld, Christian Koppka, Thomas Hannappel, and Erich Runge — Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

We present DFT and Kinetic Monte Carlo results concerning the formation of rotational twins domains (RTDs) of GaP on Si(111). Gallium phosphate is used as a buffer layer on silicon for the growth of III-V nanowires (NWs) on top. Here, (111)-oriented substrates are commonly used, as NWs preferably grow in [111] direction and NWs vertical to the substrate are advantageous for most device architectures. Heteroepitaxial layer growth on Si(111), however, is almost always accompanied by the occurrence of RTDs, which is a crystal defect having detrimental effects on NW growth and therefore on optoelectronical properties. Recently, Koppka et al.[1] could experimentally show that adjusting the growth conditions (temperature, V/III ratio, miscut angle of the substrate, etc.) can tremendously suppress the formation of RTDs to less than 5 vol%. In this talk, we aim for an ab initio understanding of the underlying atomic mechanisms.

[1] C. Koppka et al., Crystal Growth & Design 2016 (doi: 10.1021/acs.cgd.6b00541).

O 73.2 Wed 10:45 REC/PHY C213

Glancing Angle Deposited Silver Nanostructures for Surface Enhanced Raman Scattering Based Sensors — •Christoph Grüner[1], Sachin K. Srivastava[2], Atef Shalabney[2], Ibrahim Abdulhalim[2], Mousa Abu Tier[3], and Bernd Rauschenbach[1,4] — [1]Leibniz Institute of Surface Modification, Permoserstraße 15, 04318 Leipzig, Germany — [2]Department of Electro Optic Engineering, Ben Gurion University of the Negev, Beer Sheva-84105, Israel — [3]Physics Department, Al-Quds University, Jerusalem, Palestine — [4]University Leipzig, Institute of Experimental Physics II, Linnéstr. 5, 04103 Leipzig

Fast and certain determination and quantification of environmental toxics or human blood constituents is of great interest today. Such applications require highly sensitive and specific sensors for biological agents. Self-assembled nanostructure arrays can serve as such sensors. A simple and elegant method to produce these kind of structures is Glancing Angle Deposition (GLAD). This is a physical vapor deposition process, which utilizes the self-shadowing effect that appears at highly oblique particle incidence angles. Thereby, a highly porous films consisting of thin, separated nanostructures is created. The large surface area of these films opens the opportunity to fabricate Surface Enhanced Raman Scattering (SERS) based sensors. This study is focused on growth, surface functionalization and optimization of nanostructured thin silver GLAD films on the examples of highly specific sensors for endocrine disruptors and glycated hemoglobin.

O 73.3 Wed 11:00 REC/PHY C213

Direct visualization of oxidation and reduction of FeO/Au(111) studied by time-resolved STM — •Yijia Li and Jeppe Lauritsen — Gustav Wieds Vej 14, 8000 Aarhus C

Iron oxide (FeO) is of significant interest due to its catalytical reactivity in several reactions such as CO oxidation and water-gas shift reaction, and as precursors for the formation of Fe-based Fischer Tropsch catalysts. The nature and the reaction mechanism of the active sites are fundamental questions to heterogeneous catalysis. Therefore, scanning tunneling microscopy (STM) which is capable to identify the active sites at atomic scale level is employed. Here we studied the oxidation and reduction of FeO islands on Au(111) by oxygen and hydrogen using in-situ STM measurements. It is found that the edges of FeO islands play an essential role for incorporating additional oxygen atoms and O adatoms form triangular bright features assigned to adatom defect loops. The excess O atoms are in different coordination with lattice O atoms and can be removed by molecular hydrogen dosing. On the other hand, upon hydrogen exposures FeO islands are reduced with hydroxyls formed initially on the surface and vacancy defect loops created later on. These vacancy defects can be refilled by oxygen dosing. The reversible appearance of FeO islands depending on whether it is in oxidizing or reducing atmosphere are observed dynamically by time-resolved STM movies and help to distinguish the active sites in redox reactions.

O 73.4 Wed 11:15 REC/PHY C213

On the autocatalytic growth and magnetic properties of Fe nanostructures fabricated via focused electron beam induced processing — •Fan Tu, Martin Drost, Florian Vollnhals, Esther Carrasco, Andreas Späth, Rainer Fink, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen, Germany

Electron beam induced deposition (EBID) was used in combination with autocatalytic growth (AG) processes to lithographically fabricate high purity ($>$ 95%) Fe deposits from the precursor iron-pentacarbonyl in our UHV system [1-3]. In this paper correspondingly fabricated EBID-Fe deposits were investigated in detail by high resolution transmission electron microscopy (HRTEM) and scanning transmission X-ray microscopy (STXM). STXM operated in X-ray magnetic circular dicroism mode at the PoILux beamline (Swiss Light Source) allows in addition to the microscopic insights for a detailed magnetic characterization of the Fe structures depending on their actual shape [3]. We report on the thickness and lateral dimension dependent magnetic coercivity, the chemical nature and the atomic order of the Fe deposits.

This work was funded by the DFG through grant MA 4246/1-2, research unit FOR 1878/funCOS; and the Excellence Cluster Engineering of Advanced Materials granted to the FAU Erlangen-Nürnberg.

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

[2] H. Marbach, Appl. Phys. A., 117 (2014) 987.

[3] F. Tu, et al., Nanotechnology, 27 (2016) 355302.

O 73.5 Wed 11:30 REC/PHY C213

Nanostructured metallic films grown by glancing angle deposition on non-patterned substrates — •Susann Liedtke, Christoph Grüner, and Bernd Rauschenbach — Leibniz Institute of Surface Modification, Permoserstraße 15, 04318 Leipzig, Germany

Glancing angle deposition (GLAD) represents a simple and elegant method to fabricate nanostructured thin films. GLAD combines an oblique angle between incoming particle flux and substrates normal as well as substrate rotation to sculpture nanostructure morphology. On the one hand, the presentation addresses general underlying growth principles of such nanostructured films, for example the nucleation process, self-shadowing and competitive growth. On the other hand, the role of surface diffusion on the morphology of Al-, Ti-, Cr- and Mo-nanostructures grown on unstructured Si(100) substrates at room temperature is discussed. In fact, the selection of these metals covers a wide range of melting points from Al (660 °C) to Mo (2617 °C). Since melting point and surface diffusion are connected, a comparison between those metallic nanostructures reveals possible reasons for the significant differences obtained in growth behavior. The nanostructures are investigated by scanning electron microscopy and x-ray diffraction measurements.

O 73.6 Wed 11:45 REC/PHY C213

Grazing Incidence Small-Angle X-Ray Scattering on Small Sample Volumes Using Large Beams — •Mika Pflüger[1], Victor Soltwisch[1], Jürgen Probst[2], Frank Scholze[1], and Michael Krumrey[1] — [1]Physikalisch-Technische Bundesanstalt, Abbestraße 2-12, 10587 Berlin, Germany — [2]Helmholtz-Zentrum Berlin, Albert-Einstein-Straße 15, 12489 Berlin, Germany

Grazing Incidence Small-Angle X-Ray Scattering (GISAXS) is a versatile tool for the contactless and destruction-free investigation of nanostructured surfaces. However, due to the shallow incident angles used in GISAXS, the spotsize of X-ray beams on the sample is significantly elongated compared to the beam height. Traditionally, this has limited GISAXS measurements to long (several mm) samples. We will present GISAXS measurements of lamellar gratings in Si, with line lengths down to 4 μm. First, we present measurements of single grating targets on an otherwise empty substrate. Using a modified reciprocal-space construction of the intersection of the Ewald sphere with the grating we are able to quantitatively describe the recorded scattering patterns.

For most applications, such as metrological fields in semiconductor manufacturing, target structures are not completely isolated on the sample. We demonstrate that the scattering from the μm sized targets can be separated in reciprocal space from the scattering of the surrounding structures. The possibility to measure very small targets opens GISAXS for new applications in nanoscience and industry.

O 73.7 Wed 12:00 REC/PHY C213

The bismuth bilayer on Bi2Se3(0001) prepared by atomic hydrogen etching studied by scanning tunneling microscopy — •Vasilii Sevriuk[1], Holger Meyerheim[1], Arthur Ernst[1], Mikhail Otrokov[2], Dirk Sander[1], and Evgueni Chulkov[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastian, Spain

Scanning tunneling microscopy (STM) and spectroscopy (STS) has been used to study a Bi bilayer (BL) on Bi2Se3(0001) prepared by atomic hydrogen etching of the Bi2Se3 substrate. This Bi BL has been previously characterized by surface x-ray diffraction [1]. STM images show predominantly an atomically flat surface of the Bi BL, which almost fully covers Bi2Se3. Ten percent of the surface area are covered by depressions, and protrusions are observed on 5% of the surface. The depressions are 0.4 nm deep, and this corresponds to the thickness of the Bi BL. The lateral size of the depressions is from 5 to 10 nm. There are mainly two types of the protrusions with heights of 0.35 and 0.08 nm. We ascribe this to a second Bi BL and to Se atoms on the Bi BL surface, respectively. STS spectra shows a signature of the surface Dirac cone in the electronic structure of the Bi BL/Bi2Se3 structure at -0.2 V sample bias. STS maps reveal the presence of surface areas with different electronic structures. We analyze this data with the help of the first principles calculations.

O 73.8 Wed 12:15 REC/PHY C213

Donor-acceptor-donor molecules for on-surface polymerization — •Dmitry Skidin[1], Frank Eisenhut[1], Justus Krüger[1], Tim Erdmann[2,3], Anton Kiriy[2,3], Brigitte Voit[2,3], Francesca Moresco[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [3]Leibniz-Institut für Polymerforschung Dresden e. V., 01069 Dresden, Germany

One of the main tasks of the modern molecular electronics is the formation of supramolecular functional units for the circuitry at nanoscale. In this regard flexible molecular wires with finite band gap and high conductivity are of essential importance. Therefore, the molecules with alternating donor and acceptor units are perspective precursors for the formation of such wires. [1]

We employ conjugated diketopyrrolopyrrole-based molecules of the donor-acceptor-donor type to grow organic polymers on the surface. After the deposition of individual brominated monomers on Au(111) surface the sample is annealed to promote polymerization via Ullmann coupling. Structural and electronic properties of the stabilized molecular wires can be studied using low-temperature scanning tunneling microscopy and spectroscopy. STM lifting experiments are performed to investigate the conductance of the wires.

References:
1. C. Nacci, F. Ample, D. Bleger, S. Hecht, C. Joachim and L. Grill, Nat. Commun., 2015, 6, 7397.

O 73.9 Wed 12:30 REC/PHY C213

Formation of CuO_2 chains embedded into the Ir(100) surface — •Lutz Hammer[1], Pascal Ferstl[1], Alexander Schneider[1], Florian Mittendorfer[2], and Josef Redinger[2] — [1]Solid State Physics, FAU Erlangen-Nürnberg — [2]Applied Physics, TU Wien

We have investigated the oxidation of submonolayer deposits of copper on an Ir(100) surface by means of STM, quantitative LEED and DFT. Postoxidation of Cu deposits of 0.25 ML or less at temperatures around 800 K leads to the formation of regularly spaced, monatomic wires of twofold oxygen-coordinated Cu atoms. The Cu wires substitute Ir rows of the (100) terraces but are laterally shifted by half a surface unit vector with respect to the Ir positions and lifted up by 0.3 Å for steric reasons. They are flanked at both sides by rows of oxygen atoms being coordinated to one Cu and two Ir atoms each. Between the Cu oxide wires the Ir(100)2×1-O superstructure develops in narrow stripes leading to a combined surface periodicity of $n \times 2$ (or c$(2n \times 2)$) with n = 4, 5, 6 ... depending on the initial Cu coverage. CuO_2 chains closer than fourfold Ir distance are not found which points towards a stabilization of the structure by the intermediate 2×1-O phase. Structural parameters derived from a LEED intensity analysis ($R_P = 0.09$) of the most dense phase (n = 4) coincide within a few picometers with the predictions of corresponding DFT model calculations.

O 73.10 Wed 12:45 REC/PHY C213

Formation of dendritic and point-like silicon-oxide clusters during Chemical Vapor Deposition growth of graphene on copper foils — •Umut Kamber, Cem Kincal, and Oğuzhan Gürlü — Istanbul Technical University, Istanbul, Turkey

Chemical Vapor Deposition (CVD) is a widely employed method to produce large area graphene on metal surfaces. It has been known since the first CVD growth of graphene on copper foils in a quartz tube that some droplet like silicon-oxide contaminants appear on the surfaces. Therefore, optimizing the CVD process for defect free graphene is one of the most intensely studied subtopic in graphene research. We performed systematic experiments by changing CVD conditions to control the shapes and sizes of silicon-oxide particles. We developed a methodology to generate different shapes and sizes of nano scale fractal structures on both graphene/Cu system as well as on bare Cu foils. Parameters most effective on the number of impurities and the formation of fractals were determined to be hydrogen flow during annealing, annealing time and the amount of methane dosing. Lateral Force Microscopy (LFM) measurements were performed in order to investigate whether these particles formed at the graphene/Cu interface or on the graphene layer.

O 74: SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - hybrid and structured electrolytes

Time: Wednesday 11:45–12:45 Location: IFW A

O 74.1 Wed 11:45 IFW A

Morphology and conductivity of nanohybrid block copolymer electrolyte for lithium-ion batteries — •Ezzeldin Metwalli, Maximilian Kaeppel, Simon Schaper, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Polymer electrolyte membranes are promising alternatives to conventional liquid electrolytes in lithium-ion batteries [1]. A key challenge is to achieve a highly ionic conductive solid-state polymer membrane that maintains high-modulus, toughness, and chemical stability. The ionic conductivity in relation to the morphology of a ternary system composed of polystyrene-block-polyethylene oxide (PS-b-PEO) diblock copolymer (DBC) electrolyte, lithium salt and ionic liquid (IL) was investigated. An optimized functional morphology of the hybrid membrane was achieved by enabling highly interpenetrated hard PS and soft PEO/IL domains. The high-modulus glassy PS domain of the nanostructured hybrid membranes offers mechanical stability, while the Li-containing PEO/IL hybrid domain enables the requisite high ionic conductivity. The IL doping enhances the solubilization of the undissociated lithium salt at the PS/PEO domain interface. The pronounced conductivity enhancement of the current Li-ion/IL/DBC hybrid electrolyte compared to other previously reported DBC electrolyte systems is discussed. [1] E. Metwalli et al., ChemPhysChem 2015, 16, 2882.

O 74.2 Wed 12:00 IFW A

Preparation of Electrodes for Li-Ion Batteries from Inexpensive Dirty Silicon — •Richard Schalinski[1], Stefan L. Schweizer[1], and Ralf B. Wehrspohn[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle 06099, Germany — [2]Fraunhofer Institute for Mechanics of Materials IWM, Halle 06120, Germany

With the increased development of renewable energies and electric vehicles in our society, there is a greater demand for high capacity, safe and inexpensive storage technologies. Li-ion batteries are the technology of choice for the use in portable devices. To increase the capacity density of these batteries, nanostructured silicon was introduced as a material for the negative electrode. Commonly, either expensive silane or electrical grade silicon is used as the starting material. We introduce an alternative route by using inexpensive metallurgical grade silicon (purity 98%) as a starting material and purify it using metal assisted chemical etching followed by ball milling to obtain silicon nanoparticles. The Si-nanoparticles where mixed with different binders (CMC, PVdF, Na-Alginate) to form slurries, which were coated onto Cu-substrates. The dried electrodes where investigated by SEM and introduced to further electrochemical testing in a half cell setup. A variation of the chemical contents and pretreatments of the substrates were carried out to optimize the capacity and cyclability of the electrodes.

O 74.3 Wed 12:15 IFW A

Polymer paterning: Solid polymer electrolytes for lithium batteries — Preston Sutton, Ilja Gunkel, and •Ulli Steiner — Adolphe Merkle Institute, Fribourg, Switzerland

Patterning materials at the nanoscale can dramatically influence the performance of batteries. At the Adolphe Merkle Institute (AMI) we are applying expertise in structural control to improve electrodes and electrolytes alike. Two goals of our research are: 1- Take advantage of polymer self-assembly as a facile method to attain predictable morphologies in block copolymers (BCPs) quantifying ionic conductivity as a function of grain size and crystallinity. 2- Use BCPs to decouple mechanical properties from ionic conductivity in electrolytes.

O 74.4 Wed 12:30 IFW A

Modulation of the optical properties of LiMn2O4 via Li-ion transport — •Yug Joshi, Susann Nowak, and Guido Schmitz — Institut für Materialwissenschaft, Universität Stuttgart

Extensive research has been carried out in the fields of Li-ion batteries and electrochromic materials. The present study combines both in investigating the changes in the optical properties of the lithium manganese oxide (LMO), a spinel structured cathode material during an electrochemical reaction. To study this behaviors ion-beam sputtering is used to deposit LMO as the active layer onto a layer of platinum serving as a current collector, over an oxidized silicon wafer. The multilayered sample is then characterized using optical spectroscopy at different lithiation states. The measured data is fitted using Cauchy's model to extract the complex refractive index (refractive index and absorption coefficient) of LMO and its dependence on the lithium content. The reversibility of the optical changes is verified by in-situ optical measurements during multiple charging and dis-charging cycles of LMO. The study reveals a reversible change of the complex refractive index during an electrochemical reaction in the wavelength range of 850-1600nm, making it a suitable candidate for the application of optical switching.

O 75: Ultrafast Electron and Spin Dynamics

Time: Wednesday 15:00–18:45 Location: TRE Phy

O 75.1 Wed 15:00 TRE Phy

Ultrafast electronic band gap control in an excitonic insulator — •Selene Mor[1], Marc Herzog[2], Denis Golez[3], Philipp Werner[3], Martin Eckstein[4], Claude Monney[5], and Julia Stähler[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Potsdam Univ., Potsdam, Germany — [3]Fribourg Univ., Fribourg, Switzerland — [4]MPG for Structural Dynamics, Hamburg, Germany — [5]Zurich Univ., Zurich, Switzerland

Ultrafast control of material properties is of both fundamental and technological interest. Here, we investigated the sub-picosecond dynamics of the electronic structure of Ta_2NiSe_5 by means of time- and angle-resolved photoelectron spectroscopy (trARPES). The system was proposed to support an excitonic insulator (EI) phase below $T_c \approx 328$ K. Such an EI phase is expected to occur in small gap semiconductors with strong electron-hole interaction as excitons can form spontaneously and condense into a ground state with a larger gap. trARPES below T_c reveals a strong excitation-density-dependent valence band depopulation, until absorption saturates at a critical fluence $F_C = 0.2$ mJ cm^{-2}. Below F_C the band gap shrinks transiently due to *photo*enhanced screening of Coulomb interaction, while it widens above F_C for and relaxes after ≈ 1.5 ps. Hartree-Fock calculations reveal that the band gap widening can be explained by *photo*enhancement of the density of the exciton condensate, an effect that persists until the system undergoes interband relaxation. These results prove the possibility to manipulate condensates of excitons with light and to gain ultrafast control of the size of semiconductor band gaps.

O 75.2 Wed 15:15 TRE Phy

Ultrafast photoinduced valence transition in the heavy-fermion compound $YbInCu_4$ — •Lars-Philip Oloff[1], Lukas Wenthaus[2], Kerstin Hanff[1], Giuseppe Mercurio[3], Michael Bauer[1], Wilfried Wurth[2,3], and Kai Rossnagel[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany — [2]DESY Photon Science, 22607 Hamburg, Germany — [3]Department of Physics and Center for Free-Electron Laser Science CFEL, University of Hamburg, 22761 Hamburg, Germany

Upon cooling to a temperature below 42 K, the heavy-fermion compound $YbInCu_4$ undergoes an isostructural transition from a semimetallic, paramagnetic phase with an Yb valence of +3 to a metallic, non-magnetic phase with an Yb valence of +2.85. Here, we combine HHG and FEL-based time-resolved photoemission spectroscopy techniques to gain novel insights into the valence transition in the (sub-)surface region. Through the combination of time-resolved ARPES and time-resolved XPS, we are able to directly track different characteristic spectroscopic signatures of the photoinduced valence change in the (transient) valence and core electronic structure on the femtosecond to picosecond timescale. Our results constitute the first *direct* experimental observation of an ultrafast photoinduced valence change in a heavy-fermion compound.

O 75.3 Wed 15:30 TRE Phy

Ultrafast dynamics in Fe-pnictides analyzed by femtosecond time-resolved x-ray spectroscopy — •Andrea Eschenlohr[1], Mohammadmahdi Afshari[1], Klaus Sokolowski-Tinten[1], Niko Pontius[2], Hidenori Hiramatsu[3], Hideo Hosono[3], Jörg Fink[4], and Uwe Bovensiepen[1] — [1]Univ. Duisburg-Essen — [2]Helmholtz Zentrum Berlin — [3]Tokyo Institute of Technology — [4]IFW Dresden

The electronic properties of Fe-pnictide high temperature superconductors are strongly influenced by the Fe-As distance, which is linked to the superconducting critical temperature [1] and can be modified not only through doping and external pressure, but also transiently by the coherent A_{1g} phonon mode [2]. Element- and orbital-specific x-ray absorption spectroscopy (XAS) provides information on the local electronic structure. By employing femtosecond (fs) x-ray pulses from the BESSY II Femtoslicing source, we perform fs time-resolved XAS of $BaFe_2(AsP)_2$. We observe pump-induced changes at the Fe L_3 edge that are described by the interplay of a transient decrease in absorption, shift in binding energy and peak broadening. This complex behavior will be discussed in the context of electronic and phononic excitations in the Fe-pnictides, in particular photodoping and related changes of the transient chemical potential [3].

We acknowledge funding by the DFG through SPP 1458 and Sfb 1242, and the BMBF through FEMTOSPEX.

[1] Mizuguchi et al., Supercond. Sci. Technol. **23**, 054013 (2010). [2] Rettig et al., PRL **114**, 067402 (2015); Gerber et al., Nat. Commun. **6**, 7377 (2015). [3] Yang et al., PRL **112**, 207001 (2014).

O 75.4 Wed 15:45 TRE Phy

Polarization control of ultrafast photocurrents in the Dirac cone of the topological insulator Sb_2Te_3 — Johannes Reimann[1], Kenta Kuroda[1,2], •Jens Güdde[1], and Ulrich Höfer[1] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, 35032 Marburg — [2]Institute for Solid State Physics (ISSP), University of Tokyo, 277-8581 Chiba, Japan

We present energy-momentum mapping of the photocurrent in the Dirac cone of the topological insulator Sb_2Te_3 by means of time- and angle-resolved two-photon photoemission (2PPE) after optical excitation with ultrashort linear and circular polarized mid-infrared laser pulses. Recently, we have demonstrated that linear polarized mid-infrared pulses permit the generation of photocurrents with ps-lifetime in the initially unoccupied part of the Dirac cone of Sb_2Te_3 by a direct optical excitation [1]. Here, we show that the magnitude and direction of this current depend on the azimuthal orientation of the sample and reflect the threefold symmetry of the surface. For orientations where no photocurrent is generated by linear polarized light, we are instead able to generate a photocurrent by circular polarized light and fully control its direction and magnitude by varying the light helicity.

[1] K. Kuroda *et al.*, Phys. Rev. Lett. **116**, 076801 (2016).

O 75.5 Wed 16:00 TRE Phy

On the origin of photocurrents in the topological insulator Bi$_2$Se$_3$ — •Sophia Ketterl[1], Sebastian Otto[2], Martin Bastian[1], Cornelius Gahl[1], Beatrice Andres[1], Jan Minar[3], Hubert Ebert[3], Thomas Fauster[2], Jürgen Braun[3], and Martin Weinelt[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen — [3]Ludwig-Maximilians-Universität München, Butenandtstr. 5-13, 81377 München

Topological insulators (TIs) host metallic topological surface states (TSS) with helical spin structure. This makes them promising materials for the generation of spin-polarized currents. The TI Bi$_2$Se$_3$ is intrinsically n-doped and thus the TSS at the Γ point with a Dirac cone (DC) dispersion is occupied. Two-photon photoemission (2PPE) experiments have shown that Bi$_2$Se$_3$ exhibits a second, unoccupied DC in the band gap between the second and third conduction band [1].

We studied the excitation of photocurrents with circularly polarized light in the second DC with 2PPE and one-step photoemission calculations. The second DC can be populated from the first DC. We find dichroic photoemission for circularly polarized pump pulses, both at resonant and off-resonant excitation. Only for excitation out of the occupied conduction band, we observe an asymmetric electron population indicating a photocurrent. Thus our results question the topological origin of photocurrents in Bi$_2$Se$_3$ for near-IR excitation [2].
[1] D. Niesner *et. al.*, *Phys. Rev. B* **86**, 205403 (2012).
[2] C. Kastl *et. al.*, *Nat. Commun.* **6**, 6617 (2015).

O 75.6 Wed 16:15 TRE Phy

Spin and Valley Dynamics of Free Carriers in Epitaxial Single-Layer WS$_2$ — •Antonija Grubisic-Cabo[1], Soren Ulstrup[2], Deepnarayan Biswas[3], Jonathon M. Riley[3], Maciej Dendzik[1], Charlotte E. Sanders[1], Marco Bianchi[1], Cephise Cacho[4], Dan Matselyukh[4], Richard T. Chapman[4], Emma Springate[4], Phil D. C. King[3], Jill A. Miwa[1], and Philip Hofmann[1] — [1]Aarhus University, DK — [2]ALS Berkeley, USA — [3]University of St. Andrews, UK — [4]CLF, STFC Rutherford Appleton Laboratory, UK

The semiconducting single-layer (SL) transitional metal dichalcogenides (TMDCs) have been identified as ideal materials for accessing and manipulating spin- and valley-degrees of freedom. The current understanding of the valley properties and excited carrier dynamics relies largely on a photoluminescence and differential absorption measurements. Since excitons dominate the optical response of SL TMDCs, studies of free carriers can only be made indirectly. Here, we use time-resolved ARPES to directly measure free carriers in epitaxial SL WS$_2$ grown on Ag(111). We observe that the optically generated free carrier density in a single valley can be increased by a factor of 2 using circularly polarized light. Moreover, by varying the photon energy of the excitation, we can tune the free carrier density in a given spin-split band. This allows us to selectively excite free electron-hole pairs with a given spin and within a single valley.

O 75.7 Wed 16:30 TRE Phy

Resolving initial stages of carrier thermalization in graphite using time-resolved ARPES with sub-15 fs temporal and near Fourier-limited spectral resolution — •Gerald Rohde[1], Ankatrin Stange[1], Arne Müller[1], Marcel Behrendt[1], Kerstin Hanff[1], Lars-Philip Oloff[1], Lexian Yang[2], Petra Hein[1], Kai Rossnagel[1], and Michael Bauer[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [2]Department of Physics, Tsinghua University, Beijing, People's Republic of China

Carrier dynamics in graphitic materials have been subject of theoretical and experimental investigations in recent years. State-of-the-art experimental approaches address the time scales of excitation and relaxation of hot carrier distributions, aiming to break their evolutions down into the underlying fundamental scattering processes as ultimately governed by electron-electron and electron-phonon interaction. Using time- and angle-resolved photoelectron spectroscopy with sub-15 fs temporal and near Fourier-limited spectral resolution, we report here on the build-up of an out-of-equilibrium electron distribution in graphite within 13 fs and its further evolution during the thermalization towards a Fermi-Dirac distribution. We discuss potential processes causing this transition and compare the results to corresponding data reported for graphene [1]. Moreover, indications for a momentum redistribution of the hot carriers on ultrafast time scales are presented following a momentum-selective photoexcitation.
[1] I. Gierz *et al.*, Phys. Rev. Lett. **115**, 086803 (2015).

O 75.8 Wed 16:45 TRE Phy

Recent developments in the one-step description of time-resolved photoemission — •Jürgen Braun[1], Michael Potthoff[2], and Hubert Ebert[1] — [1]Dept. Chemie, LMU Universität München, Germany — [2]I. Institut für Theoretische Physik, Universität Hamburg, Germany

Recently a theoretical frame for the description of pump-probe photoemission has been developed. The approach is based on a general formulation using the Keldysh formalism for the lesser Green function to describe the real-time evolution of the electronic degrees of freedom in the initial state after a strong pump pulse that drives a system out of equilibrium [1]. As a first application, the theoretical description of two-photon photoemission (2PPE) for Ag(100) within the SPR-KKR-approach is briefly reviewed [2]. This formalism has now been generalized to the ferromagnetic case. First examples of fully spin-polarized 2PPE calculations on Fe(110) will be presented. Finally, a new approach is sketched that allows to account also for dynamical correlations in the non-equilibrium state caused by the pump pulse by means of a corresponding two-time dependent self-energy $\Sigma(z, z')$.

[1] J. Braun, R. Rausch, M. Potthoff, J. Minar, and H. Ebert, Pump-probe theory of angle-resolved photoemission, Phys. Rev. B **91**, 035119 (2015)

[2] J. Braun, R. Rausch, M. Potthoff , and H. Ebert, One-step theory of two-photon photoemission, Phys. Rev. B **94**, 125128 (2016)

O 75.9 Wed 17:00 TRE Phy

Interplay between metal-organic interface state and donor-acceptor interface mediated charge separation on PTCDA/TiOPc/Ag(111) — •Alexander Lerch[1], Frederik Schiller[1,2], and Ulrich Höfer[1] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — [2]Centro de Física de Materiales, San Sebastian, Spain

Charge separation of excitons in the well ordered model system PTCDA on titanyl phthalocyanine (TiOPc) on Ag(111) was investigated by means of time-resolved two-photon photoemission (2PPE). An optical parametric oscillator provided pump pulses with photon energies ranging from 1.6 to 2.5 eV. This allowed for selective excitation of TiOPc or PTCDA. Between TiOPc and Ag(111) a shockley derived interface state (IS) approximately 0.3 eV above the Fermi energy forms. We observe a strong coupling of the first molecular layers to the IS and determine transfer times into the IS ranging from approximately 20 fs out of the second to 160 fs out of the third and fourth molecular layers. Systematic thickness-dependent measurements quantify the distance dependence of this coupling. Whereas the IS dominates the dynamics in the second layer, the PTCDA/TiOPc acceptor-donor interface (D/A) competes for electrons from excitons in the third to fourth layer. In the fifth to sixth layer no significant IS assisted separation on a timescale below 12 ns can be detected any longer. Our results highlight the competition between IS and D/A mediated charge separation of excitons in few-layer organic systems on metal substrates.

O 75.10 Wed 17:15 TRE Phy

Ultrafast electron dynamics and small polaron formation in solid DMSO on Cu(111) — •Sarah King, Katharina Broch, and Julia Stähler — Department of Physical Chemistry, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

The ultrafast electron solvation dynamics in DMSO have been investigated using time- and angle-resolved two-photon photoemission spectroscopy of condensed DMSO films on a Cu(111) single crystal with different coverages, between 1 and 10 monolayer (ML) equivalents. At DMSO coverages higher than 1 ML, initially a delocalized electronic state is formed in DMSO at 2.85 ± 0.05 eV relative to the Fermi level, with an effective mass of approximately 1.8 times the mass of a free electron. This state simultaneously undergoes localization and energetic stabilization where the peak energy shifts to lower energies at a rate of approximately 1 eV/ps as the peak dispersion flattens. By 200 fs after formation, this state exhibits negative dispersion and ten-fold slower peak shifting before decaying completely within 1 ps. We preliminarily attribute the dynamics in peak energy and localization to small polaron formation in DMSO. The decay-time of the small polaron state is concomitant with the rise-time in a DMSO/vacuum surface state at 2.30 ± 0.05 eV, which has an extremely long decay time of *seconds* and exhibits reactivity with oxygen. As DMSO is a common electrolyte, our results on non-equilibrium electronic states in DMSO are important for understanding electrochemistry.

O 75.11 Wed 17:30 TRE Phy

Optically induced quasi-particle dynamics and transient polarization of a C_{60} film — •Sebastian Emmerich[1], Benjamin Stadtmüller[1], Dominik Jungkenn[1], Norman Haag[1], Christina Schott[1], Steffen Eich[1], Markus Rollinger[1], Mahalingam Maniraj[1], Martin Aeschlimann[1,3], Mirko Cinchetti[1,3], and Stefan Mathias[2] — [1]University of Kaiserslautern and Research Center OPTIMAS, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Physikalisches Institut I, Universität Göttingen, 37077 Göttingen, Germany — [3]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

The performance of organic based electronic devices is determined by the energy level alignment as well as by the excitation dynamics of electrons in these materials. Although both aspects are intrinsically linked by the polarizability of organic materials, they have mainly been discussed separately so far. In this work, we present new insight into the ultrafast dynamics of thin C_{60} films on Ag(111). The combination of time- and angle resolved photoemission with a fs-XUV light source allows us to follow the transient evolution of the unoccupied as well as of the occupied band structure after the fs-optical excitation with visible light. The unoccupied part of the C_{60} band structure reveals the well-known quasi-particle dynamics of the exciton formation and its decay in C_{60}. Most interestingly, we observe a transient change of the linewidth of the occupied molecular orbitals upon optical excitation. This effect is attributed to the transient polarization of the molecular film due to the exciton formation in distinct C_{60} sites.

O 75.12 Wed 17:45 TRE Phy

Vibrational relaxation and migration dynamics of excitons in sexithiophene/Au(111) — Wibke Bronsch[1], Sebastian Baum[1], Kristof Zielke[1], Malte L. Wansleben[2], Martin Weinelt[1], and •Cornelius Gahl[1] — [1]Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin — [2]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12 10587 Berlin

The primary optical excitations in organic semiconductors are excitons. The corresponding absorption bands are commonly strongly broadened due to coupling to vibrational excitations, as known from optical spectroscopy. In organic electronics, the dynamics of such excitonic states concerning their energetic evolution as well as their migration through the material are decisive for the performance of a device. We investigated the exciton dynamics by time-resolved two-photon photoemission (2PPE) spectroscopy in the model system of sexithiophene (6T) on the Au(111) surface. In crystalline 6T films, vibrational excess energy is dissipated on a time scale of <100 fs resulting in an excitonic state which is stable in energy for >100 ps. In amorphous 6T films, however, the energetic relaxation from a broad initial distribution of excited states is strongly slowed down and reaches an excitonic state with a binding energy comparable to that in the crystalline film on a time scale >10 ps. This slow process is attributed to migration of excitons towards sites with higher binding energy. Thus the morphology of the organic layer strongly influences the excited state dynamics and energetics relevant for organic electronics.

O 75.13 Wed 18:00 TRE Phy

Femtosecond electron dynamics in the momentum space — •Florian Haag[1], Johannes Seidel[1], Tobias Eul[1], Norman Haag[1], Mirko Cinchetti[2], Martin Aeschlimann[1] und Benjamin Stadtmüller[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany — [2]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

Excited electrons play a crucial role for many fundamental chemical and physical phenomena occurring at surfaces, (hybrid) interfaces, or in bulk materials. New insight into this field can be obtained by the combination of time-resolved two-photon photoemission spectroscopy with momentum microscopy. This novel approach of time-resolved 2 photon momentum microscopy offers the possibilities to follow the electron dynamics in the accessible momentum space and hence to determine momentum resolved lifetimes of excited electrons.

As most fundamental examples, we have studied the momentum resolved electronic lifetime of polycrystalline and single crystalline metal crystals. Using various combinations of light polarization for the pump and probe pulse allows us to distinguish the electron dynamics of bulk and surface bands. Our results will significantly contribute to a better understanding of momentum space dynamics of excited electrons and of inelastic und quasi-elastic scattering phenomena at interfaces and in solids.

O 75.14 Wed 18:15 TRE Phy

Spatio-Temporal Probing of Lattice Dynamics in Graphite by Ultrafast TEM — •Armin Feist[1], Nara Rubiano da Silva[1], Wenxi Liang[2], Claus Ropers[1], and Sascha Schäfer[1] — [1]IV. Physical Institute - Solids and Nanostructures, Göttingen, Germany — [2]Huazhong University of Science and Technology, Wuhan, China

Over the past decades, ultrafast techniques have shaped a rich picture of material dynamics in spatially homogenous systems. Extending these concepts, ultrafast transmission electron microscopy (UTEM) provides access to nanoscale processes on their intrinsic femtosecond time and nanometer length scales [1,2].

Here, we apply UTEM to investigate ultrafast nanoscale lattice dynamics localized at the edge of a single-crystalline graphite thin film [3]. Time-dependent convergent beam electron diffraction (CBED) of nanoscale sample areas gives access to the complex distortions of the crystal structure. Specifically, the initial optically generated, spatially-inhomogeneous strain distribution relaxes via coherent out-of-plane breathing and in-plane shear motion coupled to a propagating compressive strain wave. We spatio-temporally map these dynamics with 30 nm spatial and sub-picosecond temporal resolution. By employing UTEM, energy transfer and dissipation in complex nanostructured systems can be tracked over a wide range of time scales, spanning from femtosecond optical excitations to coherent lattice vibrations with nanosecond lifetimes.

[1] A. H. Zewail, *Science*, **328**, 187 (2010). [2] A. Feist *et al.*, arXiv: 1611.05022. [3] A. Feist *et al.*, in preparation.

O 75.15 Wed 18:30 TRE Phy

Lattice Response of Pb/Si(111) Layers and Islands upon Femtosecond Optical Excitation — •Tobias Witte, Tim Frigge, Bernd Hafke, Boris Krenzer, and Michael Horn-von Hoegen — University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Employing time resolved reflection high energy rlectron diffraction (tr-RHEED) the non-equilibrium dynamics of the phonon system after optical excitation of ultrathin Pb films and islands on Si(111) has been investigated. The sample is pumped by fs-IR-laserpulses, while the transient response is probed by a 30 keV electron pulse. Surface sensitivity is achieved via gracing incidence of the high energy electrons. fs-laserpulses cause impulsive excitation of the electron system of the Pb films and islands, respectively. The hot electron system thermalizes and heats the lattice system by electron-phonon coupling. The thermal motion of the (surface-) atoms is observed through the transient Debye-Waller effect. As Pb is known to exhibit strong electron-phonon coupling in the bulk the time constant for the energy transfer to the lattice system is - in the framework of the two temperature model (TTM) - expected to be in the sub-ps regime. In contrast, a rather slow time constant of $\tau = 3.2$ ps was observed at the surface. Moreover, incoherent lattice excitation of the islands occurs even slower at a timeconstant of $\tau = 4.6$ ps. These results demonstrate how low-dimensionality and quantum-size effects reduce the energy flow mediated by electron-phonon coupling.

O 76: Plasmonics and Nanooptics VII: Applications and Other Aspects

Time: Wednesday 15:00–18:00 Location: TRE Ma

O 76.1 Wed 15:00 TRE Ma

Hydrogen Sensing using Chemically Grown Plasmonic Nanorods in a Dust-on-Film Geometry — •Domenico Paone[1], Martin Mayer[2], Nikolai Strohfeldt[1], Florian Sterl[1], Tobias König[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart — [2]Institute of Physical Chemistry and Polymer Physics, Dresden

Noble metal nanostructures are able to confine electromagnetic radiation on a subwavelength nanometer scale. The resonant excitation of localized surface plasmons in such nanostructures gives rise to strong light absorption and scattering. These optical properties can be used in a rich variety of practical applications such as gas sensing. In this work, we present a dust-on-film sensing geometry by drop coating gold nanoparticles on active hydrogen absorbing films. The nanoparticles are fabricated by a seed-mediated growth method that enables the synthesis of nanorods with a wide variation of lengths. We employ these nanorods as optical antennas to investigate locally the hydrogen catalysis and absorption of palladium and magnesium films. To study our dust-on-film system, we perform single-particle dark-field spectroscopy on the individual gold nanorods. We are able to find pronounced spectral shifts upon exposure to different hydrogen concentrations, leading the way toward the development of inexpensive chemical reaction sensors with high sensitivity.

O 76.2 Wed 15:15 TRE Ma

Directional Emission from Active Dielectric Nanoantennas — •Manuel Peter[1], André Hildebrandt[2], Christian Schlickriede[3], Thomas Zentgraf[3], Jens Förstner[2], and Stefan Linden[1] — [1]Physikalisches Institut, University of Bonn, Nußallee 12, D-53115 Bonn, Germany — [2]Department of Electrical Engineering, University of Paderborn, Warburger Strasse 100, D-33098 Paderborn, German — [3]Department of Physics, University of Paderborn, Warburger Strasse 100, D-33098 Paderborn, Germany

Here, we report on the directional light emission from an active dielectric nano antenna. The leaky-wave antennas are made from Hafnium dioxide. Colloidal semiconductor quantum dots with an emission wavelength of 780 nm are deposited with a lithographic technique from an aqueous solution into the feed gap of the antenna. Quantum dots serve as dipole sources. Their fluorescence is guided by the director that acts as a leaky waveguide which emits the light in a narrow angle distribution into the substrate. A reflector is used to increase the efficiency of the antenna. By imaging the back-focal plane of a high NA microscope objective, we can directly map the angular distribution of the fluorescence. In our experiment we observe a strong effect of the antennas with a main lobe of the fluorescence pointing into the substrate with a longitudinal angle of θ=21°. Additionally we will present results on the polarization of the directed light and the change of directivity for antennas with different dimensions. All the measured angular intensity distributions are in good agreement with the numerical calculations.

O 76.3 Wed 15:30 TRE Ma

Plasmonic analog of electromagnetically induced absorption leads to giant thin-film Faraday rotation — •Dominik Floess, Mario Hentschel, Thomas Weiss, and Harald Giessen — 4th Physics Insitute and Research Centre SCoPE, University of Stuttgart, Stuttgart, Germany

We demonstrate the realization of a hybrid magnetoplasmonic thin film structure that resembles the classical optical analog of electromagnetically induced absorption. In transmission geometry our Au nanostructure embedded in an EuS film induces giant Faraday rotation of up to 14° for a thickness of below 150 nm for $B = 5\,\mathrm{T}$. Crucial for our achievement is the introduction of EuS as a new material for magnetoplasmonics. At low temperatures, it enables the realization of complex magnetoplasmonic structure geometries, which would not be feasible with commonly used magneto-optic materials. Our concept will lead to important, highly integrated, non-reciprocal photonic devices for light modulation, optical isolation, and magnetic field optical sensing. The simple fabrication of EuS nanostructures also enables more sophisticated and intriguing future designs of magnetoplasmonic systems and three-dimensional magneto-optic metamaterials.

O 76.4 Wed 15:45 TRE Ma

Anderson localization in disordered plasmonic waveguide arrays — •Cherpakova Zlata, Felix Bleckmann, and Stefan Linden — Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 12, 53115 Bonn, Germany

We report on the observation of Anderson localization in disordered arrays of evanescently coupled dielectric-loaded surface plasmon polariton (SPP) waveguides. The samples are fabricated by negative-tone gray-scale electron beam lithography. On-diagonal disorder is introduced to the arrays by randomly altering the waveguides effective refractive index which is a monotonous function of the waveguide height. Thus, by choosing the maximum variation of the waveguide height we can control the degree of disorder. SPPs were excited by shining a highly focused laser beam on the grating, deposited on top of the central waveguide. The spatial evolution of the SPP field intensity is monitored by real space leakage radiation microscopy (LRM). The corresponding momentum-resolved spectra which reveal the information on the energy spectrum of an equivalent condensed matter system is measured as well by making use of Fourier space LRM. With these techniques we experimentally demonstrate the transverse localization of the SPP with increasing degree of disorder both in real and Fourier space.

O 76.5 Wed 16:00 TRE Ma

Ultrafast imaging of electric fields around nanostructures — •Jan Vogelsang, Germann Hergert, Petra Gross, and Christoph Lienau — Institut für Physik, Carl von Ossietzky Universität, 26129 Oldenburg, Germany

The combination of high spatial resolution electron microscopes and high temporal resolution laser spectroscopy promises experiments in unexplored spatio-temporal regimes. E.g., many fundamental photoinduced processes such as coherent charge and energy transport phenomena occur on few-fs time scales. However, in today's ultrafast electron microscopes the time resolution is so far limited to ~100fs: The electrons propagate over mesoscopic distances, which gives rise to electron pulse broadening due to dispersion.

Recently, we demonstrated a new, plasmon-driven electron source that tackles this challenge: Adiabatic nanofocusing of surface plasmons on sharply etched metallic tapers concentrates light in a nanometric volume and efficiently induces electron emission. Direct illumination of the emission site is avoided and hence the apex-sample-distance can be chosen arbitrarily small (Nano Lett. 15, 4685, 2015).

Here, we show first ultrafast electron micrographs with few-nm spatial and few-ten-fs temporal resolution. We record an ultrafast change of the electric field near carbon nanostructures after laser excitation. It deflects the probing electrons which directly maps the field distribution to the 2d electron detector. The results prove that the simple, but efficient working principle of a lensless point-projection microscope is ideal for maintaining the ultrashort duration of electron pulses.

O 76.6 Wed 16:15 TRE Ma

Spectral imaging of topologically protected edge states in plasmonic waveguide arrays — •Felix Bleckmann[1], Andrea Alberti[2], and Stefan Linden[1] — [1]Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 12, 53115 Bonn, Germany — [2]Institut für Angewandte Physik, Rheinische Friedrich-Wilhelms-Universität Bonn, Wegelerstr. 8, 53115 Bonn, Germany.

The Su-Schrieffer-Heeger (SSH) model, i.e., a chain of lattice sites coupled via alternating strong and weak bonds, is the prototypical one-dimensional system with nontrivial topological character. It supports two different dimerizations with distinct topological properties. At any interface between both, one topologically protected edge state exists.

We report on the observation of topologically protected edge states in evanescently coupled plasmonic waveguide arrays employed to implement the SSH model. The arrays are fabricated on top of a gold film by negative-tone grey-scale electron-beam lithography. Alternating strong and weak bonds were realized by choosing two different separations between neighboring plasmonic waveguides. We created an interface between the two dimerizations of the SSH model by repeating the larger separation twice.

Surface plasmon polaritons are excited directly at the interface. Their spatial evolution as well as their momentum-resolved spectra are measured by making use of real and Fourier space leakage radiation microscopy. We demonstrate that the topologically protected edge state is localized at the interface and has a midgap position in the momentum-resolved spectrum.

O 76.7 Wed 16:30 TRE Ma

Resonant Plasmonic Antenna-Enhanced Far-IR and Terahertz Spectroscopy — •Ksenia Weber[1], Maxim Nesterov[1], Thomas Weiss[1], Michael Scherer[2], Mario Hentschel[1], Jochen Vogt[3], Christian Huck[3], Weiwu Li[4], Martin Dressel[4], Harald Giessen[1], and Frank Neubrech[3] — [1]4th Physics Institute, University of Stuttgart, Stuttgart — [2]InnovationLab GmbH, Heidelberg, Germany — [3]Kirchhoff Institute for Physics, Heidelberg University, Germany — [4]1st Physics Institute, University of Stuttgart, Stuttgart

Terahertz spectroscopy is a technique with a vast range of sensing applications, based on material-specific absorption features of molecular vibrations. However, the low absorption cross section of these excitations strongly limits its sensitivity. The possibility to increase the sensitivity of spectroscopic methods via the enhanced electromagnetic near fields provided by plasmonic nanoantennas has been shown before for surface-enhanced infrared spectroscopy (SEIRA). In the present work we transfer the concept of SEIRA to single digit terahertz frequencies. We use plasmonic nanoantennas for the enhancement of molecular vibrations with frequencies in a spectral region from 4.5 to 45 THz We therefore fabricated arrays of rectangular gold antennas by electron beam lithography and coated them with thin layers of the fullerenes C$_{60}$ and C$_{70}$, as well as the amino acid threonine. The samples were investigated with Fourier transform infrared spectroscopy using a bolometer as detector. An increased SEIRA enhancement of one two orders of magnitude is found for antennas resonant at 6.7 THz when compared to 45 THz, corresponding to a λ^3 scaling.

O 76.8 Wed 16:45 TRE Ma

Watching hydride formation in single plasmonic magnesium nanoparticles — •Florian Sterl, Heiko Linnenbank, Nikolai Strohfeldt, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Magnesium (Mg) has recently demonstrated its potential for active plasmonics in the visible wavelength range via the absorption of hydrogen. We have shown that this can be achieved by using Mg nanoantennas with a catalytic palladium (Pd) capping layer. Upon hydrogenation, Mg forms non-metallic magnesium hydride (MgH$_2$). In this system, the plasmonic resonance can be switched off and back on via exposure to hydrogen and oxygen gas, with switching times on the order of tens of seconds. On one hand, this leads to potential applications such as tunable plasmonic displays. On the other hand, the system can be used to investigate the hydrogenation of Mg.

MgH$_2$ is considered a promising candidate for solid-state hydrogen storage, owing to its high hydrogen content of up to 7.6 wt%, and can also be considered a model system for other energy storage materials. We aim for a better understanding and characterization of the hydrogen diffusion in Mg at the nanoscale, using different techniques: We investigate the time dynamics of the Mg-MgH$_2$ phase transition using the optical far field of Mg/Pd nanoantennas, and probe the optical near field of individual Mg nanostructures to observe the evolution of hydrogenated domains during this transition. We furthermore address the mechanical deformation due to the hydrogen-induced expansion of the Mg crystal lattice.

O 76.9 Wed 17:00 TRE Ma

Palladium Nanopatches - Size-dependent Hydrogen Kinetics — •Nikolai Strohfeldt[1], Florian Sterl[1], Ronald Griessen[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Stuttgart, Germany — [2]Faculty of Sciences, Division of Physics and Astronomy, VU University, Amsterdam, The Netherlands

Nanoparticles exhibit many potentially interesting properties that are relevant for key applications such as storage of energy in batteries or data in non-volatile memories. Especially the storage of hydrogen in nanomaterials has stimulated the development of powerful new investigation methods. Electron-beam lithography makes it possible to create essentially monodisperse ensembles of particles, which can conveniently be studied with optical and plasmonic methods. In nanoparticles, H desorption occurs fully coherently only for small crystalline nanocubes (typically smaller than 50 nm) at temperatures sufficiently close to the critical temperature. For larger particles, it is partially incoherent, where dilute α-PdH$_x$ and high concentration β-PdH$_x$ phases coexist. In polycrystalline particles, larger than 200 nm, the H absorption occurs at much lower pressures than in nanocubes. With a newly developed localized surface plasmon resonance method we succeeded in determining the size dependence of the hydrogen induced in-plane and out-of-plane expansion. With increasing size the in-plane expansion of these particles is increasingly hampered. The knowledge gathered with Pd-H nanoparticles is at the basis of recent developments of active plasmonic elements based on the Y-H and Mg-H systems.

O 76.10 Wed 17:15 TRE Ma

Polaronic nature of charge carriers at the LAO/STO interface — •Vladimir N. Strocov[1], Claudia Cancellieri[2], Adrian Husanu[1], Ulrich Ashauer[3], and Andrey Mishchenko[4] — [1]Swiss Light Source, Paul Scherrer Insitute, Switzerland — [2]EMPA, Switzerland — [3]University of Bern, Switzerland — [4]RIKEN Center for Emergent Matter Science, Japan

2D electron system emergent at the paradigm buried oxide interface LaAlO$_3$/SrTiO$_3$ (LAO/STO) is explored with soft-X-ray ARPES, which combines resolution in electron energy and momentum with enhanced probing depth and chemical specificity [1]. Accentuated with resonant photoexcitation of the interface Ti^{3+} ions, ARPES response of the interface charge carriers resolves the manifold energy band structure of t_{2g}-derived subbands formed in the interface quantum well. The temperature dependent peak-dip-hump spectral lineshape manifests polaronic nature of the interface electrons, where the breathing-mode LO3 phonon at 118 meV limits low-temperature mobility of the interface charge carriers, and the polar TO1 one, changing its frequency from 18 to 14 meV across the antiferrodistortive phase transition, causes a dramatic mobility drop with temperature [2]. Doping with oxygen vacancies, affecting electron-phonon coupling, opens ways to tune the interfacial mobility at oxide interfaces in view of their potential device applications.

1. V.N. Strocov *et al*, Synchr. Rad. News 27, N2 (2014) 31
2. C. Cancellieri *et al*, Nature Comm. 7 (2016) 10386

O 76.11 Wed 17:30 TRE Ma

Attosecond time-resolved photoelectron spectroscopy of hybrid nanoresonators — •Julia Hengster and Thorsten Uphues — ARS, CFEL, Luruper Chaussee 149, 22761 Hamburg

Understanding plasmons as collective oscillations of the free-electron gas density important questions related to their propagation, damping, charge and energy localization came up. Nevertheless the behaviour of hybrid nanostructures approaching the monolayer limit raises a new type of questions concerning their plasmonic behaviour in space and time, following the complex dynamics of the electromagnetic field.

Attosecond time-resolved experiments are on the way to resolve subcycle electron dynamics from plasmonic interaction of ultrashort driving pulses in surfaces and nanostructures. Our approach of attosecond photoscopy demonstrates a reliable route to extend attosecond technology to surface and nanostructure dynamics. Hybrid nanostructures exhibit complex plasmonic properties sensitive to parameters as geometrical aspect ratios or material compositions. Vertically aligned disk nano-resonators belong to a group of tailored systems demonstrating field enhancement with strong localization. We found a remarkably sensitive behaviour in the coupling of surface and bulk plasmons with respect to the outer geometry of the resonators with ultrafast subcycle dynamics.

As proof-of-concept we demonstrate attostreaking from gold films with significant deviation to gas-phase streaking. Furthermore we developed non-destructive preparation procedures for nanoparticle samples as requirement for attosecond photoscopy.

O 76.12 Wed 17:45 TRE Ma

Monitoring of structural changes of polypeptides using resonant surface enhanced infrared spectroscopy — •Rostyslav Semenyshyn[1], Mario Hentschel[1], Jochen Vogt[2], Christian Huck[2], Christoph Stanglmair[3], Claudia Pacholski[3], Frank Neubrech[1,2], and Harald Giessen[1] — [1]4th Physics Institute, University of Stuttgart — [2]Kirchhoff Institute for Physics, University of Heidelberg — [3]Max Planck Institute for Intelligent Systems, Stuttgart

Infrared (IR) vibrational spectroscopy is a powerful tool for the identification of chemical and structural composition of molecules. Its detection limit can be improved by several orders of magnitude using surface-enhanced IR absorption (SEIRA) with resonant nanoantennas. Here, we demonstrate the capability of SEIRA for the ultra-sensitive detection of minute amounts of a polypeptide, namely poly-L-lysine (PLL). Furthermore, we applied SEIRA to monitor structural changes of the molecules introduced by injecting sodium dodecyl sulfate as well as varying the pD value. For this purpose, we functionalized nanoantenna arrays with mercaptoundecanoic acid (MUA) and mercaptoundecanol (MUoL) in order to bind PLL molecules to the gold surface. The combination of MUA and MUoL ensures a sufficient flexibility, allowing for structural changes. Such changes are detected based on a detailed analysis of the amide-I vibrations. Hence, we tuned the plasmonic resonances of nanoantennas to the amide-I band of PLL and performed in-vitro SEIRA measurements in D_2O based solutions. Following this approach, we monitored the reversible change between α-helix and β-sheet structural states of PLL in low concentrations.

O 77: 2D Materials Beyond Graphene IV

Time: Wednesday 15:00–17:45 Location: WIL A317

Invited Talk O 77.1 Wed 15:00 WIL A317
Carbon Nanomembranes (CNM) : 2D Materials Beyond Graphene — •Armin Gölzhäuser — Universität Bielefeld, Physik Supramolekularer Systeme und Oberflächen, Universitätsstr. 25, 33615 Bielefeld

Carbon Nanomembranes (CNMs) are thin (~1nm), synthetic two-dimensional (2D) layers or sheets with tailored physical, chemical or biological function [1]. Their fabrication scheme utilizes a sequence of molecular monolayer assembly on a solid surface and radiation induced cross-linking in two dimensions. The cross-linked 2D-layer is then released from the surface, forming a self-supporting nanomembrane with properties that are determined by properties of the monolayer. Depending on the desired applications, CNMs can be engineered with a controlled thickness, elasticity and surface functionalization. Helium ion microscopy, spectroscopic methods and functional tests are applied to investigate the structure and composition as well as permeation properties. Helium Ion Lithography is used the fabrication of well-defined nanopores [2] and perforated CNMs are tested as ballistic membranes for the separation of gases and liquids.

[1] A. Turchanin and A. Gölzhäuser: Carbon Nanomembranes, Adv. Mater. 28, 6075 (2016).

[2] D. Emmrich, A. Beyer, A. Nadzeyka, S. Bauerdick, J. C. Meyer, J. Kotakoski and A. Gölzhäuser: Nanopore fabrication and characterization by helium ion microscopy, Applied Physics Letters 108, 16310 (2016).

O 77.2 Wed 15:30 WIL A317
A hybrid MoS2 material for nanopore sensing: interface and asymmetry — Ganesh Sivaraman[1], Fabio A.L. de Souza[2], Rodrigo G. Amorim[3,4], Wanderla L. Scopel[2], Ralph H. Scheicher[3], and •Maria Fyta[1] — [1]Institute for Computational Physics, Stuttgart University — [2]Departamento de Fisica, Universidade Federal do Espirito Santo, Brazil — [3]Department of Physics and Astronomy, Materials Theory, Uppsala University, Sweden — [4]Departamento de Física, Universidade Federal Fluminense, Brazil

An important class of 2D nanomaterials beyond graphene is the family of transition metal dichalcogenides (TMDs) such as molybdenum disulfide (MoS2). In MoS2 a semiconducting (2H) and a metallic (1T) phase can co-exist. We investigate the electronic and transport properties of a hybrid MoS2 monolayer composed by a 1T strip embedded in the 2H MoS2 phase. Using density functional theory based calculations with the non-equilibrium Greens functions (NEGF) approach, we study in detail the structural and electronic properties of hybrid MoS2 and its interface. A clear anisotropy in the electronic and transmission properties of the hybrid material was found and linked to the microstructure of its interfaces. We also show the relevance of such a material to sensing DNA with MoS2 nanopores. In order to understand the formation of this nanopore, a single point-defect analysis is performed also assessing the stability of the hybrid system and the different pore terminations. The current modulation around a nanopore when placing DNA in the pore manifests the strong potential of hybrid MoS2 in next generation biosensing devices.

O 77.3 Wed 15:45 WIL A317
Semiconductor to Metal Transition in WS_2/Ag(111) — •Charlotte E. Sanders[1], Maciej Dendzik[1], Albert Bruix[1], Matteo Michiardi[2], Arlette S. Ngankeu[1], Marco Bianchi[1], Bjørk Hammer[1], Jill A. Miwa[1], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, Denmark — [2]Department of Physics and Astronomy, University of British Columbia, Canada

Substrate effects play an important role in determining electronic structure in two-dimensional materials (2DMATs). A common effect of a metallic substrate on a semiconducting 2DMAT is renormalization of the band gap, induced by metallic screening, as recently observed in MoS_2/Au(111) [1]. Here we report a substrate effect that goes beyond band gap change due to screening. For WS_2/Ag(111), hybridization between electronic states of Ag and WS_2 leads to a non-zero density of states at the Fermi level (FL), and thus to a transition of WS_2 from a direct band gap semiconductor to a metal. This is evidenced by the asymmetric lineshape observed in core-level photoemission spectra. It is associated particularly with the emergence of states at the FL near the Q point of WS_2, as can be seen in measurements by angle-resolved photoemission spectroscopy (ARPES). Meanwhile, ARPES and time-resolved ARPES confirm that the WS_2 conduction band minimum at K remains well defined and stays above the FL. Electronic structure calculations based on density functional theory shed further light on the reasons for these strong changes in band structure. [1] Phys. Rev. B 93, 165422 (2016)

O 77.4 Wed 16:00 WIL A317
A many-body view on the not-so-passive role of the substrate: trions and screening in transition metal dichalcogenides — •Matthias Drüppel[1], Thorsten Deilmann[2], Peter Krüger[1], and Michael Rohlfing[1] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Center for Atomic-Scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The strongly enhanced Coulomb interaction due to reduced dimensionality has established transition metal dichalcogenides (TMDC) as promising candidates for next-generation opto-electronic devices. However, in almost all experiments and applications, the monolayer is deposited on a substrate for mechanical stability or - in bulk/few layer materials - interacts with neighboring layers. In this talk we show that the surrounding of the monolayer does *not* play a passive role. In contrast, it distinctly modifies the TMDC excitations.

We subsequently apply DFT → GW → Bethe-Salpeter equation (BSE) to access the optical properties. Our results show how additional charge carriers, that are often induced by substrates, lead to trion formation that might dominate optical spectra. We take our *ab-initio* approach and directly compare trion and exciton spectra, finding that trions split into inter- and intra-valley trions. Additionally, a drastically enhanced screening by a substrate renormalizes both the exciton and trion binding energies and the fundamental band gap. In bilayer and bulk materials, excitons can be excited with electron and hole located on different layers, forming inter-layer excitons.

O 77.5 Wed 16:15 WIL A317
Simple Screened Hydrogen Model of Excitons in Two-Dimensional Materials — •Thomas Olsen, Simone Latini, Filip Rasmussen, and Kristian Thygesen — Technical University of Denmark

We present a generalized hydrogen model for the binding energies (E) and radii of excitons in two-dimensional (2D) materials that sheds light on the fundamental differences between excitons in two and three dimensions. In contrast to the well-known hydrogen model of three-dimensional (3D) excitons, the description of 2D excitons is complicated by the fact that the screening cannot be assumed to be local. We show that one can consistently define an effective 2D dielectric constant by averaging the screening over the extend of the exciton. For an ideal 2D semiconductor this leads to a simple expression for E that only depends on the excitonic mass and the 2D polarizability α. The model is shown to produce accurate results for 51 transition metal dichalcogenides. Remarkably, over a wide range of polarizabilities the binding energy becomes independent of the mass and we obtain $E = 3/4\pi\alpha$), which explains the recently observed linear scaling of exciton binding energies with band gap. It is also shown that the model accurately reproduces the non-hydrogenic Rydberg series in WS2 and can account for screening from the environment.

O 77.6 Wed 16:30 WIL A317

Investigation of hexagonal boron-nitride (hBN) on SiC — •Markus Franke[1,2], François C. Bocquet[1,2], Janina Felter[1,2], and Christian Kumpf[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology, 52425 Jülich, Germany

Among 2D materials, hexagonal boron-nitride (hBN) seems to be a promising candidate for a new substrate material to achieve a highly ordered layer of free-standing graphene. It forms a flat hexagonal lattice structure with a lattice constant similar to that of graphene, but (in contrast to graphene) has a wide band gap ($> 5\,\mathrm{eV}$) and is therefore insulating. It should be free of charge traps and dangling bonds and its flat surface should prevent overlying 2D materials from corrugating.

Here, we report on the growth of hBN layers on the wide band gap semiconductor silicon carbide (SiC) by annealing SiC wafers in a borazine ($B_3N_3H_6$) atmosphere. The properties of this system are investigated by XPS, ARPES and HREELS.

O 77.7 Wed 16:45 WIL A317

Plasmonic Superconductivity in Layered Materials — Malte Rösner[1,2], Roelof G. Groenewald[1], Gunnar Schönhoff[2], Jan Berges[2], Stephan Haas[1], and •Tim O. Wehling[2] — [1]Department of Physics and Astronomy, University of Southern California, USA — [2]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Germany

Due to a lack of screening in two dimensions the Coulomb interaction is generally enhanced and consequently plays a major role to understand many-body effects within layered materials. In the field of superconductivity it is usually introduced as an approximate, static, and adjustable parameter μ^* which describes only effectively the Coulomb repulsion which is therefore responsible for reduced transition temperatures.

Here, we overcome this inadequate handling and present an ab initio based material-realistic Coulomb description for doped single layers of MoS_2 which captures simultaneously material-intrinsic, substrate, and dynamical screening processes. Using this model we can reliably describe the resulting plasmonic excitations including both, their coupling to the electrons and their dependence on the environmental screening and doping level. Utilizing Eliashberg theory we show that the low-energy plasmonic modes originating from the dynamically screened Coulomb *repulsion* can actually lead to an effective Coulomb *attraction* and thus to an enhanced transition temperature (T_c). Furthermore, we find an optimal ratio between the substrate screening and the electron doping which maximizes T_c of the induced plasmonic superconducting state.

O 77.8 Wed 17:00 WIL A317

MoS2 film conductivity change on periodically poled LiNbO3 substrate determined by nano-FTIR spectroscopy — •Piotr Patoka[1], Georg Ulrich[1], Peter Hermann[2], Bernd Kästner[2], Ariana Nguyen[3], Arne Hoehl[2], Ludwig Bartels[3], Peter Dowben[4], Gerhard Ulm[2], and Eckart Rühl[1] — [1]Physikalische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, Berlin, 10587, Berlin, Germany — [3]Dept. of Chemistry, Univ. of California Riverside, Riverside, CA 92521, USA — [4]Dept. of Physics and Astronomy, Univ. of Nebraska, Lincoln, Lincoln, NE 68588-0299 USA

Coupling of ultra-broadband synchrotron radiation from the Metrology Light Source (MLS) to a scattering-type scanning near-field optical microscope (s-SNOM) allows for contactless conductivity evaluation in the mid-infrared regime. The system is based on an atomic force microscope, such that the optical signal can be directly correlated with topographic information. Using this method, we investigated the influence of a ferroelectric substrate (LiNbO3) enhanced by its surface phonon on thin films of MoS2. Recent electric transport measurements suggest changes in the carrier density due to substrate polarization.[1] The present findings obtained from s-SNOM studies offer a complimentary way of contactless investigations of conductivity changes.[2]

[1] Nguyen, A. et al., Nano Lett. 15, 3364-3369 (2015).

[2] Hermann, P. et al., Opt. Express 21, 2913-2919 (2013).

O 77.9 Wed 17:15 WIL A317

Band gap transition in few-layer ReS$_2$ investigated by photoemission k-space microscopy — •Mathias Gehlmann[1], Lukasz Plucinski[1], Slavomír Nemšák[1], Irene Aguilera[2], Gustav Bihlmayer[2], Pika Gospodarič[1], Markus Eschbach[1], Ewa Młyńczak[1], Giovanni Zamborlini[1], Vitaliy Feyer[1], Florian Kronast[3], Philipp Nagler[4], Tobias Korn[4], Christian Schüller[4], Stefan Blügel[2], and Claus Michael Schneider[1] — [1]PGI-6, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — [2]PGI-1/IAS-1, Forschungszentrum Jülich GmbH and JARA, D-52425 Jülich, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, D-12489 Berlin, Germany — [4]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

ReS_2 is a promising candidate for novel electronic and sensor applications. The low crystal symmetry of this van der Waals compound leads to highly anisotropic optical and vibrational behavior. However, the details of the electronic band structure of this fascinating material are still largely unexplored. We present a momentum resolved study of the electronic structure of monolayer, bilayer, and bulk ReS_2. Using photoemission k-space microscopy in combination with density functional theory calculations we demonstrate a significant 3D delocalization of the valence electrons in bulk ReS_2. Furthermore, we directly observe the evolution of the valence band dispersion in our photoemission experiments as a function of the number of layers, revealing a varying character of the band gap.

O 77.10 Wed 17:30 WIL A317

Structural Analysis of h-BN on Cu(111) — •Martin Schwarz[1], Manuela Garnica[1], Jacob Ducke[1], Peter Deimel[1], David Duncan[2], Ari Seitsonen[3], Francesco Allegretti[1], Johannes Barth[1], and Willi Auwärter[1] — [1]Physik Department, Technische Universität München, James Franck Str. 1, 85748 Garching, Germany — [2]Diamond Light Source, Didcot, Oxfordshire, OX11 0DE, United Kingdom — [3]Département de Chimie, École Normale Supérieure, 24 rue Lhomond, F-75005 Paris, France

Atomically thin boron nitride (h-BN) layers on metallic supports represent promising platforms for the adsorption of atoms, clusters, and molecular nanostructures [1-2]. Specifically, STM studies revealed an electronic corrugation of h-BN/Cu(111), guiding the self-assembly of molecules and their energy level alignment. A comprehensive characterization of the h-BN/Cu(111) interface including the spacing between the h-BN sheet and its support - elusive to STM measurements - is crucial to rationalize the interactions within these systems. To this end, we employed complementary techniques including scanning tunneling microscopy (STM), high resolution atomic force microscopy (AFM), low energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), X-ray standing wave (XSW) and density functional theory (DFT). Thus, our multi-method study yields a complete, quantitative structure determination of the sp2 bonded BN layer on Cu(111).

[1] Joshi, Sushobhan, et al. NL 12.11 (2012): 5821-5828

[2] Urgel, J. I. et al. JACS 137.7 (2015): 2420-2423

O 78: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - V

Time: Wednesday 15:00–18:15 Location: GER 38

O 78.1 Wed 15:00 GER 38

First-principle Linear Response in Real Space — •Honghui Shang[1], Danilo S. Brambila[1], Christian Carbogno[1], Patrick Rinke[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Aalto University, Helsinki, Finland

Density-functional perturbation theory (DFPT) has developed into an important computational tool for assessing the linear electronic response of crystalline solids to perturbations, e.g., from electric fields or nuclear displacements [1]. In this work we present a full real-space reformulation of DFPT and its implementation [2] in the all-electron, numeric atom-centered orbital electronic structure theory code FHI-aims. We discuss the specific contributions, e.g., relativistic effects and Pulay terms, that arise in such a formulation and validate our implementation by systematically comparing with the finite-difference approach for various extended systems. The computational efficiency is then analyzed via scaling and scalability tests on massively parallel architectures (CRAY and IBM x86 clusters). Finally, we show that this real-space formalism enables an arbitrarily dense sampling of the Brillouin zone by numerically cheap Fourier transformations, which in turn facilitates an efficient evaluation of the electron-phonon coupling matrix elements. We demonstrate the efficiency by computing the relaxation time of hot carriers in Si.

[1] X. Gonze and C. Lee, *Phys. Rev. B* **55**, 10355, (1997).

[2] H. Shang, *et al.*, *Comp. Phys. Comm. (accepted)*, arXiv:1610.03756.

O 78.2 Wed 15:15 GER 38

Anharmonic Vibrations in Solids: Why and When Going Beyond Perturbative Treatments is Necessary — •Hagen-Henrik Kowalski, Maja-Olivia Lenz, Christian Carbogno, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

In *ab initio* theory, the nuclear motion is typically assessed using a truncated second order Taylor expansion for the potential energy (harmonic approximation). Recent computational and methodological advancements [1] allow to extend this expansion to the third order so to approximately treat also anharmonic effects. Little is known, however, about the role of higher order terms. In this contribution, we systematically compare how a third-order expansion performs with respect to techniques that are able to capture higher degrees of anharmonicity, e.g., the quasi-harmonic approximation and fully anharmonic molecular dynamics. For this purpose, anharmonic properties such as the thermal expansion and the Grüneisen parameters are computed for a set of materials with increasing degree of anharmonicity (Si, Mg_2Si, CuCl, and ZrO_2). This reveals that a third order expansion can still lead to quantitative and even qualitative errors at elevated temperatures and/or in highly anharmonic systems. Eventually, we discuss the impact of the chosen exchange-correlation functionals on these calculations and the implications of these findings for the computation of thermal conductivities [2].

[1] D. A. Broido, *et al.*, *Appl. Phys. Lett.* 91, 231922 (2007).

[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *ArXiv:* 1608.06917.

O 78.3 Wed 15:30 GER 38

Anharmonic and Quantum Fluctuations in Molecular Crystals from Ab Initio Simulations — •Mariana Rossi[1] and Michele Ceriotti[2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin — [2]École Polytechnique Fédérale de Lausanne, Switzerland

Molecular crystals often exist in multiple competing polymorphs which are challenging to be predicted computationally, but show significantly different physicochemical properties. This challenge is not due only to the combinatorial search space, but also to the complex interplay of subtle effects determine the relative stability of different structures. Here we estimate all contributions to the free energies of these systems with density-functional theory, including the oft-neglected anharmonic contributions and nuclear quantum effects, by using a series of different flavors of thermodynamic integration. As an example, for the two most stable forms of paracetamol we find that anharmonic contributions, different descriptions of van der Waals interactions, and nuclear quantum effects **all** matter to quantitatively determine the stability of different phases [1]. Our studies indicate that anharmonic free energies could play an important role for molecular crystals composed by large molecules and opens the way for a systematic inclusion of these effects in order to obtain a predictive screening of structures. [1] Rossi, Gasparotto, Ceriotti, *PRL* **117**, 115702 (2016).

O 78.4 Wed 15:45 GER 38

Exact solutions and approximations in the exact factorization of the electron-nuclear wavefunction — •Graeme Gossel and Neepa Maitra — Department of Physics and Astronomy, Hunter College of the City University of New York, 695 Park Avenue, New York, NY 10065.

"Recently it was shown how a molecular wavefunction may be written exactly as a single product of a nuclear and an electronic wavefunction, with a pair of corresponding equations of motion [1]. This exact factorization provides a new and rigorous starting point for developing intuitive and physical approximations to the exact coupled system. Strikingly, in this factorized picture the electronic Hamiltonian is not strictly Hermitian. Nevertheless, the norm is conserved so long as certain terms persist. This, and other constraints, inform the approximations we apply to make the process numerically feasible. In parallel we present numerical self-consistent solutions of the exact factorization equations devoid of approximations to assess accuracy and behaviour of different terms. Finally, we discuss how a well characterized and robust single-product-picture such as this may be used in TDDFT calculations.

[1] A Abedi, NT Maitra, and EKU Gross, PRL 105 (12), 123002, 2010

O 78.5 Wed 16:00 GER 38

Insight into time-propagation TDDFT excitations via Kohn–Sham decomposition — •Tuomas P. Rossi[1], Mikael Kuisma[2,3], Martti J. Puska[1], Risto M. Nieminen[1], and Paul Erhart[2] — [1]Aalto University, Espoo, Finland — [2]Chalmers University of Technology, Gothenburg, Sweden — [3]University of Jyväskylä, Jyväskylä, Finland

The real-time-propagation formulation of time-dependent density-functional theory (RT-TDDFT) is an efficient method for calculating optical excitations of large molecules and nanoparticles. However, within RT-TDDFT, the analysis of the response is often limited to photoabsorption spectra and induced densities, in contrast to linear-response formulations of TDDFT, such as the Casida method, in which one can obtain further understanding on the basis of the Kohn–Sham electron-hole decomposition of the excitations.

In this work, we show that the Kohn–Sham decomposition can be equivalently obtained from RT-TDDFT calculations. We demonstrate the approach for the optical response of organic molecules and large metallic nanoparticles. The focus is especially on plasmonic applications, for which the method enables the analysis in terms of transition contribution maps [1]. By using the decomposition, we can shed light on the microscopic origin of plasmon resonances and their damping via plasmon–single-electron coupling, while retaining the favorable scaling of RT-TDDFT compared to linear-response formulations.

[1] S. Malola *et al.*, ACS Nano **7**, 10263 (2013).

O 78.6 Wed 16:15 GER 38

Gauge-invariant Magnetic Properties from Time-Dependent Current-Density-Functional Theory — •Nathaniel Raimbault[1], Paul de Boeij[3], Pina Romaniello[2], and Arjan Berger[1] — [1]Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université Toulouse III - Paul Sabatier — [2]Laboratoire de Physique Théorique, CNRS, IRSAMC, Université Toulouse III - Paul Sabatier — [3]University of Twente, Faculty of Science and Technology, Physics of Interfaces and Nanomaterials

Standard formulations of magnetic response properties are often plagued by gauge dependencies, which can lead to unphysical results, and to a slow convergence with basis-set size. In this talk we present a novel method for obtaining magnetic properties from the current density [1]. This alternative scheme is fully gauge-invariant, numerically efficient, and can be applied to any method from which the current density can be obtained. To illustrate our method, we applied it to time-dependent current-density-functional theory (TDCDFT). While different types of magnetic properties can be calculated in this way, we here emphasize the calculation of circular dichroism spectra, which are notably important in order to characterize secondary structures in biomolecules. The circular dichroism spectra we thus obtain for methyloxirane, dimethyloxirane and α-pinene are in good agreement with experiment [2]. [1] N. Raimbault, P.L. de Boeij, P. Romaniello, and J.A. Berger, PRL 114, 066404 (2015); [2] N. Raimbault, P.L. de Boeij, P. Romaniello, and J.A. Berger, JCTC 12, 3278 (2016)

O 78.7 Wed 16:30 GER 38

Calculation of charge transfer integrals using constrained-DFT

— •Tobias Lettmann and Nikos Doltsinis — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Deutschland

For the investigation of charge transport properties of organic semiconductor materials, the fast and accurate calculation of charge transfer integrals (or transition matrix elements) is desirable. It has been suggested that the transfer integrals depend on a universal linear function of the corresponding wavefunction overlap, which can then be used to approximate the integral at a reduced computational cost[1].

We have calculated transfer integrals for dimers of poly(3-hexylthiophene) (P3HT) and diperylene bisimide (DiPBI), which are used in organic solar cells, in a large variety of intra- and intermolecular conformations and polymer lengths using a constrained-DFT approach[2]. Our results show, that there is indeed a universal relation between transfer integral and wavefunction overlap. However this relation is (i) nonlinear for large overlaps and (ii) only holds true if the transfer integral is rescaled by the number of electrons of the respective system.

[1] F. Gajdos et al.: *J. Chem. Theory Comput.*, 2014, **10**, 4653

[2] H. Oberhofer, J. Blumberger: *J. Chem. Phys.*, 2010, **133**, 244105

O 78.8 Wed 16:45 GER 38

Towards ultra long-range ab-initio calculations

— •Tristan Müller[1], Sangeeta Sharma[1,2], Eberhard K.U. Gross[1], and John K. Dewhurst[1] — [1]Max-Planck-Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — [2]Department of physics, Indian Institute for Technology-Roorkee, 247997 Uttarkhand, India

We propose a generalization of the Bloch state which involves an additional sum over a finer grid in reciprocal space around each k-point. This allows for ab-initio calculations of ultra long-range modulations in the density which may involve millions of unit cells but with an efficiency rivaling that of a single unit cell. This is due to a new algorithm developed specifically for solving the particular eigenvalue problem that this ansatz requires. Thus physical effects on the micron length scale, which nevertheless depend on details of the electronic structure on nanometer length scales, can be computed exactly within density functional theory.

O 78.9 Wed 17:00 GER 38

Local density fitting within a Gaussian and plane waves scheme for large-scale density functional theory calculations

— •Dorothea Golze[1,2], Marcella Iannuzzi[1], and Jürg Hutter[1] — [1]Aalto University, Otakaari 1, 02150 Espoo, Finland — [2]University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland

A local resolution-of-identity (LRI) approach is introduced in the Gaussian and plane waves (GPW) scheme to enable large-scale Kohn-Sham (KS) density functional theory calculations. The construction of the KS matrix in GPW scales already linearly with respect to system size by using a plane wave expansion of the density for the evaluation of the Coulomb term in combination with a local basis. The intention is to retain the linear scaling of the GPW approach, while reducing the prefactor for computing the KS matrix. The locality of the density fitting ensures an $O(N)$ scaling and is implemented by approximating the atomic pair density by an expansion in one-center fit functions. The prefactor is smaller with LRI since the computational demands for the grid-based operations become negligible, while they are dominant in GPW. We observe a speed-up of the self-consistent field (SCF) procedure by a factor of up to 30 for periodic systems dependent on the symmetry of the simulation cell and the grid cutoff. The accuracy of LRIGPW is assessed for different systems and properties. Generally, total energies, reaction energies, intramolecular and intermolecular structure parameters are well reproduced. LRIGPW yields also high quality results for extended condensed phase systems such as liquid water, ice XV and molecular crystals.

O 78.10 Wed 17:15 GER 38

From the Electron Localization Function to a Coalescent-Pair Locator

— •Stefano Pittalis[1], Daniele Varsano[1], Alain Delgado[2,3], and Carlo Andrea Rozzi[1] — [1]Istituto Nanoscienze, Consiglio Nazionale dellle Ricerche, Via Campi 213a, 41125 Modena, Italy — [2]Department of Physics, University of Ottawa, Ottawa, ON K1N 6N5, Canada — [3]Centro de Aplicaciones Tecnológicas y Desarrollo Nuclear, Calle 30 # 502, 11300 La Habana, Cuba

The Electron Localization Function (ELF), as proposed originally by Becke and Edgecombe, uses the information on the distribution of pairs of electrons with parallel spins. The ELF has been widely adopted as a descriptor of atomic shells and covalent bonds, but it is not useful to visualize the bond in H_2 – the simplest neutral molecule in the universe. Here we propose a complementary descriptor which also works for H_2 by exploiting the information on pairs of electrons with opposite spins. Remarkably, only quantities derived from occupied single-particle orbitals are required in the calculations. If time allows, implications for developing improved approximate density functionals will also be discussed.

O 78.11 Wed 17:30 GER 38

Band structure interpolation via maximally localized Wannier functions implemented in LAPW+lo basis

— •Sebastian Tillack, Andris Gulans, and Claudia Draxl — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin

The band structure is one of the most fundamental quantities of any solid that carries a lot of information about the material's properties. Obtaining a smooth dispersion from density-functional theory (DFT) and especially from the GW approximation of many-body perturbation theory may be very expensive. To this extent, we have implemented a method for generating maximally localized Wannier functions (WF) [1] from Kohn-Sham wavefunctions in the full-potential all-electron code `exciting` [2] using a (linearized) augmented plane-waves plus local-orbitals basis. These WF are used for interpolating wavefunctions and corresponding eigenenergies for arbitrary **k**-points in a computationally cheap post-processing step. The interpolated Kohn-Sham and GW bands of conventional and two-dimensional semiconductors and insulators are also used as an input to calculations of optical-excitation spectra.

[1] N. Marzari and D. Vanderbilt, *Phys. Rev. B **56***, 12847 (1997)
[2] A. Gulans, et al. *J. Phys.: Condens. Matter **26***, 363202 (2014)

O 78.12 Wed 17:45 GER 38

Chemical insight from Fermi-Löwdin orbitals

— •Torsten Hahn[1], Sebastian Schwalbe[1], Simon Liebing[1], Jens Kortus[1], and Mark Pederson[2] — [1]Institute for Theoretical Physics, TU Freiberg, Germany — [2]Department of Chemistry, Johns Hopkins University, Baltimore Maryland (MD), US

The recently developed Fermi-Löwdin orbital based method for correcting the self-interaction error in Density Functional Theory (FLO-SIC DFT) [1,2,3] is briefly introduced. Contrary to standard DFT approaches, where only auxiliary Kohn-Sham orbitals are available, FLO-SIC DFT delivers a set of well-defined, localised Fermi-Löwdin orbitals. These localised orbitals together with their optimised reference positions yield an inherently 'chemical' representation of bonding details in molecules that resembles remarkably well Lewis concept of lone and binding electron pairs. For complex examples, the method provides detailed insights into the bonding situation in terms of multi-center many-electron bonds in a natural, chemically-intuitive fashion.

[1] M. R. Pederson et al., JCP 140, 121103 (2014).
[2] M. R. Pederson, JCP 142, 064112 (2015).
[3] T. Hahn et al., JCP 143, 224104 (2015).

O 78.13 Wed 18:00 GER 38

Conditions for describing triplet states in reduced density matrix functional theory

— Iris Theophilou[1], Nektarios N. Lathiotakis[2], and •Nicole Helbig[3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vass. Constantinou 48, GR-11635 Athens, Greece — [3]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

We consider necessary conditions for the one body-reduced density matrix (1RDM) to correspond to a triplet wave-function of a two electron system. The conditions concern the occupation numbers and are different for the high spin projections, $S_z = \pm 1$, and the $S_z = 0$ projection. Hence, they can be used to test if an approximate 1RDM functional yields the same energies for both projections. We employ these conditions in reduced density matrix functional theory calculations for the triplet excitations of two electron systems. In addition, we propose that these conditions can be used in the calculation of triplet states of systems with more than two electrons by restricting the active space. We assess this procedure in calculations for a few atomic and molecular systems. We show that the quality of the optimal 1RDMs improves by applying the conditions in all the cases we studied.

O 79: Electronic Structure of Surfaces: Spectroscopy, Surface States I

Time: Wednesday 15:00–18:15 Location: WIL C307

Invited Talk O 79.1 Wed 15:00 WIL C307

Sensing the Quantum Limit in Scanning Tunneling Spectroscopy: From the Josephson Effect to Quantum Tunneling — •Christian R. Ast — Max-Planck-Institut für Festkörperforschung, Stuttgart

The tunneling current in scanning tunneling spectroscopy (STS) is typically and often implicitly modeled by a continuous and homogeneous charge flow. If the charging energy of a single-charge quantum sufficiently exceeds the thermal energy, however, the granularity of the current emerges. In this quantum limit, the capacitance of the tunnel junction mediates an interaction of the tunneling electrons with the surrounding electromagnetic environment and becomes a source of noise itself, which cannot be neglected in STS. Using a scanning tunneling microscope operating at 15 mK, we show that we operate in this quantum limit, which determines the ultimate energy resolution in STS. A theoretical description requires quantum electrodynamics to be included resulting in the $P(E)$-theory, which describes the probability for a tunneling electron to exchange energy with the environment. I will discuss this effect using a superconducting aluminium tip and a superconducting aluminium sample, where it is most pronounced. These considerations will be most important also at higher temperatures for extremely sharp spectral features, such as superconducting gaps, sharp Kondo peaks or Yu-Shiba-Rusinov states.

O 79.2 Wed 15:30 WIL C307

Photoemission tomography from extended 2D layers: the role of molecule/substrate interactions — •Peter Puschnig[1], Daniel Lüftner[1], Thomas Ules[1], Georg Koller[1], Xiaosheng Yang[2], Simon Weiss[2], Vitaliy Feyer[3], Stefan Tautz[2], Michael Ramsey[1], and Sergey Soubatch[2] — [1]Institute of Physics, University of Graz, Austria — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [3]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Germany

The valence band photoemission angular distribution (PAD) from highly oriented organic molecular layers has been shown to contain rich information on the spatial structure of orbitals and thereby also allows molecular orientations and conformations to be determined. In the past however, measured PADs have been often interpreted in terms of molecular orbitals computed for gas phase molecules.

In this contribution, we show how the photoemission tomography approach can be generalized to take into account two-dimensionally extended organic layers which are in contact with a substrate surface. To this end, we extend the initial state to a sum over Bloch states within the first Brillouin zone and further modify the plane wave final state such that the mean free path of the photoelectron is taken into account in an empirical manner. With the example of a monolayer of PTCDA on Cu(100) a detailed comparison of simulated and experimental momentum and band maps is then made which demonstrates show how the large substrate mediated intermolecular dispersion manifests itself.

O 79.3 Wed 15:45 WIL C307

Bulk and surface states on the Weyl-semimetal candidate Tellurium (Te) probed by spin integrated and spin resolved angle-resolved photoemission — •Florian Titze[1], Mattia Mulazzi[1], Maryam Nazarzadehmoafi[1], Christoph Janowitz[1], Taichi Okuda[2], Kazuki Sumida[3], and Andrei Varykhalov[4] — [1]Humboldt Universität zu Berlin — [2]Hiroshima Synchrotron Radiation Centre — [3]Hiroshima Graduate School of Science — [4]Helmholtz Zentrum Berlin

Te is a direct semiconductor with a band gap of 330 meV. At ambient conditions it crystallises in a hexagonal unit cell with 3 inequivalent atoms winding along its c-axis to form left & right helices making it non-centrosymmetric and chiral.

Lacking a symmetry centre together with a strong spin-orbit coupling induces exotic properties: The nested bands near the top of the valence band (at the H point of the Brillouin zone) provide conducting channels for holes, making Te a good thermoelectric material. Furthermore, non-degenerate bands cross near H at a point called a Weyl node, which is a source of Berry curvature. Because of this, the electron spin near H is predicted to be locked parallel to the electron momentum.

With high resolution angle-resolved photoemission spectroscopy, we mapped the electronic structure in great detail, parallel & perpendicular to the surface plane. We compared our data with bulk band structure calculations in order to identify electronic states and surface states. Finally, spin-resolved ARPES near H has been carried out to examine the predicted exotic spin texture.

O 79.4 Wed 16:00 WIL C307

Spin-dependence in photoemission from strongly spin-orbit coupled systems — •Henriette Maass[1], Hendrik Bentmann[1], Eugene E. Krasovskii[2,3,4], Thiago R. F. Peixoto[1], Christoph Seibel[1], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Departamento de Física de Materiales, Universidad del Pais Vasco UPV/EHU, 20080 San Sebastían/Donostia, Spain — [3]Donostia International Physics Center (DIPC), 20018 San Sebastían/Donostia, Spain — [4]IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Spain

Strong spin-orbit coupling governs the emergence of electronic states with an intrinsic spin polarization. Prominent examples are topological surface states which form for example on the surface of Bi_2Te_3, or Rashba-type spin-splittings in noble metals and surface alloys. Using spin- and angle resolved photoelectron spectroscopy we have investigated the spin- and orbital texture of the topological insulators Bi_2Te_3 and Bi_2Te_2Se as well as the surface alloy $BiAg_2$. Interestingly, whereas at first sight the measured photoelectron spin polarization strongly resembles the one expected for the ground state, strong modulations occur in both, the topological surface states as well as Rashba-type surface states, when the light polarization or photon energy is changed. These modulations reflect a strong influence of the symmetry of initial and final state as well as the experimental alignment on the measured photoelectron spin polarization. Our data yields insight into the relation between the result of a spin-sensitive photoemission experiment and the intrinsic spin-structure of material.

O 79.5 Wed 16:15 WIL C307

Electronic structure of a single crystal BiVO4 photocatalyst measured by angle-resolved photoemission spectroscopy — Mansour Mohammed[1,2], Matthias May[2], Christoph Janowitz[1], Michael Kanis[3], Reinhardt Uecker[4], Mario Brützmann[4], Roel van de Krol[3], and •Mattia Mulazzi[1,4] — [1]1Humboldt University in Berlin, Institute of Physics, 12489 Berlin, Germany — [2]2Assiut University, Department of Physics, Faculty of Science, 71515 Assiut Egypt — [3]3Helmoltz Zentrum Berlin für Materialien und Energie, Institute of Solar Fuels, 14109 Berlin, Germany — [4]4Leibniz Institute for Crystal Growth, 12489 Berlin, Germany

We measured by angle-resolved photoemission at low energy the valence band dispersion of BiVO4. The material, a wide-band gap n-type oxide, is a promising photoanode material for water splitting applications. A solar-to-hydrogen efficiency of ~5% was reached wiht a BiVO4 / double juntion a-Si tandem cell device. The bands measured in ARPES experiments are flat, with only a sizeable dispersion measured in the in-plane directions perpendicular to the (010) axis. We found a weak non-dispersive peak in the forbidden gap indicating localised states, which we attribute to point defects. To determine thee origin of the defects, we compared (for different photon energies) the in-gap peak and top-of-valence-band photoemission intensity ratio to the theoretical Mo and oxygen cross-sections. We found that the theory is in quantitative agreement with the experiment and attributed the in-gap peak to the Mo dopant. We discuss the consequences of the Mo states, which change the size and character of the band gap.

O 79.6 Wed 16:30 WIL C307

Effects of spin-orbit coupling on the optical responses of a material — •Tae Yun Kim[1], Andrea Ferretti[2], and Cheol-Hwan Park[1] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Centro S3, CNR-Instituto Nanoscienze, 41125 Modena, Italy

The electronic structure of a material involving heavy elements are significantly affected by spin-orbit coupling (SOC). Especially, since SOC allows the manipulation of the spin degree of freedom in a material by using light [1-4], understanding the SOC effects on the optical response is a matter of importance. In this contribution, we calculate and investigate the effects of SOC on the optical responses of a material based on a fully-relativistic pseudopotential method [5-6].

[1] C.-H. Park and S. G. Louie, Phys. Rev. Lett. 109, 097601 (2012)

[2] C. Jozwiak, C.-H. Park, K. Gotlieb, C. Hwang, D.-H. Lee, S. G. Louie, J. D. Denlinger, C. R. Rotundu, R. J. Birgeneau, Z. Hussain and A. Lanzara, Nature Physics 9, (2013)

[3] J. H. Ryoo and C.-H. Park, Phys. Rev. B 93, 085419 (2016)

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O 79.7 Wed 16:45 WIL C307

Contribution of magnetic dopants to the electronic structure of the Topological Insulator Sb_2Te_3. — •Sonja Schatz[1], Thiago R. F. Peixoto[1], Hendrik Bentmann[1], Oleg E. Tereshchenko[2], Konstantin A. Kokh[2], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Saint Petersburg State University, 198504 Saint Petersburg, Russia

Doped Topological Insulators with magnetic impurities have been shown to exhibit novel and exotic quantum phenomena. As has been reported recently, V-doped $(BiSb)_2Te_3$ features an insulating ground state below $T_C \sim 30$ K, and it forms a quantum anomalous Hall state below $T \sim 100$ mK [1]. For thin films of this system we already reported, that the existence of a $3d$ impurity band near the Fermi energy is expected to lead to the occurrence of a ferromagnetic superexchance interaction [2]. In this talk we will present studies of the Topological Insulator Sb_2Te_3 doped with different $3d$ transition metals and compare our results to first-principles calculations [3]. To investigate the electronic structure of these systems, angle-resolved photoemission and absorption experiments were performed in the soft X-ray regime at temperatures around $T \lesssim 30$ K. In particular the valence band was observed resonantly at the $2p$ absorption edge providing element specificity.

[1] C. Z. Chang *et al., Nature Materials* **14**, 473 (2015).

[2] T. Peixoto *et al., Physical Review B* **94**, 195140 (2016).

[3] J.-M. Zhang *et al., Physical Review B* **88**, 235131 (2013).

O 79.8 Wed 17:00 WIL C307

Investigation of the Mahan cones spin polarization of noble metal surfaces — •Benito Arnoldi, Johannes Stöckl, Mirko Cinchetti, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics, TU Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

The angle resolved photoemission (ARPES) yield of noble metals such as Au, Ag or Cu recorded at low photon energies is dominated by direct optical transitions between free electron like sp-bands of the bulk band structure, the so called Mahan cones [1]. During the optical transition, the momentum conservation leads to an exchange of momentum between the photoelectron and the crystal lattice by adsorption of a reciprocal lattice vector.

Here, we employ spin and angle resolved laser ARPES with linear polarized light to gain insight into the spin polarization of these direct optical transitions for different noble metal surfaces. For $h\nu \approx 6$ eV and $h\nu \approx 3$ eV in the 1 photon photoemission emission (1PPE) and 2 photon photoemission (2PPE) process for the Au(111) surface, we observe clear spin-polarization of the Mahan cones along all high symmetry directions. Similar results will be presented for the Au(110) as well as for Cu(111) surface. A comparison of our results will allow us to reveal the influence of the spin-orbit coupling on the spin-polarization of the Mahan cones of noble metal surfaces. [1]New J. Phys. 14 (2012) 083027

O 79.9 Wed 17:15 WIL C307

Retrieving the initial-state spin polarization from spin-resolved photoemission: W(110) as a case study — •Jürgen Henk[1], Koji Miyamoto[2], Henry Wortelen[2], and Markus Donath[2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle — [2]Westfälische Wilhelms-Universität, Münster

Spin- and angle-resolved photoelectron spectroscopy (SARPES) aims at measuring the spin polarization of the initial states. In systems with sizable spin-orbit coupling, however, the photoemission process itself results in an additional spin polarization of the photoelectrons. This falsification can be considerable, even for surface states with spin-momentum locking.

We show that the initial-state spin polarization can be largely retrieved by combining SARPES data for selected setups. The idea is presented for optical orientation from the Dirac-type surface state of W(110). Theoretical spectra compare well with their experimental pendants; limitations of the approach are discussed.

O 79.10 Wed 17:30 WIL C307

Surface states of transition-metal delafossite oxides — •Veronika Sunko[1,2], Helge Rosner[2], Pallavi Kushwaha[2], Lewis Bawden[1], Oliver J. Clark[1], Jonathon M. Riley[2,3], Deepa Kasinathan[2], Maurits W. Haverkort[2], Andrew P. Mackenzie[1,2], and Philip D.C. King[2] — [1]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, UK — [2]MPI-CPfS, Nöthnitzer Straße 40, 01217 Dresden, Germany — [3]Diamond Light Source, Harwell Campus, Didcot, OX11 0DE, UK

Delafossite oxides have recently attracted considerable attention because of their fascinating transport properties[1]. PdCoO2 and PtCoO2 are the most conductive oxides known at room temperature, with resistivities comparable to those of silver, copper and gold[2, 3]. This high conductivity is attributed to a single broad band crossing the Fermi level[3]. However, due to the polarity of the structure the electronic properties at the surfaces can be very different to those of the bulk[4]. We use angle resolved photoemission (ARPES) to show that the CoO2 terminated surfaces of (Pd,Pt)CoO2 do host a set of states which do not appear in the bulk, with much higher masses and stronger interactions. Comparing ARPES with density functional theory and model tight-binding calculations, we investigate the origin of these states, paying special attention to the role of the spin-orbit coupling.

[1] Moll et al., Science 351 (2016) 6277, Kikugawa et al., Nature Commun. 7 (2016) 10903 [2] Hicks et al., PRL 109 (2012) 116401 [3] Kushwaha et al., Science Adv. 1 (2015) e1500692 [4] Kim et al., PRB 80 (2009) 035116, Noh et al., PRL 102 (2009) 256404

O 79.11 Wed 17:45 WIL C307

Non-symmorphic band degeneracy at the Fermi level in ZrSiTe — •Andreas Topp[1], Judith M. Lippmann[1,2], Andrei Varykhalov[3], Viola Duppel[1], Shweta Sheoran[1], Bettina V. Lotsch[1,2,4], Christian R. Ast[1], and Leslie M. Schoop[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Department of Chemistry, Ludwig-Maximilians-Universität, D-81377 München — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Bessy II, D-12489 Berlin — [4]Nanosystems Initiative Munich (NIM) & Center for Nanoscience, D-80799 München

Three-dimensional Dirac semimetals, which accommodate massless Dirac or Weyl fermions, show exotic physical properties, e.g. an extremely high mobility and giant magnetoresistance. Compounds that contain non-symmorphic symmetries are especially interesting, because they exibit band crossings that are not affected by SOC. ZrSiS, hosting a square lattice of Si atoms, exhibits normal, as well as, non-symmorphically protected 3D Dirac crossings below and above the Fermi level [1]. Pinning these non-symmorphic crossings to the Fermi level can be difficult, since it requires a material with a half-filled band, that is usually not stable. Upon replacing S with Te, the resulting chemical uniaxial strain shifts the position of the non-symmorphic crossing. Here, we present ARPES data and DFT calculations confirming that the non-symmorphic crossing is located at the Fermi level in ZrSiTe, making this compound a strong candidate to investigate the effect of forced band degeneracies on transport properties.

[1] L. M. Schoop *et al.*, Nat. Comm. 7, 11696 (2016).

O 79.12 Wed 18:00 WIL C307

AiiDA Workflows with FLEUR for X-ray photoemission Spectroscopy — •Jens Bröder[1,2], Gregor Michalicek[1], Daniel Wortmann[1], Rudi Koslowski[2], Christian Linsmeier[2], and Stefan Blügel[1] — [1]Peter Grünberg Institute (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institut für Energie- und Klimaforschung - Plasmaphysik, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

We present the plugin of the all-electron DFT code FLEUR[1] to AiiDA[2] (Automated interactive Infrastructure and database for material science) and our first established workflows to calculate electron binding energies and core level shifts (CLS) of X-ray photoemission (XPS) spectra of pure materials for surface science.

One workflow calculates CLS in the initial state approximation of bulk and slab geometries. An other workflow uses super cell core-hole calculations to extract binding energies. Their first application will be the simulation of materials relevant for research on plasma wall interaction (PWI) in fusion. First results of different methods are compared to recent experimental data.

We acknowledge financial support in part from MAX (Materials design at the eXascale) Horizon 2020 EINFRA-5.

[1] www.flapw.de [2] G. Pizzi, et al. Comp. Mat. Sci. 111, 218-230 (2016)

O 80: SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - Structure - property relationships II

Time: Wednesday 15:45–16:45 Location: IFW D

O 80.1 Wed 15:45 IFW D

Process monitoring of charging/discharging of lithium ion battery cathodes by operando SQUID magnetometry — •Roland Würschum[1], Gregor Klinser[1], Stefan Topolovec[1], Harald Kren[2], Stefan Koller[2], Walter Goessler[3], and Heinz Krenn[4] — [1]Inst. of Mater. Phys., Graz Univ. of Technology, Graz, Austria — [2]VARTA Micro Innovation GmbH, Graz — [3]Inst. of Chem., Univ. Graz — [4]Inst. of Phys., Univ. Graz

The magnetic susceptibility χ of cathode materials, which contain transition metals, substantially changes during charging/discharging and, therefore, serves as highly sensitive fingerprint for the charge state. A novel pathway in this direction has recently opened up by developing in-situ electrochemical techniques for magnetometry. Operando magnetic χ-measurements on Li_xCoO_2 [1] and $Li_xNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (NMC) cathode materials [2] in a SQUID magnetometer during repetitive electrochemical cycling were performed enabling a continuous and bulk sensitive monitoring of the charge compensation process. Upon charging of NMC up to Li contents of $x = 1/3$ exclusively Ni undergoes oxidation, namely in two consecutive steps $Ni^{2+} \rightarrow Ni^{3+}$ for $x > 2/3$ and $Ni^{3+} \rightarrow Ni^{4+}$ for $2/3 > x > 1/3$ [2]. Co oxidation for $x < 1/3$ is found to be irreversible [2]. In the case of Li_xCoO_2, evidence is found for a nonmetal−metal transition of Anderson−type [1]. In addition to Co also O undergoes partial oxidation, as also observed for NMC.

[1] St. Topolevec et al., J. Sol. State Electrochem. 20 (2016) 1491.

[2] G. Klinser et al., Appl. Phys. Letters 109 (2016) 213901.

O 80.2 Wed 16:00 IFW D

Enhancement of Sodium Ion Battery Performance Enabled by Oxygen Vacancies — •Yang Xu, Min Zhou, Chengliang Wang, Liying Liang, Fabian Grote, Yan Mi, and Yong Lei — Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, Ilmenau 98693, Germany

The utilization of oxygen vacancies (OVs) in sodium ion batteries (SIBs) is expected to enhance performance, yet it has rarely been reported. Taking the MoO3-x nanosheet anode as an example, for the first time we demonstrate the benefits of OVs on SIB performance. Moreover, the benefits at deep-discharge conditions can be further promoted by an ultrathin Al2O3 coating. Ex-situ electrochemical impedance and X-ray photoelectron spectroscopy measurements show that the OVs increase the electric conductivity and Na-ion diffusion coefficient, and the promotion from ultrathin coating lies in the effective reduction of cycling-induced solid-electrolyte interphase. The coated nanosheets exhibited high reversible capacity and great rate capability with the capacities of 283.9 mAh g-1 at 50 mA g-1 and 179.3 mAh g-1 at 1 A g-1 after 100 cycles. This work could not only arouse future attention on OVs for sodium energy storage, but also open up new possibilities for designing strategies to utilize defects in other energy storage systems.

Reference

Y. Xu, M. Zhou, X. Wang, C. Wang, L. Liang, F. Grote, M. Wu, Y. Mi, Y. Lei, Angew. Chem. Int. Ed. 2015, 54, 8768.

O 80.3 Wed 16:15 IFW D

Polycrystalline NaxCoO2 thin films on ß-Alumina ceramics for solid state batteries — •Philipp Kehne[1], Conrad Guhl[2], René Hausbrand[2], and Philipp Komissinskiy[1] — [1]Department of Materials Science, TU-Darmstadt, Advanced thin film technology — [2]Department of Materials Science, TU-Darmstadt, Surface science

Good cycling performance was previously shown for rechargeable sodium ion batteries with layered-oxide cathode materials such as NaxCoO2 in combination with liquid electrolytes. However, studies of sodium-based solid state batteries are necessary to correlate the electronic structure of sodium-ion insertion materials with the battery performance. Here we report polycrystalline NaxCoO2 films grown on ß-Alumina polycrystalline ceramic substrates with pulsed laser deposition. The sodium content in the films can be adjusted in the range of x = 0.6 * 1.1 by varying the post-deposition annealing conditions. The ß-alumina substrates reveal ionic conductivities of 0.002 S/cm (25 °C) and can be used as electrolyte in solid-state sodium batteries. The fabricated Swagelok-type rechargeable batteries with NaxCoO2 thin-film cathodes, ß-alumina electrolyte, and sodium anodes reveal an open circuit voltage of 2.75 V and a specific capacitance of C = 80 mAh/g. Investigations of the electronic structure of the materials and interfaces in the fabricated batteries by in-situ XPS are in progress.

O 80.4 Wed 16:30 IFW D

Large-scale highly ordered Sb nanorod arrays anode with high capacity and rate capability for sodium-ion batteries — •Liying Liang, Yang Xu, Chengliang Wang, Liaoyong Wen, Yaoguo Fang, Yan Mi, Min Zhou, Huaping Zhao, and Yong Lei — Institute for Physics and IMN MacroNano, Ilmenau University of Technology, Ilmenau 98693, Germany.

The poor electrochemical performance of Na-ion batteries is the major bottleneck for future development. Hence a performance-oriented electrode structure is proposed, which is 1D nanostructure arrays with large-scale high ordering, well vertical alignment, and large interval spacing. Benefiting from these structure merits, a great enhancement on electrochemical performance could be achieved. To Sb as an example, we firstly report large-scale highly ordered Sb nanorod arrays with uniform large interval spacing (190 nm). In return for this electrode design, high ion accessibility, fast electron transport, and strong electrode integrity are presented here. Used as additive-free anode for SIBs, Sb nanorod arrays showed a high capacity of 620 mAh g-1 at the 100th cycle with a retention of 84% up to 250 cycles at 0.2 A g-1, and superior rate capability for delivering reversible capacities of 579.7 and 557.7 mAh g-1 at 10 and 20 A g-1, respectively. A full cell coupled by P2-Na2/3Ni1/3Mn2/3O2 cathode and Sb nanorod arrays anode was also conducted, which showed a good cycle performance up to 250 cycles, high rate capability up to 20 A g-1, and large energy density up to 130 Wh kg-1.

O 81: Oxide and Insulator Surfaces: Adsorption II

Time: Wednesday 16:00–18:30 Location: WIL C107

O 81.1 Wed 16:00 WIL C107

Adsorption Sites of Individual Metal Atoms on MgO Thin Films Determined by Means of STM — •Edgar Fernandes, Fabio Donati, François Patthey, and Harald Brune — Institute of Physics (IPHYS), Ecole Polytechnique Fédérale de Lausanne (EPFL), Station 3, CH-1015 Lausanne, Switzerland

Single Atoms on ultrathin insulating layers grown on metal surfaces have shown magnetic bistability up to 40 K [F. Donati & *al.*, Science **352**, 318 (2016)] and catalytic activity [B. Qiao & *al.*, Nat. Chem. **3**, 634 (2011)]. These spectacular properties are determined by the adsorption site that influences the charge state, crystal field, diffusion barrier, and magnetic ground state.

Here, we present a novel experimental method to determine the adsorption site of adatoms on thin MgO(100) layers on Ag(100) with the scanning tunnelling microscope. We determine the lattice constant and orientation of the atomic lattice from atomic resolution images recorded on pristine MgO and identify the sub-lattice imaged as protrusions by means of doping with Ca atoms that substitute and thereby mark the Mg atoms. Ho atoms adsorb on O and bridge sites, with their respective abundance depending on MgO thickness. Co and Fe atoms are on O sites while Au atoms are on bridge sites in contrast to former work [M. Sterrer & *al.*, Phys. Rev. Lett. **98**, 206103 (2007)].

O 81.2 Wed 16:15 WIL C107

Photochemical switching of azobenzene derivatives on an insulating surface — •Simon Jaekel[1], Antje Richter[2], Robert Lindner[2], Angelika Kühnle[2], Stefan Hecht[3], and Leonhard Grill[1] — [1]Department of Physical Chemistry, University of Graz, Austria — [2]Institute for Physical Chemistry, Johannes-Gutenberg University Mainz, Germany — [3]Department of Chemistry, Humboldt-University Berlin, Germany

Studying single molecular switches is of interest for a better understanding of fundamental physical and chemical processes, but also in view of their possible use in molecular nanotechnology [1].

A prototypical conformational switch is azobenzene, which changes between trans and cis isomers at the central N=N bond upon an external stimulus, showing efficient photochemical activation. In the past years, various studies have shown that adsorption on metal substrates strongly influences the switching properties [2,3], especially for activation by light [4].

We present non-contact atomic force microscopy (nc-AFM) results on the switching of individual azobenzene molecules on a calcite surface where the molecules retain their photochemical activity.

[1] C. Joachim et al., Nature 506, 651 (2000); [2] Choi et al., Phys. Rev. Lett. 96, 156106 (2006); [3] Dri et al., Nature Nanotechnology 3, 649 (2008); [4] Comstock et al., Phys. Rev. Lett 99, 038301 (2007)

O 81.3 Wed 16:30 WIL C107

DFT Study of Water Adsorption on Cation Doped (001)-MgO Surfaces — •Thomas Ruh[1], Christian Knoll[2], Danny Müller[2], Peter Weinberger[2], and Peter Blaha[1] — [1]Institute of Materials Chemistry, TU Wien — [2]Institute of Applied Synthetic Chemistry, TU Wien

Combined hydration/dehydration processes of oxide/hydroxide systems can be used for storage of industrial excess heat. An example is the system CaO/Ca(OH)$_2$ [1]. The exothermal reaction of CaO and water (to release stored energy) is fast and complete at ambient temperature; however, the reverse reaction to recover CaO requires high temperatures. For several applications a system operable at lower temperatures would be desirable.

A potential candidate is the system MgO/Mg(OH)$_2$. However, the reaction of the oxide with water is slow and incomplete at room temperature. Many studies of the adsorption behaviour of water on MgO surfaces suggest that the reaction is kinetically hindered. Hu et al [2], for instance, found in a DFT study, that adsorbed water does not dissociate on MgO surfaces, whereas on CaO surfaces hydroxyls are formed.

In the present work we investigate the effects of cation doping of the (001)-surface of MgO with different cations on the formation and subsequent stability of hydroxyls.

[1] S. Jujimoto et al., Energ. Convers. Manage., 2002, 43, 947-960 [2] X.L. Hu et al., Phys. Chem. Chem. Phys., 2011, 13, 12447-12453 [3] http://www.wien2k.at

O 81.4 Wed 16:45 WIL C107

Adsorption of Organic Molecules on Magnetite Single Crystal Surfaces — •Marcus Creutzburg[1,2], Heshmat Noei[1], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, Hamburg, Germany — [2]Fachbereich Physik, Universität Hamburg, Jungiusstraße 9, Hamburg, Germany

Magnetite (Fe$_3$O$_4$) is a very important and diverse transition metal oxide with applications in catalysis, data storage and biomedical imaging. In a recent study magnetite nanoparticles linked by oleic acid molecules show exceptional isotropic mechanical properties [1]. To give further insight on how these nanoparticles interact with organic molecules it is crucial to study flat single crystal and vicinal Fe$_3$O$_4$ surfaces. In this contribution, we present initial results on the adsorption of water and organic molecules like formic acid and oleic acid on the magnetite (111) and on the vicinal (112) surface under UHV conditions obtained by vibrational spectroscopy and X-ray photoemission spectroscopy. We show low energy electron diffraction patterns of the vicinal (112) which allows us to conclude that this surface is indeed stable and presents regularly ordered terraces and steps.

[1] A. Dreyer *et al.*, Nature Materials **15**, 522-528 (2016)

O 81.5 Wed 17:00 WIL C107

Temperature-dependent reactions of Phthalic Acid on Co$_3$O$_4$(111) — •Daniel Wechsler, Matthias Franke, Quratulain Tariq, Hans-Peter Steinrück, and Ole Lytken — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen, Egerlandstraße 3, Germany

Understanding the bonding between organic molecules and metal-oxide surfaces plays an important role in many nanotechnology devices. Functional groups, like -COOH, can act as linkers to attach molecules to surfaces in a controlled manner.

Using synchrotron-radiation X-ray photoelectron spectroscopy and temperature programmed desorption we have followed the adsorption and reactions of phthalic acid, a model system with two carboxylic acid linker groups, with Co$_3$O$_4$(111) as a function of coverage and temperature. Upon annealing from 105 to 800 K, three different temperature regions have been identified. They were assigned to intact phthalic acid, a carboxylate species forming at 350 K and finally thermal composition beginning at 750 K. Near-edge X-ray absorption fine structure measurements confirm an upright-standing adsorption geometry of the carboxylate species.

The project is supported by the DFG through FOR 1878 (funCOS).

O 81.6 Wed 17:15 WIL C107

Theoretical Description of the Adsorption of Water and Ethanol on Pt$_4$/Pt(111) and Pt$_4$/CeO$_2$(111) Substrates — •Yohanna Seminovski[1], Polina Tereshchuk[1], Adam Kiejna[2], and Juarez L. F. Da Silva[1] — [1]São Carlos Institute of Chemistry, University of São Paulo, São Carlos, SP, Brazil — [2]Institute of Experimental Physics, University of Wrocław, Wrocław, Poland

Pt-ceria, which has been proposed as catalyst for H$_2$ production in ethanol steam reforming reaction process, show formation of partially reduced Ce cations because of charge transfer from Pt transition metal towards oxide surface.[1] However, the role of the independent active adsorption sites on TM$_n$/CeO$_2$(111) substrates is not well understood yet. For instance, it is not known if the cationic Pt sites coexistent with the newly formed Ce^{3+} influence the adsorption properties of molecule on the substrates. In this work,[2] we applied DFT+U to study the active sites and the role of partial cationic charge of the Pt atoms on the adsorption properties of water and ethanol (probe molecules) on four selected substrates, Pt(111), Pt$_4$/Pt(111), CeO$_2$(111), and Pt$_4$/CeO$_2$(111). Results show each molecule preferentially located in the cationic sites of the base of the tetrahedron Pt$_4$ cluster, while in the anionic, lower-coordinated Pt atom sites located on the cluster-top or in the surface Ce and O sites the molecule adsorption is less favored. The Ce^{3+} atoms aren not found to be directly involved in the adsorption process of molecules, however these are important in the stabilization of the substrate.[1]P. Tereshchuk *et al.*, PCCP **17**, 13520 (2015) [2]Y. Seminovski *et al.*, JCP **145**, 124709 (2016)

O 81.7 Wed 17:30 WIL C107

High-resolution photoemission and X-ray absorption spectroscopy of a functionalized porphyrin adsorbed on MgO(100) — •Quratulain Tariq, Matthias Franke, Daniel Wechsler, Hans-Peter Steinrück, and Ole Lytken — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen, Egerlandstraße 3, Germany

Ultra-thin layers of functional organic molecules on oxide surfaces have a huge scientific and technological potential in molecular electronics. Porphyrins, in particular, represent an interesting class of compounds that can be modified synthetically by variation of the metal center, by attaching different substituents to the macrocycle, or by introduction of specific linker groups for the attachment on surfaces. In present work, a cobalt porphyrin bearing carboxylic groups, 5,10,15,20-tetrakis (4-carboxyphenyl) porphyrin (CoTCPP), was anchored on MgO(100)/Ag(100) thin films, at room temperature. High-resolution synchrotron radiation photoelectron spectroscopy (SRPES) and near-edge X-ray absorption fine structure (NEXAFS) spectroscopy are used to characterize the system, as a function of coverage and temperature. SRPES analysis for different coverages reveals that CoTCPP binds to the surface via formation of bidentate carboxylate. From NEXAFS spectroscopy, it is found that for sub-monolayer coverage, CoTCPP adsorbs almost parallel to the oxide substrate, whereas for monolayer and higher coverages, CoTCPP adsorbs at an angle from the surface plane (with a possible tilt angle of $< 45°$ relative to the surface normal). This project is supported by the DFG through FOR 1878 (funCOS).

O 81.8 Wed 17:45 WIL C107

Adsorption of Oxygen on $Ca_3Ru_2O_7$(001) — •Daniel Halwidl[1], Wernfried Mayr-Schmölzer[1,2], Florian Mittendorfer[1,2], David Fobes[3], Jin Peng[3], Zhiqiang Mao[3], Michael Schmid[1], Josef Redinger[1,2], and Ulrike Diebold[1] — [1]Institute of Applied Physics, TU Wien, Wiedner Hauptstraße 8-10, A-1040 Vienna, Austria — [2]Center for Computational Materials Science, TU Wien, Wiedner Hauptstraße 8-10, A-1040 Vienna, Austria — [3]Department of Physics and Engineering Physics, Tulane University, New Orleans, LA, USA

Complex ternary perovskite oxides are increasingly used in solid oxide fuel cells and catalysis [1]. Therefore it is highly desirable to obtain a better understanding of their surface chemical properties. We use low-temperature STM, nc-AFM, XPS and DFT to investigate the adsorption of oxygen on the layered perovskite $Ca_3Ru_2O_7$.

Single oxygen molecules appear fuzzy in STM, but are resolved in nc-AFM at LHe and LN_2 temperature. At higher coverages the molecules form a (2×1) overlayer that covers almost the whole surface. Local contact potential difference (LCPD) measurements suggest that the oxygen molecules are charged, in agreement with DFT calculations predicting adsorption as superoxo species. Desorption of the O_2 occurs at approximately 220 K, again in agreement with the calculated adsorption energy of $E_{ads} = 0.7$ eV.

This work was supported by the Austrian Science Fund (FWF project F45) and the ERC Advanced Grant “OxideSurfaces”.

[1] M. A. Pena, and J. L. G. Fierro, Chem. Rev. 101, 1981 (2001)

O 81.9 Wed 18:00 WIL C107

Water adsorption on top of the hematite(0001) surface at medium and high coverage regimes — •Roman Ovcharenko and Elena Voloshina — Institut für Chemie, Humboldt-Universität zu Berlin, Berlin, Germany

On the pristine hematite(0001) half-iron termination isolated water molecules form an dissociated structure with an OH group attached to a surface iron ion and a protonated surface oxygen ion [1]. At increasing water loading the water-water interaction starts to play a crucial role in the adsorption behaviour and energetics. Thus, according to our PBE+U+D2 calculations, for the 1/2 monolayer (ML) coverage fully dissociated and mixed adsorption structures are energetically degenerated. Nevertheless, both water molecules and OH-groups adsorb at different coordinatively unsaturated metal sites and do not tend to form a dimer structure as it was found for the magnetite(111) surface [2]. When increasing water loading further up to 3/4 ML, a tendency to form mixed adsorption structures become even more pronounced. This is different to water adsorption on top of the isomorphic corundum (0001) surface, where by increasing water loading each following molecule was found to dissociatively adsorb at new metal site up to the full monolayer. Thus, the hematite(0001) surface, partially inheriting the properties of both magnetite and aluminium oxide, demonstrates unique chemical reactivity towards water adsorption at medium and high coverage regimes. [1] R. Ovcharenko et al., Phys. Chem. Chem. Phys. 18, 25560 (2016) [2] X. Li et al., J. Phys. Chem. C 120, 1056 (2015)

O 81.10 Wed 18:15 WIL C107

Adsorption of Oxygen on Ruthenate Perovskite Surfaces — •Florian Mittendorfer, Wernfried Mayr-Schmölzer, Josef Redinger, Daniel Halwidl, and Ulrike Diebold — Institute of Applied Physics, TU Vienna

The surface chemistry of perovskite oxides plays a central role for promising applications, such as solid oxide fuel cells. In a recent study, we could demonstrate a high chemical activity of strontium ruthenate surfaces for the adsorption of CO [1] and H_2O[2].In this presentation, I will discuss the adsorption of oxygen (O_2) on the (001) surface of the Ruddlesden-Popper perovskites $Sr_3Ru_2O_7$(SRO) and $Ca_3Ru_2O_7$ (CRO) on the basis of density functional theory (DFT) calculations. Oxygen adsorbes as a charged molecular species on both surfaces, yet our results display pronounced differences between the two systems. In the low coverage case, the calculations predict a slight tilting of the O_2 molecule on the SRO (001) surface, and the surface is uniformly covered at higher coverages. In contrast, the additional tilting of the Ru octahedra at the bare CaO terminated CRO (001) surface leads to a striped pattern of wide and narrow rows. This pattern strongly influences the respective adsorption energies of the O_2 molecule, as the adsorption in the wide channels is significantly more stable than the adsorption in the narrow channels. Thus, in agreement with experiment, the saturation coverage is already reached at an oxygen coverage of 0.5 ML, where the occupation of symmetry- equivalent sites leads to the formation of a zig-zag arrangement of the O_2 molecules. [1] Phys. Rev. Lett 113, 116101 (2014) [2] Nature Materials 15, 450 (2016)

O 82: Nanostructures at Surfaces: Graphene and Other Aspects

Time: Wednesday 16:00–18:30 Location: REC/PHY C213

O 82.1 Wed 16:00 REC/PHY C213

Sublimation of non-IPR fullerene dimers — •Jürgen Weippert[1], Lea Hohmann[1], Artur Böttcher[1], and Manfred M. Kappes[1,2] — [1]Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Non-IPR fullerenes were generated in vacuum by electron impact ionization and fragmentation of IPR fullerenes (C60, C70). The corresponding solids were formed by low energy ion beam deposition of the mass-selected Cn cages onto HOPG. The materials grow via formation of a network of covalently interlinked oligomers. This morphology is responsible for the unique properties of these novel materials such as an (n-dependent) band gap, high thermal stability, hardness and Young*s modulus.... Recently we found, that the sublimation of some non-IPR solids proceeds via a second channel: in addition to the dominant emission of monomers we also observe the emission of dimers. These show a significantly higher sublimation enthalpy than found for related monomers. Furthermore, we can relate the monomer geometries to the emission intensity in competition with thermal hardening of the network.

O 82.2 Wed 16:15 REC/PHY C213

Amorphous hydrogenated carbon (a-C:H) depositions on polyoxymethylen (POM) - polymer substrate effects for identical depositions — •Christian B. Fischer, Alberto Catena, Liz M. Rösken, and Stefan Wehner — Department of Physics, University Koblenz-Landau, 56070 Koblenz, Germany

The polymer polyoxymethylene (POM) has been gradually covered with a-C:H films by radio frequency plasma-enhanced chemical vapor deposition (RF-PECVD) with acetylene plasma after initial oxygen plasma cleaning. Both steps where performed on the same sample plate together with selected polymers like high-density polyethylene (HDPE) and polyethylene terephthalate (PET). The focus of this investigation is to study specific effects during an identical carbon coating on these chemically different polymer substrates. Especially the interlayer forming behavior between these two materials is of primary interest. Surface morphology was conducted by atomic force microscopy (AFM), the chemical composition by diffusive reflectance infrared Fourier transform (DRIFT), near-edge X-ray absorption (NEXAFS) and micro-Raman spectroscopy. Findings indicate the absence of a solid interlayer formation for POM as found for the other two polymers. Furthermore, the developing a-C:H network on POM is remarkably different to the carbon film structure on HDPE and PET. Altogether these results reveal that different plastic substrates strongly affect the resulting structure of the a-C:H coating during identical depositions.

O 82.3 Wed 16:30 REC/PHY C213

Recent advances in Secondary Ion Mass Spectrometry in the Helium Ion Microscope — •Florian Vollnhals, David Dowsett, Jean-Nicolas Audinot, and Tom Wirtz — Advanced Instrumentation for Ion Nano-Analytics (AINA), Luxembourg Institute of Science and Technology (LIST), L-4422 Belvaux, Luxembourg

The Helium Ion Microscope (HIM) has become an ideal tool for imaging with an ultimate resolution down to 0.5 nm using He and nanopatterning of structures with sub 20 nm feature using Ne ions. [1]

As standard analytical techniques like EDX are are not compatible with HIM, we have developed a Secondary Ion Mass Spectrometry (SIMS) add-on for Zeiss' Orion Nanofab.[2] SIMS is based on the identification of characteristic secondary ions emitted due to the irradiation of a surface with a primary ion beam. As the probe size in the HIM is substantially smaller (both for He and Ne) than the sputtering interaction volume, the lateral resolution is limited only by fundamental considerations and not by the probe size. The available mass range of up to 500 amu in combination with a mass resolution greater than 400 allows for compositional analysis of nanoscale structures.

We will present our progress in instrumental and method development of HIM-SIMS as well as data obtained on the prototype systems. He and Ne ion beams will be shown to be viable primary species for SIMS, approaching the physical resolution limits of $<$20 nm.

[1] L. Scipioni et al., J. Vac. Sci. Technol. B 27 (2009), 3250

[2] T. Wirtz et al., in "Helium Ion Microscopy", Springer (2016), p. 297-323

O 82.4 Wed 16:45 REC/PHY C213

Amorphous TiO2 Inverse Opal Anode for High-rate Sodium Ion Batteries — •Min Zhou, Yang Xu, Liying Liang, Huaping Zhao, Benrong Hai, and Yong Lei — Ilmenau University of Technology, Ilmenau 98693, Germany

With the increased demands of available energy, potential applications of sodium-ion batteries have motivated significant progress in energy storage field. Compared with Li ions, large radius of Na ions results in different electrochemical behaves. Hence, synergistic understanding of the differences is greatly significant. Surface availability of ions is critical to rate performance in SIBs. Here, amorphous TiO2 inverse opal is employed as a proof-of-concept example to illuminate the influences of surface ion availability and the relationship between solvent wettability and rate capability. Enhanced solvent wettability contributes to superior rate capabilities, regardless of the type of electrolyte and the ion concentration in electrolyte. Our concept offers a potential to realize full potential of designing electrode materials for SIBs by adjustable surface kinetics. Similar attentions may be used to mitigate problems caused by ion affinity or other limitations from tremendous Na ions, and enable sodium-ion batteries to be more amenable for large-scale implementations.

O 82.5 Wed 17:00 REC/PHY C213

An extended continuum model for epitaxial growth of graphene: A phase field crystal approach — •Rainer Backofen[1], Sai Tang[2], and Axel Voigt[1] — [1]Institut für Wissenschaftliches Rechnen, TU Dresden, 01062 Dresden, Germany — [2]MPI für Eisenforschung, 40237 Düsseldorf, Germany

Epitaxial growth of graphene on single crystalline metal substrates lead to a large variety of different shaped graphene flakes. E.g. hexagonal, rectangular or butterfly shaped flakes are observed depending on the symmetry of the substrate. This macroscopic morphologies of the crystal have been successfully reproduced by a phase field model following the ideas of step flow modeling introduced by Burton, Cabrera and Frank [1]. In this model, the anisotropy of adatom diffusion and line energy of the growing crystal is adjusted to achieve the different morphologies. We present a phase field crystal model (PFC), that directly introduce the interaction with the substrate on the atomistic length scale and lead to different growth shapes. Thus, the anisotropy of of the macroscopic properties are a direct result of the interaction with the substrate. Additionally, defects and elastic deformations are naturally included. This approach combines a multimode extension of PFC, [2], to account for the crystalline structure and a vapor phase PFC model, [3], to control the phase transition at the substrate. With this model we can show how the local interaction to the substrate leads to different shapes of the growing crystal.

[1] Esteban et al., Nano Lett., 2013, 13(11) [2] Mkhonta et al., PRL 111, 035501 [3] Schwalbach et al., PRE 88, 023306

O 82.6 Wed 17:15 REC/PHY C213

Graphene on Ir(110), a twofold-symmetric substrate for van der Waals epitaxy applied to growth of organometallic nanowires — •Felix Huttmann, Stefan Kraus, and Thomas Michely — II. Physikalisches Institut, Universität zu Köln, Germany

Standard substrates for van der Waals heteroepitaxy, such as graphene on hcp or fcc metal surfaces or H-terminated Si, all possess threefold or sixfold rotational symmetry, and if an adsorbed film does not have such symmetry, this leads to the formation of rotational domains, in conflict with the common goal to achieve an effectively single-crystalline film. We have encountered this problem in the growth of carpets of organometallic nanowires of europium cyclooctatetraene (EuCot) on the graphene/Ir(111) surface, where the lack of a global orientation of the nanowires forbids the study of orientation-dependent properties using spatially averaging techniques. Here, we investigate the growth of graphene on Ir(110), a surface with only twofold rotational symmetry. While clean Ir(110) exhibits facetting, exposure to ethylene at elevated temperatures leads to re-flattening of the surface. Two well-ordered overlayer phases are formed depending on the growth temperature of either 1250 K or 1380 K. The high-temperature phase is atomically flat over terrace sizes on the order of 100 nm and permits to grow the EuCot nanowires oriented along the [001] direction of the substrate. A single global orientation of almost all nanowires is thus achieved as intended. On the scale of a few hundred nanometers, a structure of ridges and valleys with step edge bundles in between limits the smoothness of the graphene/Ir(110) surface and provides room for improvement.

O 82.7 Wed 17:30 REC/PHY C213

Atomic structure and element distribution of graphene/Ir(111) supported Pt/Rh metal clusters — •Dirk Franz[1,2], Nils Blanc[3,4], Johann Coraux[4], Heshmat Noei[2], Roman Shayduk[2], and Andreas Stierle[1,2] — [1]Universität Hamburg, D-20355 Hamburg, Germany — [2]DESY NanoLab, D-22607 Hamburg, Germany — [3]Institut NEEL, CNRS, F-38042 Grenoble, France — [4]CEA-UJF, INAC, F-38054 Grenoble, France

Ultrasmall metallic nanoparticles exhibit altered structural, chemical and magnetic properties as compared to their bulk counterparts making them attractive for applications as highly active heterogeneous catalysts or high storage density magnetic media. To pinpoint structure-functionality relationships for systems containing nanoparticles with diameters smaller than 2 nm an atomic scale understanding of their structure is mandatory.

It was previously shown that different 2D metal cluster arrays can be grown using the moiré of graphene/Ir(111) as a template [1]. We have employed several surface sensitive techniques (SXRD, GISAXS, XPS) to investigate the structure of Pt/Rh particles (shape, epitaxy, strain, element distribution) with less than 50 atoms after growth on a graphene/Ir(111) support and in oxidizing/reducing gas environments. SXRD and GISAXS benefits essential from the ordered arrangement of the clusters and is able to reveal the average atomic structure of these small clusters.

[5] A. T. N'Diaye, et al., New J. Phys. 11, 103045 (2009).

[6] D. Franz, et al., Phys. Rev. Lett. 110, 065503 (2013).

O 82.8 Wed 17:45 REC/PHY C213

Self-assembly of para-hexaphenyl-dicarbonitrile on graphene on Cu(111) — •Nico Schmidt, Stefano Gottardi, Juan-Carlos Moreno-Lopez, Jun Li, Leonid Solianyk, Leticia Monjas Gomez, Anna Hirsch, and Meike Stöhr — University of Groningen, Groningen, the Netherlands

Graphene is a 2D material exhibiting various outstanding features.

Self-assembled molecules on graphene are often studied with respect to altering the electronic properties, i.e., making graphene more suitable for applications. However, the underlying substrate, on which graphene is grown, has been shown to still have an impact on the formation of the molecular adlayer.

In this study, para-hexaphenyl-dicarbonitrile was deposited onto graphene grown on Cu(111) via chemical vapor deposition. The resulting densely-packed network was found to be stabilized by a combination of dipolar coupling and hydrogen bonding. However, the molecular assembly showed no correlation with the varying orientation of the underlying graphene. This showcases the necessity to carefully assess the influence of the substrate in molecule/graphene interfaces. All experiments were carried out under UHV conditions using low-temperature scanning tunneling microscopy and low-energy electron diffraction.

O 82.9 Wed 18:00 REC/PHY C213

Electronic and optical properties of ultra-thin graphene nanoribbons — •Boris Senkovskiy[1], Danny Haberer[2], Alexander Fedorov[1], Markus Pfeiffer[3], Sayed Alavi[3], Nicolae Atodiresei[4], Vasile Caciuc[4], Klas Lindfors[3], Felix Fischer[2], and Alexander Grüneis[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]Department of Chemistry, University of California at Berkeley, Berkeley, USA — [3]Institute for Physical Chemistry, University of Cologne, Germany — [4]Peter Grünberg Institute and Institute for Advanced Simulation, Jülich, Germany

The present work demonstrates that electronic and optical properties of ultra-thin graphene nanoribbons are strikingly different from its 2D or 3D counterparts. A semiconductor-to-metal transition in armchair graphene nanoribbons of N=7 carbon atoms width causes drastic changes in the electronic system. By using angle-resolved photoemission spectroscopy of lithium doped nanoribbons, a quasiparticle band gap renormalization from 2.4 eV to 2.1 eV is observed. Reaching high doping levels (0.05 electrons/atom), it is found that the effective mass of the conduction band carriers increases by a factor of four to a value equal to the free electron mass. This giant increase in the effective mass by doping can have palpable impact on the electronic properties of the system. Having carried out the bubble transfer of massively aligned nanoribbons from the gold to the insulating substrate we investigate the optical properties of the material. It is shown that incorporation of sp3 defects induces polarized photoluminescence from intrinsically 'dark' graphene nanoribbons.

O 82.10 Wed 18:15 REC/PHY C213

Formation of Coupled Organic-Inorganic Nanostructures Studied by X-ray Scattering Techniques — •Santanu Maiti[1], Alexander Andre[2], Marcus Scheele[2], and Frank Schreiber[1] — [1]Institute of 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 18, 72076 Tuebingen, Germany

Electronically coupled hybrid nanostructures of alternating semiconductor nanocrystal (NC) and monolayer of organic semiconductor (OSC) molecules can exhibit interesting charge carrier transport across the superlattice network. Ordered superlattices of coupled organic-inorganic nanostructures (COINs) are a promising material class to realize and exploit the directional transport as well as exciting optical properties1,2. A combined x-ray reflectivity and grazing incidence scattering (GISAXS and GIWAXS) study during COINs formation (ex- and in-situ) of PbS NCs with different OSCs (CuTAPc/TTFDA) has been carried out3-5. The assembly of nanoparticles and their ordering before and after the ligand exchange process at the air-liquid interface has been monitored. A significant change of about 0.6 and 0.5 nm along the in-plane and out-of-plane direction respectively has been observed after COINs formation. 1. M. P. Boneschanscher et al., Science 344, 1377 (2014); 2. M. Scheele et al., PCCP 17, 97 (2015); 3. S. Maiti et al., J. Phys.: Condens. Matter, 25, 395401 (2013); 4. J. Novak et al., ACS Appl. Mater. Interfaces 8, 22526 (2016); 5. A. Andre et al., Chem. Mater. 27, 8105 (2015).

O 83: Overview Talk: Bernd Meyer

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

Invited Talk O 83.1 Thu 9:30 TRE Phy

Molecular adsorption on oxide surfaces: Insights from first-principles calculations — •Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

In the past decade, much progress was made in characterizing and understanding chemical processes occurring at oxide surfaces. Compared to metals, oxides show a much wider variety of phenomena upon adsorption and reaction of molecules. The more versatile behavior of oxide surfaces can be attributed to more pronounced changes in the electronic structure, a reduced screening and the more important role of surface defects. In this talk I will review recent theoretical studies in this field, starting with examples of how the adsorption of small molecules can lead to phenomena such as surface metalization and how new types of substrate-mediated adsorbate–adsorbate interactions can result in the formation of unexpected complex adsorbate structures. I will then turn to the functionalization of oxide surfaces by larger organic molecules and the characterization of hybrid organic–inorganic interfaces, which play an important role in molecular electronics and dye-sensitized solar cells. Finally, first ab initio molecular dynamics simulations on chemical processes at the oxide/liquid interface will be discussed.

O 84: Focus Session: Semiconductor Materials and Nanostructure for Photocatalysis

Time: Thursday 9:30–12:30 Location: POT 51

Invited Talk O 84.1 Thu 9:30 POT 51

Solar-driven photoelectrochemical water splitting and carbon dioxide reduction — •Joel Ager — Joint Center for Artificial Photosynthesis, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA USA — Department of Materials Science and Engineering, UC Berkeley

Solar to fuel conversion, if it could be performed in a sustainable manner, could provide an alternative to mankind's currently unsustainable use of fossil fuels. Solar fuel generation by photoelectrochemical (PEC) methods is a potentially promising approach to address this fundamental and important challenge.

While there are number of laboratory-scale solar to hydrogen (STH) conversion devices whose efficiencies exceed 10%, there are very few reports of long term operational stability. In this context, the long term stability of protective coatings for water oxidation photoanodes will be discussed, with an emphasis on the experimental procedures required to predict the operational lifetime.

Electrochemical carbon dioxide reduction is comparatively less mature as a technology and hence the challenges are more basic. Indeed, there are very few report of systems which produce usable fuel products with high selectivity. Recently, building on work performed with Cu nanocubes, we have designed Cu nanostructures which achieve up to 70% conversion of carbon dioxide to C2+ products. When coupled with high efficiency solar cells, overall energy conversion efficiencies exceeding that of natural photosynthesis can be achieved.

O 84.2 Thu 10:00 POT 51

Tuning the electronic structure of Nb3O7(OH) by titanium doping for enhanced light-induced water splitting — Wilayat Khan[1], •S. Betzler[2], O. Sipr[3], Ch. Scheu[4], and J. Minar[5] — [1]New Technologies-Research Center, University of West Bohemia, Univerzitní 8, 306 14 Plzen, Czech Republic — [2]Department of Chemistry and Center for NanoScience, LMU Munich, Butenandtstraße 11, 81377 Munich, Germany — [3]NTC, University of West Bohemia, Plzen, Czech Republic — [4]Max-Planck-Institut fur Eisenforschung GmbH, Max-Planck-Straße 1, Du*sseldorf, Germany — [5]NTC, University of West Bohemia, Plzen, Czech Republic

Water photolysis is a clean and renewable source for hydrogen fuel and is therefore considered as a potentially important part of the solution of the energy crises. An extensive work has been performed on transition metal oxides semiconductors like TiO2, WO2 and Fe2O3, which can be used as electrode materials. Recently, Nb3O7(OH) has been proposed as a promising material for this propose due to its stability and suitable band gap [1]. Here we report on the modification of the structure and electronic properties of Nb3O7(OH) due to the Ti doping. Our theoretical study is based on the density functional theory using FP-LAPW method. The Ti-doped Nb3O7(OH) showed a direct band gap at the G point in the calculated band structures. In addition, Ti doping modifies the optical properties of the host material in a desirable way. Theoretical study is accompanied by a corresponding detailed experimental EELS study. [1] W. Khan et. al., J. Phys. Chem. C, 2016, 120 (41), 23329-23338

O 84.3 Thu 10:15 POT 51

Semiconductor surface stabilization under photoelectrochemical conditions — •Waqas Saddique, Klaus Stallberg, Gerhard Lilienkamp, and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

The production of hydrogen by solar energy via water splitting in photoelectrochemical (PEC) cells is a field of current research and challenges in materials research. III-V semiconductors with suitable band gaps are candidates for water splitting but frequently subjected to corrosion during the water splitting process and suffer from corrosion-related decrease in efficiency. GaP has an indirect band gap of 2.26 eV which covers both the hydrogen and oxygen evolution potentials. So GaP can in principle be used as photocathode and photoanode, respectively. We have studied structural and chemical properties and modifications of an n-GaP(100) photoanode after extended photoelectrochemical activity. A 4 nm thin oxide film was produced at the surface of an n-GaP(100) photoanode via oxidizing the surface at specific PEC conditions and subsequently hydrogenating the surface to passivate defects in the oxide film. This specific process results in the formation of a stable Ga surface oxide, which inhibits corrosion while allowing the light and the charge carriers to pass through the thin oxide for the completion of the PEC process. No other prior surface treatments or catalysts were required for this process. An open-circuit potential Voc of 1.2 V vs the reversible hydrogen electrode (RHE) was also determined.

Invited Talk O 84.4 Thu 10:30 POT 51

Quantum confined colloidal semiconductor nanocrystals for solar fuels — •Frank Jäckel — Stephenson Institute for Renewable Energy and Department of Physics, University of Liverpool, UK

Co-catalyst decorated colloidal semiconductor nanocrystals are currently receiving increasing interest as a potentially cheap and scalable means for the photocatalytic generation of solar fuels such as solar hydrogen. [1,2] At the same time, colloidal semiconductor nanocrystals offer size-tuneable optical and electronic properties which allow the realisation of material properties beyond the bulk. In this talk, I will address how quantum confinement can be used to optimise quantum efficiencies and the use of the solar spectrum for photocatalytic hydrogen generation.[3] I will also present new approaches towards solving the stability-efficiency-dilemma frequently encountered in these systems. [4]

[1] M. Berr, A. Vaneski, A. S. Susha, J. Rodriguez-Fernandez, M. Döblinger, F. Jäckel, A. L. Rogach, and J. Feldmann, Appl. Phys. Lett. 97 093108 (2010).

[2] T. Simon, N. Bouchonville, M. J. Berr, A. Vaneski, A. Adrovic, D. Volbers, R. Wyrwich, M. Döblinger, A. S. Susha, A. L. Rogach, F. Jäckel, J. K. Stolarczyk, J. Feldmann, Nature Materials 13 1013 (2014).

[3] W. Li, G. O*Dowd, T. J. Whittles, D. Hesp, Y. Gründer, V. R. Dhanak, F. Jäckel Nanoscale 7 16606 (2015).

[4] W. Li, J. Lee, F. Jäckel ACS Appl. Mater. & Interf. 8 29434 (2016).

Coffee Break

O 84.5 Thu 11:30 POT 51

Photo-catalytic carbon dioxide reduction with InGaN photoelectrodes — •Viktoria Kunzelmann, Andreas Zeidler, Andrea Winnerl, and Martin Stutzmann — Walter Schottky Institut, Technische Universität München, Garching, Deutschland

Carbon dioxide (CO_2) has reached a critical level in atmosphere and counts as one of the reasons for global warming. Reducing this greenhouse gas to hydrocarbon fuels would help solving environmental issues and simultaneously address challenges such as energy storage and resource shortage. Using a photo-catalytic reaction to convert CO_2 into fuels is one way to address this issue. Due to the chemical inertness of CO_2 and the instability of suitable catalysts, efficient CO_2 reduction is still challenging. Using gallium nitride (GaN) as a photo-electrode is promising, since GaN is relatively stable under operating conditions and provides electrons with sufficient energy. Tuning the band gap by alloying GaN with indium might additionally enhance desired reduction processes. The current work concerns charge transfer processes on the interface of p- and n-type GaN or indium gallium nitride (InGaN), grown by molecular beam epitaxy, and an electrolyte. The characterization of the photo-electrode material is done by: atomic force and scanning electron microscopy for topography analysis, Kelvin probe force microscopy to analyze the surface potential landscape of the samples, surface photo-voltage measurements to evaluate the change of the electronic band structure due to illumination and Hall effect measurements to clarify the charge charrier density. Additionally, first results of photoelectrochemical measurements will be presented.

O 84.6 Thu 11:45 POT 51

Omnidirectional Photoelectrochemical Activity of Ultrathin CdS film on Periodic Three-Dimensional Composite Pillar/Truncated-Pyramid Au arrays — •Rui Xu, Liaoyong Wen, Huaping Zhao, Shipu Xu, Max Sommerfeld, Yang Xu, Yan Mi, Yaoguo Fang, and Yong Lei — Institute of Physics & Institute of Micro- and Nanotechnologies (ZIK MacroNano), Ilmenau University of Technology, 98693 Ilmenau, Germany

Photonic mode and surface plasmon resonance show prominent promise in improving light utilization of solar energy-related devices. In order to incorporate both features simultaneously, we designed and manufactured ordered array of three-dimensional metal pillar/truncated-pyramid (PTP) nanostructures. The experiments along with simulation indicate that the Au PTP arrays demonstrate multiple SPR and PM originated from the two structural elements leading to superior and broadband anti-reflection performance. To take these advantages, a conformal 90-nm-thick CdS film was coated on the PTP nanostructures and the resultant photoanode reaches a respectable light absorption over 90% in the overall optical operation regime. More importantly, the efficient light-trapping is omnidirectional and the calculated average absorptivity keeps almost the same in at least 50 degree range. The PTP photoanode demonstrated a dispersive light absorption, which worked in concert with CdS surface extension and strong light absorption to achieve a tremendous current promotion by a factor of 2.8 from the flat counterpart at -0.2 V (vs. Ag/AgCl).

Invited Talk O 84.7 Thu 12:00 POT 51

Photo-electrochemistry modelling beyond idealised surfaces and the computational hydrogen electrode — •Harald Oberhofer — Technical University Munich Garching, Germany

The role computer modelling plays today in understanding and optimising catalysts for photo-electrochemical reactions is undisputed. Yet, state of the art simulation approaches tend to rely on a number of assumptions and simplifications which—according to newest results—may not be fully justified. For example, simulation of the all-important electro-catalytic water oxidation reaction is mainly based on idealised surfaces and the computational hydrogen electrode (CHE) approach, which evaluates the thermodynamic feasibility of a catalyst looking at pathway where each hydrogen abstraction is coupled to the removal of one electron (PCET). The precise reactive site of the catalyst is thereby viewed as irrelevant, based on the premise of idealised surfaces. Yet, especially on semi-conducting catalysts both the assumption of PCET and of pristine, defect-free catalyst surfaces are not necessarily fulfilled.

The great success of the CHE approach is in part due to its low computational cost allowing a computational screening of suitable catalyst materials. Any other scheme going beyond PCET and pristine surfaces should therefore match this advantage, ideally avoiding costly numerical sampling of solvent degrees of freedom. Yet, recent developments in thermodynamic modelling as well as embedding techniques, both liquid and solid-state, especially considering the interface between catalyst and solvent, point the way towards photo-electrochemistry modelling beyond the computational hydrogen electrode.

O 85: Thin Films, Nanostructures and Nanoparticles I

Time: Thursday 10:15–13:00 Location: ZEU 114

O 85.1 Thu 10:15 ZEU 114

Nanostructured diblock copolymers as templates for metal sputter deposition — •Marc Gensch^{1,2}, Björn Beyersdorff^{1}, Wiebke Ohm^{1}, Matthias Schwartzkopf^{1}, Calvin Brett^{1,2}, Deniza Chekrygina^{2}, Pallavi Pandit^{1}, Andreas Stierle^{1,2}, and Stephan Roth^{1,3} — ^{1}DESY, Notkestr. 85, D-22607 Hamburg — ^{2}University of Hamburg, Luruper Chaussee 149, D-22761 Hamburg — ^{3}KTH, Teknikringen 56-58, SE-100 44 Stockholm

Nanostructured polymer metal composites demonstrate great perspective for flexible electronic and plasmonic applications [1]. Therefore, the growth kinetics and optical properties for silver deposition on co- and homopolymers were characterized by GISAXS, specular reflectance spectroscopy (UVVis), AFM and resistivity measurements. As substrates, solvent annealed PS-b-PMMA diblock copolymers of different molecular weights and their corresponding homopolymers were used. Thus, the influence of the block length and the diblock domains could be investigated. The study reveals the selective wetting of silver on one of the blocks from the copolymer thin films. The silver layers show a clear plasmon resonance. GISAXS measurements indicate a difference in the embedding of silver clusters depending on the polymer substrate. [1] S. V. Roth et al., ACS Appl. Mater. Interfaces 7, 12470 (2015).

O 85.2 Thu 10:30 ZEU 114

***In situ* GISAXS of gyroid terpolymer films during selective solvent annealing** — James A. Dolan^{1}, Karolina Korzeb^{2}, Raphael Dehmel^{1}, Bodo D. Wilts^{2}, Karl C. Gödel^{1}, Morgan Stefik^{3}, Ulrich Wiesner^{3}, Timothy D. Wilkinson^{1}, Jeremy J. Baumberg^{1}, Ullrich Steiner^{2}, and •Ilja Gunkel^{2} — ^{1}University of Cambridge, Cambridge, UK — ^{2}Adolphe Merkle Institute, Fribourg, CH — ^{3}Cornell University, Ithaca, NY, USA

Solvent annealing is an effective means to generate order in polymer systems. When solvent enters a film, the resultant plasticization drastically increases the mobility of the polymer chains. Annealing diblock copolymers in selective solvents has already been shown to induce morphological transitions from spheres to cylinders, gyroids, or lamellae. However, for the next more complicated family of linear block copolymers, triblock terpolymers, the morphological effect of selective solvent annealing is not well understood. Therefore, we present the results of *in situ* GISAXS during selective solvent annealing of gyroid-forming polyisoprene-*b*-polystyrene-*b*-poly(ethylene oxide) triblock terpolymer films. The selectivity was adjusted by using mixed vapor ratios of tetrahydrofuran and methanol. Distinct from diblock copolymers, we found that irrespective of the solvent vapor ratios used for annealing, the gyroid morphology remained. However, the selectivity of the solvent did either increase or decrease the unit cell size of the gyroid in both swollen and dried films.

O 85.3 Thu 10:45 ZEU 114

Selective metal deposition on block copolymer nanotemplates: A new perspective — •Ezzeldin Metwalli^{1}, Yuan Yao^{1}, Volker Körstgens^{1}, Matthias Schwartzkopf^{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

The characteristic metal affinity towards one block of self-assembled block copolymer (BC) templates plays an essential role to fabricate highly-order and well-defined metal nanopatterns. Deposition of inert metal atoms on several BC nanotemplates shows an extreme selectivity towards the glassy polymer nanodomain [1]. An explanation based on a difference in the metal-polymer interaction energy cannot adequately explain such extreme affinity. To better investigate this phenomenon, RF magnetron sputtering system was used to deposit gold metal in its atomic state on glassy poly(methylmethacrylate) and soft poly(ethylhexylacrylate) amorphous homopolymers as well as the corresponding statistical copolymer P(EHA-stat-MMA). At time resolution of 15 milliseconds, the nucleation/growth kinetics of gold nanoparticles on these polymer films was monitored using in situ grazing incidence small angle X-ray scattering (GISAXS). The coalescence behavior of the inert metal is mainly dominated by an improved atom mobility within the glassy polymers. This study on polymer thin films provides a new perspective into the long-time debated high selectivity characteristics of metals towards one block of BC based nanotemplates. [1]S. V. Roth et al., ACS Appl Mater Inter 2015, 7, 12470.

O 85.4 Thu 11:00 ZEU 114

In situ GISAXS study of Aluminum thin film growth on PS-b-PMMA and its constituent homopolymers — Björn Beyersdorff^{1}, •Matthias Schwartzkopf^{1}, Wiebke Ohm^{1}, Alexander Hinz^{2}, Thomas Strunskus^{2}, Oleksandr Polonskyi^{2}, Franz Faupel^{2}, Volker Körstgens^{3}, Franzika Löhrer^{3}, Peter Müller-Buschbaum^{3}, and Stephan V. Roth^{1,4} — ^{1}Deutsches Elektronen-Synchrotron DESY — ^{2}Christian-Albrechts-Universität zu Kiel — ^{3}Technische Universität München — ^{4}KTH Royal Institute of Technology

Installation of nanostructured metal films with tailored optical properties is of high importance in many areas of modern science and technology. Aluminum (Al) nanostructures for instance are very promising for surface-enhanced Raman Scattering (SERS) due to their wide tuneability of the plasmon resonance [1]. When depositing metal by sputter deposition on a nanostructured diblock copolymer substrate, a different adatom mobility on the two polymer blocks leads to selective wetting of one block and thus to an imitation of the polymer structure by the metal atoms [2,3]. We report on the sputter deposition of Al on a PS-b-PMMA diblock copolymer thin film and its two constituent homopolymers PS and PMMA by means of grazing incidence small-angle X-ray scattering (GISAXS). Cluster growth kinetics on the diblock and the homopolymer films is analyzed and compared to ex situ samples investigated by AFM. [1] Gérard et al, J. Phys. D: Appl. Phys., 48, 184001 (2015), [2] Lopes et al, Nature 414, 735 (2001), [3] Roth et al, ACS Appl. Mater. Interfaces 7 (23), 12470 (2015)

O 85.5 Thu 11:15 ZEU 114

Structural evolution of gold-teflon nanocomposite multilayer structure — •Pallavi Pandit^{1}, Ajay Gupta^{2}, Sigrid Bernstorff^{3}, Matthias Schwartzkopf^{1}, Deniza Chekrygina^{4}, and Stephan Roth^{1} — ^{1}DESY, Notkestr. 85, D-22607 Hamburg — ^{2}Amity University, 201313 Noida India — ^{3}Elettra, SS 14, I-34149 Basovizza Trieste — ^{4}UHH, Lurup. chaus. 149, D-22761 Hamburg

The combination of metal nanoparticles in polymer metrics has gained sustained research interest as their fine control of size and shape leads to the fabrication of materials with novel electronic, magnetic and catalytic properties. This offers some level of controllable performance. Thermal annealing as well can artificially modify the morphology of embedded metal nanoparticles. In this study the structural evolution of gold/PTFE multilayer nanocomposite has been studied using in-situ temperature dependent Grazing incidence Small and wide angle X-ray scattering. Nanoparticles exhibited a lognormal size distribution in multilayer structure. A rather well defined inter-particle correlation is observed in lateral and vertical direction. Linear dependence of the size of nanoparticles on square root of annealing time suggests a diffusion control growth of nanoparticles. After annealing at 573 K the nanoparticles distribution become isotropic in both the directions. UV-Vis reflectance spectroscopy has been used to study the Surface Plasmon Resonance of gold nanoparticles. The SPR frequency exhibits a systematic variation with gold content as well as with thermal annealing.

15 min break

O 85.6 Thu 11:45 ZEU 114

Printed nanostructured polymer films embedded with magnetic nanoparticles — •Senlin Xia^{1}, Ezzeldin Metwalli^{1}, Matthias Opel^{2}, Paul A. Staniec^{3}, Eva M. Herzig^{4}, and Peter Müller-Buschbaum^{1} — ^{1}TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [3]Beamline I22, Diamond Light Source, Harwell, OX11 0DE, United Kingdom — [4]TU München, Munich School of Engineering, Herzig Group, Lichtenbergstr. 4, 85748 Garching

Nanostructured polymer films containing magnetic nanoparticles (NPs) are promising materials due to their potential applications in the areas of high-density storage and magnetic sensors. Owing to the advantages, like large-scale production and energy saving, printing techniques were employed to fabricate hybrid films composed of maghemite NPs and PS-b-PMMA diblock copolymer (DBC). External magnetic fields were applied during the printing process to guide the NPs within the polymer matrix. The mesoscopic structure of PS-coated maghemite NPs within the DBC films was investigated as a function of the NP concentration using optical microscopy, AFM, SEM and GISAXS. The PS-coated NPs were selectively dispersed in the PS domains of the lamella-structured hybrid films. At high NP concentrations, the coalescence of NPs into large micro-sized metal-oxide wires was observed. The superparamagnetic behavior of the hybrid film was proved using a superconducting quantum interference device magnetometer.

O 85.7 Thu 12:00 ZEU 114

vinyl-terminated Au nanotriangles as platform for the fabrication of hybrid Au@pNIPAM particles for improved SERS responses. — Miguel Casado-Rodriguez[1], Christian Kuttner[2], Manuel Lopez-Romero[1], Andreas Fery[2,3], and •Rafael Contreras-Caceres[2] — [1]Universidad de Malaga, Departamento de. Quimica Organica. Facutlad de Ciencias. Universidad de Malaga 29071. Malaga. Spain — [2]Leibniz-Institut fu*r Polymerforschung, Dresden e.V. Hohe Strasse 6, 01069 Dresden, Germany — [3]Physical Chemistry of Polymeric Materials, Technische Universita*t Dresden, 01069 Dresden, Germany

We present a new approach for a water-based seedless synthesis of vinyl-terminated triangular Au nanotriangles. This method enables temperature controllable Au size by using 3-butenoic acid as reducing agent. We initially analyze the influence of the temperature on the particle size. Interestingly, the presence of terminal double bonds on the Au nanotriangle surface (coming from 3BA) is exploited for the fabrication of core@shell hybrid systems by free radical polymerization of N-isopropylacrylamide (AuNT@pNIPAM). Additionally, Au overgrowth using AuNTs@pNIPAM as seeds permits the fabrication of Austars@pNIPAM particles. The SERS enhancement capabilities of these two core*shell hybrids demonstrate that Au cores with tips and high curvature sites produced the highest plasmonic responses.

O 85.8 Thu 12:15 ZEU 114

Nanostructure tuning of sputter deposited Al layers on polystyrene using bias voltage — •Stephan V. Roth[1,2], Matthias Schwartzkopf[2], Björn Beyersdorff[2], Calvin Brett[2], Marc Gensch[2], Wiebke Ohm[2], Andre Rothkirch[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Franziska C. Löhrer[4], Volker Körstgens[4], Adrian Haussmann[4], Lorenz Biessmann[4], and Peter Müller-Buschbaum[4] — [1]KTH, Teknikringen 56-58,SE-100 44 Stockholm — [2]DESY, Notkestr. 85, D-22607 Hamburg — [3]CAU, Kaiserstr.2, D-24143 Kiel — [4]TUM, James-Franck-Str. 1, D-85748 Garching

Nanostructuring the polymer-metal interface in thin films is crucial for organic photovoltaics, flexible electronics and sensors. Hence, we investigated in real-time the different growth kinetics of nanostructured Aluminum layers on polystyrene thin film substrates during DC sputter deposition at applied bias voltages from 0V to -400V and at industrial coating rates. Using grazing incidence X-ray scattering and UV-Vis spectroscopy, we were able to directly correlate the crystallinity, the nanogranular structure and the optical properties at all growth stages during in situ sputter deposition at the applied bias voltages. Electron microscopy confirmed a transition in the nanogranular structure at a bias voltage around -300 V from a densely packed via a worm-like transient stage to a large cluster layer. Our results offer a versatile route for fabricating tailored metal arrays, ranging from nanoparticulate layers to full scale electrical contacts.

O 85.9 Thu 12:30 ZEU 114

In situ GISAXS analysis of spray deposited biopolymer thin films — Wiebke Ohm[1], Björn Beyersdorff[1], Matthias Schwartzkopf[1], Pallavi Pandit[1], Calvin Brett[1], Marc Gensch[1], Shun Yu[2], Nitesh Mittal[2], Daniel Söderberg[2], and •Stephan Roth[1,2] — [1]Deutsches Elektronen-Synchrotron Hamburg, Notkestraße 85, 22607 Hamburg — [2]KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden

Flexible biopolymer substrates based on cellulose nanofibrils (CNFs) are gaining increasing interest for nanotechnology such as organic electronics or solar cells since they present a renewable and sustainable alternative for synthetic polymers. In view of efficient industrial scalable fabrication, both the controlled arrangement of the CNFs during deposition and the use of industrial compatible deposition processes are essential.

We thus applied air-brush spray deposition of aqueous dispersions of CNF/water as a versatile deposition technique for preparing of cellulose thin films [1]. In situ grazing incidence small angle x-ray scattering (GISAXS) and atomic force microscopy measurements revealed the inner structure of these cellulose films. The effect of different types of CNFs was explored, enzymatic cellulose as well as TEMPO oxidized cellulose with different surface charges. The influence of different incidence angles of the spray was studied to reveal the impact on ordering of the CNFs. [1] Roth, J. Phys.: Condens. Matter 28, 403003(2016)

O 85.10 Thu 12:45 ZEU 114

An in-situ STXM approach to understand soft x-ray induced chemical modification in polymers — •Markus Meyer[1], Andreas Späth[1], Benjamin Watts[2], and Rainer H. Fink[1] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg, Physikalische Chemie II, Erlangen, Germany — [2]SwissLight Source (SLS), Paul Scherrer Institut, Villigen, Switzerland

Certain binding motifs in organic molecules are very sensitive to UV or XUV irradiation which induces severe chemical modifications. Scanning transmission x-ray microspectroscopy (STXM) was used to follow the evolution of effects like mass loss (due to bond rupture) and chemical changes of sample in an all but in-situ fashion. In our studies we investigated carbonyl group containing ultrathin free-standing films of PMMA, PLA and polycarbonate. The aim is a comprehensive study on x-ray induced chemical modification of the target for resonant and non-resonant excitations. It is found that the cleavage of chemical bonds does not follow a defined reaction pathway, thus directly leading to the formation of new C=C double bonds. In contrary, our studies provide clear evidence of small molecule fragments leaving the sample, thereby changing the chemical nature of the pristine material. This process is accompanied by deposition of residual gas onto the sample of interest as an unavoidable secondary process. Theoretical considerations are applied in a simulation and are able to retrace and to confirm the findings of the in-situ STXM analysis going well beyond recent publications [1]. [1] Leontowich, A. et al, JElectronSpectrosc, 58-64, 206, 2016

O 86: Graphene: Electronic Properties, Structure and Substrate Interaction I

Time: Thursday 10:30–13:00 Location: WIL A317

O 86.1 Thu 10:30 WIL A317

Charge Puddles in Graphene near the Dirac Point — •Sayanti Samaddar[1,2,3], Indra Yudhistira[4], Shaffique Adam[4,5], Hervè Courtois[2,3], and Clemens Winkelmann[2,3] — [1]II. Physikalisches Institut, RWTH Aachen Otto-Blumenthal-Straße, Turm 28 D-52074 Aachen, Germany — [2]Université Grenoble Alpes, Institut NEEL, F-38042 Grenoble, France — [3]CNRS, Institut NEEL, F-38042 Grenoble, France — [4]Centre for Advanced 2D Materials and Department of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117551, Singapore — [5]Yale-NUS College, 16 College Avenue West, Singapore 138527, Singapore

The charge carrier density in graphene on a dielectric substrate such as SiO2 displays inhomogeneities, the so-called charge puddles. Because of the linear dispersion relation in monolayer graphene, the puddles are predicted to grow near charge neutrality, a markedly distinct property from conventional two-dimensional electron gases. By performing scanning tunneling microscopy/spectroscopy on a mesoscopic graphene device, we directly observe the puddles' growth, both in spatial extent and in amplitude, as the Dirac point is approached. Self-consistent screening theory, together with the consideration of the impact of the STM tip as an electric gate, provides a unified description of both the macroscopic transport properties and the microscopically observed charge disorder.

O 86.2 Thu 10:45 WIL A317

***Ab-initio* study of the effective Coulomb interactions and Stoner ferromagnetism in hydrogenated graphene** — •Ersoy Sasioglu[1], Hanif Hadipour[2], Christoph Friedrich[3], Stefan Blügel[3], and Ingrid Mertig[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale) Germany — [2]Department of Physics, University of Guilan, 41335 Rasht, Iran — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425Jülich, Germany

Hydrogenation provides a novel way to tune the electronic and optical properties of the graphene. Recent scanning tunneling microscopy experiments have demonstrated that local graphene magnetism can be selectively switched on and off by hydrogen dimers [1]. Employing *ab-initio* calculations in conjunction with the constrained random-phase approximation [2] we study the strength of the effective Coulomb interaction U in hydrogenated graphene. It is found that the calculated U parameters are smaller than the ones in pristine graphene and depend on the hydrogen concentration. Moreover, the U parameters are very sensitive to the position of hydrogen atoms adsorbed on the graphene lattice. We discuss the instability of the paramagnetic state towards the ferromagnetic one on the basis of calculated U parameters within the Stoner model. Spin-polarized calculations reveal that the experimentally observed itinerant ferromagnetism in hydrogenated graphene can be well described by the Stoner model.

[1] H. González-Herrero *et al.*, Science **352**, 437 (2016).

[2] E. Şaşıoğlu *et al.*, Phys. Rev. B **83**, 121101(R) (2011).

O 86.3 Thu 11:00 WIL A317

Characterization of CVD-grown graphene on germanium at the atomic scale — •Andreas P. Becker, Wolfang M. Klesse, Mindaugas Lukosius, and Thomas Schroeder — IHP microelectronics GmbH, Frankfurt (Oder), Germany

Graphene is a two-dimensional carbon allotrope where the atoms are arranged in a honeycomb lattice. Especially its extraordinarily high carrier mobility, plasmonic activity and impermeability make it a promising candidate for novel applications in microelectronics, such as high-frequency transistors, sensors and optical modulators.

Direct growth of graphene on silicon is hampered by the formation of covalent bonds. CVD growth of high-quality graphene on transition metal substrates and subsequent transfer of the sheets has proved feasible, however, tenacious metallic contamination obstructs its use in the front-end-of-line of CMOS technology.

As a resort, graphene can be grown on germanium buffer layers, which is one current research focus of the IHP. Specifically, samples grown in the cleanroom are already being routinely investigated by e. g. scanning electron microscopy (SEM) and Raman spectroscopy. But only scanning probe microscopy (SPM) allows to scrutinize graphene layers at the atomic scale and can therefore be an essential complement to such established methods of quality assessment on larger scales.

Accordingly, I will present our latest results on the ex- and in-situ structural characterization of such gr/Ge structures by means of SPM depending on the growth parameters and post-growth annealing procedures.

O 86.4 Thu 11:15 WIL A317

Observation of photoemission "dark lines" for Ir(111) and graphene/Ir(111) via high-resolution ToF k-microscopy — •Anna Zaporozhchenko-Zymaková[1,2], Dmytro Kutnyakhov[1,3], Katerina Medjanik[1], Christian Tusche[4], Olena Fedchenko[1], Sergey Chernov[1], Martin Ellguth[1], Sergej A. Nepijko[1], Hans-Joachim Elmers[1,2], and Gerd Schönhense[1,2] — [1]Inst. für Physik, Univ. Mainz — [2]MAINZ graduate school — [3]DESY, Hamburg — [4]PGI-6, Forschungszentrum Jülich

ToF k-microscopy [1,2] has been used to analyze emergent photoelectron diffraction effects for UHV/Ir(111) and graphene/Ir(111). We observed a regular pattern of dark lines with circular shape and six-fold symmetry that have been overlooked in previous experiments. Quantitative evaluation along with a model calculation reveals that electrons initially located within the first Brillouin zone can with finite probability be scattered by a reciprocal lattice vector into a state that propagates parallel to the surface. Such electrons vanish due to inelastic scattering events in the vicinity of the surface. This leads to a reduced intensity observed as dark lines. The relevant reciprocal lattice vector corresponds to the lattice of the topmost layer (in our case Ir or graphene). The dark lines appear in a certain photon energy range satisfying the congruence of lattice constant and wavelength. The parallel momentum of the dark lines decreases with increasing photon energy in agreement with the model. The effect has been observed with both p- and s-polarized light at BESSY II (10m NIM). [1] Chernov et al., Ultramic. 159, 453 (2015); [2] Tusche et al., APL 108, 261602 (2016).

O 86.5 Thu 11:30 WIL A317

Landau Level Spectroscopy of Twisted Graphene Layers on Ir(111) — •Sabina Simon[1], Felix Förschner[1], Vivien Enenkel[1], Fabian Geml[1], Yuriy Dedkov[1], Timo Knispel[2], Charlotte Herbig[2], Thomas Michely[2], and Mikhail Fonin[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Institute of Physics II, University of Köln, 50937 Köln, Germany

Epitaxial growth on metal substrates is known to be one of the most powerful approaches in producing large-scale, high-quality, monolayer graphene. Yet it remains a major challenge to realize the growth of multilayers.

This work is devoted to the investigation of multilayered graphene systems epitaxially grown on a transition metal, namely Ir(111). We address the growth and the structure of large scale twisted graphene bilayers by intercalation of atomic carbon under graphene on Ir(111). We show that the intercalated graphene buffer layer provides sufficient decoupling from the metal substrate, giving a possibility to access the local electronic properties of graphene by means of Landau level spectroscopy. We further discuss the influence of the twist angle on the local electronic properties of the top graphene layer, upon the analysis of the doping level, Fermi velocity of charge carriers, and quasiparticle lifetimes.

O 86.6 Thu 11:45 WIL A317

Epitaxial growth of graphene via flash annealing of SiC studied by STM, AFM and LEED — •Ismail Baltaci, Malte Schulte, Eugenia Wodopian, Patrick Mehring, and Carsten Westphal — Experimentelle Physik 1, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund

Due to its unique electronic and structural properties graphene is of particular interest for the semi-conductor industry, e.g. as a new material in transistor applications.

In this study we concentrate on an epitaxial growth based on cyclic heating of SiC by direct current, known as flash annealing. In order to yield large and homogeneous graphene layers multiple parameters have to be taken into account such as heating and cooling rates as well as the number of heating cycles.

Determining the number of graphen layers on SiC is achieved by utilizing Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM) and Low Energy Electron Diffraction (LEED). Especially the structural differences between buffer layer and graphen is visualized by STM and LEED measurements. Furthermore, we report on the growth mechanism of graphene.

O 86.7 Thu 12:00 WIL A317

Surface-assisted self-assembly of graphene nanoribbons — •Axel Enders[1,2], Paulo Costa[2], Jacob Teeter[2], Daniel Miller[3], Eva Zurek[3], and Alexander Sinitskii[2] — [1]Experimentalphysik Va, Universität Bayreuth — [2]University of Nebraska, Lincoln NE 68588, USA — [3]State University of New York at Buffalo, Buffalo 14260, USA

The physical properties of graphene are sensitive to the presence of structural defects, dopants and edges. This creates opportunities to design an electronic bandgap in graphene, which is most consequently exploited in graphene nanoribbons (GNRs), which have edges that are amenable to structural and chemical modification. It is shown that surface-assisted self-assembly is a powerful strategy to build GNRs from the bottom up. As in solution-based self-assembly, also on surfaces the edge structure and chemistry of GNRs is determined by the precursor molecules. But on surfaces the substrate itself can be a control parameter during growth, as can be the method of deposition. Specifically here the self-assembly of 6,11-dibromo-1,2,3,4-tetraphenyltriphenylene and related, appropriately modified precursor molecules was studied on Au(111) and on Cu(111) surfaces. The precursors were deposited under ultrahigh vacuum by two different methods for comparison, which are thermal evaporation and nanoimprinting. Among the significant findings of these studies are the substrate-dependent epitaxial alignment of the ribbons, considerably lower dehalogenation temperatures on Cu(111), and entirely different GNR architectures that can emerge from the same precursors under different conditions.

O 86.8 Thu 12:15 WIL A317

Lifting Graphene by Alkali Intercalation — •Caio Silva[1], Jiaqi Cai[1], Wouter Jolie[2], Daniela Dombrowski[1,2], Ferdinand Farwick zum Hagen[2], Antonio Martínez-Galera[2], Christoph Schlueter[3], Tien-Lin Lee[3], and Carsten Busse[1,2] — [1]Institut für Materialphysik, Münster, Germany — [2]II. Physikalisches Institut, Köln, Germany — [3]Diamond Light Source Ltd, Didcot, United Kingdom

Intercalation is a versatile tool to tune the properties of graphene grown epitaxially on metal surfaces. Especially alkali metals are efficient to decouple graphene from its substrate and, in addition, induce a strong n-doping on graphene.

In the present work, we used the x-ray standing wave (XSW) techinique to compare the structures resulting from intercalation of a small (Li) and a rather large (Cs) alkali metal between graphene and Ir(111). We noted an opposing behavior during deintercalation: In the case of Cs, different phases $[(\sqrt{3}\times\sqrt{3})R30^{\circ}_{Ir}, (2\times 2)_{gr}]$ coexist, each with a characteristic height of graphene with respect to Ir(111), as revealed by XSW. In the case of Li, however, we find just a single phase of gr/Li/Ir(111) for a wide range of intercalant coverage (1 - 0.2 ML), with a distance between the graphene sheet and the metal surface that is independent on the amount of Li intercalated in between. We explain the contrast between Li and Cs by differences in the delamination energy that has to be paid in order to intercalate the different species.

O 86.9 Thu 12:30 WIL A317

Giant magneto-photoelectric effect at a graphene edge — •Friedemann Queisser, Ralf Schützhold, Jens Sonntag, Annika Kurzmann, Martin Geller, and Axel Lorke — Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße, Duisburg 47048, Germany

Graphene is a promising material for optical or infrared absorption, as its pseudo-relativistic energy-momentum relation allows for a broad absorption bandwidth. An efficient charge separation can be achieved at a graphene edge in a magnetic field. By solving the Dirac equation, it can be shown that particles and holes move in antipodal directions along the edge [1]. Motivated by the proposed mechanism, an surprisingly high magneto-photocurrent has been measured in suspended graphene [2]. The observed photoresponsitivity (100 incident photons create up to 17 particle-hole pairs) strongly exceeds the predicted value. A possible mechanism to explain the amplification of the magneto-photoeffect relies on the strong Coulomb interaction in graphene: Due to the huge effective fine-structure constant ($\alpha_{\mathrm{graphene}} \gg \alpha_{\mathrm{QED}}$) and the enlarged phase space at the graphene edge, inelastic (Auger-type) scattering amplifies the magneto-photocurrent.

[1] F. Queisser and R. Schützhold *Phys. Rev. Lett.* **111**, 046601 (2013)

[2] J. Sonntag, A. Kurzmann, M. Geller, F. Queisser, A. Lorke, R. Schützhold, arXiv:1505.01762

O 86.10 Thu 12:45 WIL A317

Magnetism in graphene induced by transition metal and rare earth atomic layers — •Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany

On the Ir(111) surface graphene is physisorbed with a local chemical modulation [1] whose structural and electronic properties can be engineered via atomic intercalation [2,3,4] or molecular adsorption [5,6]. In particular, our *ab initio* density functional theory (DFT) simulations performed for $3d$ transition metal (TM) atoms such as Co [3] and Fe [4] intercalated at the interface between graphene and Ir(111) clearly demonstrated that the graphene layer exhibits a spin-split electronic structure. On the other hand, the strong hybridization between the π electronic states of graphene and the d ones of the TM monolayer significantly changes the magnetic properties of the intercalated atoms. Moreover, we investigated if this physical picture remains valid also in the case of the rare earth (RE) atoms with spatially localized magnetic moments such as $4f$ Eu intercalated between graphene and the Ni(111) surface.

This work is supported by DFG through SFB 1238 (Project C01).

[1] C. Busse *et al.*, Phys. Rev. Lett. **107**, 036101 (2011).
[2] W. Jolie *et al.*, Phys. Rev. B **89**, 155435 (2014).
[3] R. Decker *et al.*, Phys. Rev. B **87**, 041403(R) (2013).
[4] R. Decker *et al.*, J. of Phys.: Cond. Matter. **26**, 394004 (2014).
[5] R. Brede *et al.*, Nature Nanotech. **9**, 1018 (2014).
[6] F. Huttmann *et al.*, Phys. Rev. Lett. **115**, 236101 (2015).

O 87: Metal Substrates: Structure, Epitaxy and Growth

Time: Thursday 10:30–13:00 Location: WIL C307

Invited Talk O 87.1 Thu 10:30 WIL C307

Structure and redox dynamics of ultrathin ceria films and nanostructures — •Jan Ingo Flege — Institute of Solid State Physics, University of Bremen, Bremen, Germany — MAPEX Center for Materials and Processes, University of Bremen, Bremen, Germany

Cerium oxide is of considerable importance for a wide range of technological applications including, e.g., energy harvesting, storage, and conversion, chemical sensing, and heterogeneous catalysis. Epitaxially grown ceria thin films and nanostructures represent important model systems allowing for the investigation of their peculiar materials properties using surface science methodology. In this presentation, I will focus on the growth and characterization of cerium oxide ultrathin films and microparticles on transition metal surfaces and the subsequent monitoring of their structural and chemical modifications in reactive environments using low-energy electron microscopy and related methods. Starting from the frequently employed ceria(111)/Ru(0001) inverse model catalyst [1], it will be demonstrated that nanoscale structural transformations that occur upon chemical reduction, thermal annealing, or reoxidation can be followed in real-time. Furthermore, it will be shown that in situ probing during epitaxial growth facilitates a deeper understanding of the prevailing mechanisms, which may be exploited to selectively synthesize ceria(001) nanostructures and microparticles [2, 3] for model catalytic studies.

[1] D. C. Grinter et al., Appl. Catal., B 197, 286 (2016).
[2] J. Höcker et al., J. Phys. Chem. C 120, 4895 (2016).
[3] J. I. Flege et al., Nanoscale 8, 10849 (2016).

O 87.2 Thu 11:00 WIL C307

Growth and Magnetism of Fe Thin Films on Rh(111) — •Matthias Vogt, Nicolai Seubert, Martin Schmitt, Jeannette Kemmer, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We present a growth study of monolayer and bilayer Fe films on Rh(111) monitored by scanning tunneling microscopy. The arrangement of the Fe layers on the surface can be influenced to a certain extent by varying the post-annealing temperature, but Fe tends to form high islands with small terrace size under these conditions. Large flat Fe terraces were only observed when the sample was heated during evaporation. Whereas the first layer seems to grow pseudomorphic, the second layer exhibits zig-zag–shaped arrays, which seem to be suppressed in areas with high defect densities. They share many aspects with the Fe double-layer on Ir(111) reported previously [1] and resemble a periodic herringbone pattern. For the Fe double-layer on Rh(111) the periodicities amount to about 1.58 nm between the ribs and about 14.5 nm from backbone to backbone. The results of measurements performed with magnetically coated probe tips will be presented and discussed to identify the underlying Fe spin structure.
[1] P.-J. Hsu *et al.*, Phys. Rev. Lett. **116**, 017201 (2016).

O 87.3 Thu 11:15 WIL C307

Spectroscopic observation and molecular dynamics simulation of Ga surface segregation in liquid Pd-Ga alloys — •Mathias Grabau[1], Jannis Erhard[2], Nicola Taccardi[3], Sandra Krick Calderon[1], Andreas Görling[2], Peter Wasserscheid[3], Christian Papp[1], and Hans-Peter Steinrück[1] — [1]Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg (FAU) — [2]Theoretische Chemie, FAU — [3]Chemische Reaktionstechnik, FAU

Pd-Ga alloys with 0.8, 1.8 and 4.7 at.% of Pd were examined as a function of temperature between 400 and 750 K using angle-resolved x-ray photoelectron spectroscopy (XPS). The Pd surface concentration is found to depend on temperature. This is explained by the transition from a liquid phase to a two-phase system, consisting of a buried solid Ga_5Pd phase and a liquid Pd-Ga alloy, which leads to Pd depletion of the liquid phase. In the liquid phase, Pd was depleted from the vacuum/liquid interface, as deduced from the comparison of XPS data obtained in 0 and 80° emission; this observation is independent of temperature and Pd concentration of the liquid phase. It is interpreted as an inhomogeneous depth distribution function of Pd, that is, Pd depletion in the topmost layer and enrichment in the next layer. In line with experiment, a DFT-based molecular dynamics simulation (MD) shows interfacial stratification of Ga and an inhomogeneous Pd distribution along the surface normal. The experimental data was evaluated by using a rigid layer model leading to excellent agreement with the results of the MD simulation. We acknowledge the financial support by the Cluster of Excellence 'Engineering of Advanced Materials'.

O 87.4 Thu 11:30 WIL C307

Correlogram Correlation for Surface Topology Evaluation by White Light Interferometry — •Ilia Kiselev[1], Michael Drexel[1], Egor Kiselev[2], and Michael Hauptmannl[1] — [1]Breitmeier Messtechnick GmbH, Englerstr. 24, 76275 Etlingen — [2]Physikalisches Institut, Karlsruhe Institut of Technology, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe

Established methods to gauge the surface height by the white light interferometry do not use the full Information contained in a correlogram. As the result, the envelope evaluation methods suffer from susceptibility to noise, whereas the phase methods are prone to the *2-pi ambiguity*. The suggestion here is to determine the surface position via the correlation of the local correlogram with a reference correlogram. It is easy to see that the method is to be the most stable to noises of different kinds: it benefits using the complete correlogram information. Theoretical Cramer-Rao estimations as well as evaluations of measured data samples demonstrates the prevalence of the method. Tolerance to noise of this method is by more than one order of magnitude higher, than that of the envelope methods and exceeds that of the phase method; available data which indicates the 2-pi jumps by phase method provide smooth results by this one. Another advantage of the suggested method is the immediate availability of a suitability criterion for a local correlogram * the correlation coefficient with the reference one.

O 87.5 Thu 11:45 WIL C307

Diffusion properties of lithium and magnesium studied using DFT: growth phenomena and the effect of an electric field — •Markus Jäckle[1,2] and Axel Gross[1,2] — [1]Helmholtz Institut Ulm - Elektrochemische Energiespeicherung, 89069 Ulm, Germany — [2]Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

The formation of dendrites poses a significant problem with respect to the performance and safety of batteries as it can lead to short-circuits during battery operation. Metal growth processes are intimately linked to diffusion behaviour. Therefore, we have extended our initial theoretical first-principles study of the self-diffusion properties of lithium, sodium and magnesium [1] by investigating a broader variety of diffusion processes. Thereby we intend to contribute to a better understanding of this phenomenon which may help avoiding battery failure due to dendrite growth.

According to our new calculations, the previously established picture of an inhomogeneous lithium surface and a homogeneous magnesium surface [1] is still correct. Our new results suggest a significant influence of the across-step diffusion barrier, which will be elucidated in the presentation.
[1] M. Jäckle and A. Groß, J. Chem. Phys. **141**, 174710 (2014).

O 87.6 Thu 12:00 WIL C307

Metallic Nanopore Arrays as Ideally Nanostructured Electrode for Supercapacitors — •Huaping Zhao, Ranjith Vellacheri, Min Zhou, Yang Xu, and Yong Lei — Institut für Physik & IMN MacroNano* (ZIK), Technische Universität Ilmenau, Ilmenau, Germany

Supercapacitors have attracted great interest as an electrical energy storage system because of their high power density, fast charge-discharge rate, and excellent cycle stability. Besides the active materials themselves, the electrode structure also plays an important role in determining the charge storage capability and rate capability of supercapacitors. Considering that the energy storage of supercapacitors is through either ionic adsorption-desorption or fast and reversible surface redox reactions at the electrode/electrolyte interface, a promising supercapacitor electrode should have large specific area to realize high charge storage capability. Meanwhile, it should provide shorter ion diffusion path and lower electron transfer resistance that enable the achievement of high rate capability. Here, we demonstrate metallic nanopore arrays fabricated using a two-step replication process from porous anodic alumina membrane as an ideally nanostructured electrode for supercapacitors. With metallic nanopore arrays as supercapacitor electrode, the large specific surface area could ensure high capacitance, while the highly oriented and stable nanoporous structure can facilitate ion transport, thus high charge storage capability and high rate capability of supercapacitor were achieved simultaneously.

O 87.7 Thu 12:15 WIL C307

Low temperature bias-assisted RF-sputtering process for heteroepitaxial growth of iridium (100) on sapphire (11-20) — Frank Meyer[1], Eduard Reisacher[1], Johannes Preussner[1], Andreas Graff[2], Alexander Fromm[1], Lukas Gröner[1], and •Frank Burmeister[1] — [1]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg i. Br., Germany — [2]Fraunhofer-Institut für Mikrostruktur von Werkstoffen und Systemen IMWS, Halle, Germany

Heteroepitaxially grown iridium (100) on sapphire (11-20) is one of the most promising systems for large scale heteroepitaxial diamond growth [1]. However, due to the high melting point of iridium (2466°C) and low adatom mobility, in various e-beam or sputter deposition experiments, epitaxial growth has only been observed at substrate temperatures above 600°C. Very recently, Tolstova et al. [2] were able to significantly reduce the temperature necessary for growing epitaxial platinum and gold films on MgO by using RF-sputtering with an additionally applied substrate bias. In this study we investigated the influence of the additional substrate bias on the growing Ir film. Crystallinity and morphology were characterized using X-ray diffraction and electron backscattering diffraction. We found that in the first seconds of the deposition process, an additional substrate bias creates a thin iridium seeding layer, which enables epitaxial growth of iridium (100) on sapphire (11-20) already at temperatures slightly above 300°C. [1] Z. Dai et al., Appl. Phys. Lett., 82, 3847 (2003) [2] Y. Tolstova et al. Scientific Reports 6, 23232, (2016)

O 87.8 Thu 12:30 WIL C307

Transformation of the Pt(001)-hex to a smooth and clean Pt(001)-(1x1) — Rene Hammer[1], Florian Schumann[1], •Oliver Krahn[1], Stefan Förster[1], Klaus Meinel[1], and Wolf Widdra[1,2]

— [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck Institut für Mikrostrukturphysik, D-06120 Halle, Germany

The quasihexagonal reconstruction of the (001) surfaces of gold and platinum have been under intense investigation for decades. Yet the non-reconstructed (1x1) structure is important for particular applications. Here, we study by STM, SPA-LEED and HREELS the structural transformation of the Pt(001)-hex to an unreconstructed (1x1) surface by gas adsorption. The lifting of the hex occurs along the reconstruction rows. Surplus Pt atoms are pushed on top of the surface leading to one-dimensional chains growing along [110] at low temperatures (77 K). These chains decay into islands at room temperature and result in a roughening of the Pt(001)-(1x1) surface. Surface smoothing by intralayer diffusion above 150 °C fails because the hex layer recovers from the islands. Island growth is only attained by step edge diffusion at around 100 °C promoting a Smoluchowski ripening of the islands. When island size reaches 10 nm, Ostwald ripening at 350 °C can be applied. This leads to a smooth surface with large two-dimensional islands. Finally an annealing process at 150 °C in O_2 atmosphere results in a well-ordered and adsorbate-free (1x1) surface.

O 87.9 Thu 12:45 WIL C307

Electron energy loss spectroscopy with parallel readout of energy and momentum — •F. C. Bocquet[1,2], H. Ibach[3], J. Sforzini[1,2], S. Soubatch[1,2], and F. S. Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology — [3]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany

Electron Energy Loss Spectroscopy (EELS) has been a very successful technique for the past three decades for studying elementary excitations at surfaces (e.g. vibrational modes, phonons, plasmons) and providing sub-meV resolution [1]. In this work, we demonstrate that the combined use of a hemispherical electron analyzers equipped with a multichannel plate (MCP) as detector, together with a modified version of the conventional double monochromator allows a faster detection of electron in the off-specular geometry. We show the first results obtained on the phonon dispersion of clean Cu(111) [2]. The full dispersion curve has been obtained in a single 7-minutes long measurement, which is a clear improvement with respect to standard spectrometer that would require several hours of acquisition.

References [1] H. Ibach, J. Elec. Spec. Relat. Phenom. 64 819 (1993) [2] H. Ibach, et al. submitted (arXiv:1611.09709)

O 88: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VI

Time: Thursday 10:30–13:45 Location: GER 38

O 88.1 Thu 10:30 GER 38

Implicit solvation functionality in FHI-aims: Kirkwood multipole expansion model — •Markus Sinstein, Karsten Reuter, and Harald Oberhofer — Technische Universität München, Germany

Implicit solvation models describe a liquid environment in form of a dielectric continuum. Used within first-principles calculations for the solute such models provide a numerically most efficient way to effectively capture solvation effects. To this end we have implemented the multipole expansion (MPE) model introduced originally by Kirkwood into the full-potential density-functional theory (DFT) code FHI-aims. This implementation fully exploits the optimized multi-center multipole decomposition of the density performed within FHI-aims and therewith leads generally to an insignificant overhead as compared to the underlying DFT calculation for the solute.

Aiming to minimize the number of free parameters inevitably connected with such implicit models, we use an iso-density definition of the solvent cavity. As to the other parameters, we present an efficient parametrization scheme based on experimentally measured hydration energies of small organic molecules. Finally, we discuss extensions of the solvation model to address extended solid-liquid interfaces.

O 88.2 Thu 10:45 GER 38

Using Dipsersion-Corrected Density Functional Theory to Understand the Phase Diagram of Alkanethiolates on Gold — •Joakim Löfgren, Henrik Grönbeck, Kasper Moth-Poulsen, and Paul Erhart — Chalmers University of Technology, Gothenburg, Sweden

A key challenge in modern computational materials chemistry is the description of van der Waals interactions in density functional theory simulations, where the failure of conventional exchange-correlation functionals is well-known. While, in the recent years, several methods have been proposed for overcoming these difficulties, the applications are becoming increasingly more demanding as well. An important example is that of ligand-protected nanoparticles, which typically feature metallic, covalent as well as dispersive interactions that should all, ideally, be treated on an equal footing. In this work we show that significant progress can be made in this direction: with the aid of the recently-developed vdW-DF-cx functional we study the phase diagram of self-assembled monolayers of alkanethiolates on gold. This system is important for practical applications and as a general representative of self-assembly at a metal surface. In particular, a quantitative description of the dispersion-driven phase transition between a lying-down and a standing-up monolayer is obtained using an ab inito thermodynamics framework. The results are shown to be in good agreement with experimental data and highlight that accurately accounting for dispersive interactions is both feasible and a crucial part of modeling self-assembled systems.

O 88.3 Thu 11:00 GER 38

Finite-temperature properties of the thermoelectric clathrate $Ba_8Al_xSi_{46-x}$ — •Maria Troppenz, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

Intermetallic clathrate compounds are promising candidates for high-efficiency thermoelectric (TE) applications. Here, we study $Ba_8Al_xSi_{46-x}$ in the composition range $x \in [6, 16]$ [1]. Recent theoretical studies [2] show a strong dependence of the electronic properties on configuration, i.e. the atomic arrangement of the substitutional Al atoms in the crystal framework. At the Zintl composition ($x = 16$), the ground-state configuration is semiconducting. However, configurations higher in energy are metallic. Understanding this metal-semiconductor transition is essential, as semiconducting behavior is a prerequisite for TE applications. In this work, we employ the cluster expansion technique combined with Monte-Carlo simulations and the Wang-Landau method [3] to access finite-temperature properties. We find that the transition is driven by a partial order-disorder transition of the substituents. Most importantly, it is found that the transition temperature (~ 800 K) at the Zintl composition is close to the typical temperatures at which the figure of merit of TE clathrates is maximal. Signatures of the transition in the entropy, order parameter, specific heat, and canonical distribution are analyzed for the full composition range.

[1] J. H. Roudebush *et al.*; *Inorg. Chem.* **51**, 4161 (2012)
[2] M. Troppenz, S. Rigamonti and C. Draxl; preprint.
[3] F. Wang and D. P. Landau, *Phys. Rev. Lett.* **86**, 2050 (2001)

O 88.4 Thu 11:15 GER 38

Electronic structure and solid-state optical properties of indigo from time-dependent optimally tuned range-separated hybrid functional theory — •Bernd Kollmann[1], Arun Kumar Manna[2], Daniel Lüftner[1], Leeor Kronik[2], and Peter Puschnig[1] — [1]Institute of Physics, NAWI Graz, University of Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, Israel

Indigo is a natural dye with a long history in organic chemistry. Recent applications of indigo as a functional building block for organic electronics, like in solar cells or field effect transistors, have renewed the interest in the chemical and physical properties of this molecule. We report on its electronic structure for the isolated molecule as well as for the alpha- and beta- bulk molecular crystal phases. Further we investigate the optical properties of the bulk molecular crystal phases. For the molecule we employ an optimally tuned range-separated hybrid functional (OT-RSH) within density functional theory. Comparing the theoretical results obtained with different levels of theory and with experiment emphasizes the need for going beyond simple semi-local DFT-functionals in order to obtain the correct orbital ordering. For the bulk crystals we take into account the screening in the bulk by using an optimally tuned screened range-separated hybrid (OT-SRSH) approach. Regarding the optical properties of the bulk molecular phases we employ time-dependent density functional theory (TDDFT) to calculate the absorption spectra, whereby TDDFT represents an accurate low-cost substitute to many-body perturbation theory.

O 88.5 Thu 11:30 GER 38

Thermodynamic properties from ab-initio calculations - Ti as a case study — •Guy Makov — Materials Dept, Ben-Gurion University of the Negev, Beer Sheva, Israel

Ab-initio calculations of thermophysical properties and of phase stability as a function of pressure and temperature are considered in titanium as a case study. Ti is of interest due to its multiple phases and unusual thermophysical properties. At low temperatures Ti has been reported to exhibit negative anisotropic thermal expansion. In addition, there have been reports of two additional phases at high pressure and room temperature, and a possible transition to a bcc phase at very high pressures.

Despite extensive studies there remains both experimental and theoretical uncertainty in determining the phase diagrams and selected properties. Density Functional Theory total energy calculations complemented by Density Functional Perturbation Theory (DFPT) calculations of phonon spectra are obtained as a function of pressure. The free energy and thermal properties (heat capacity and thermal expansion) of Ti phases, phase equilibria and high pressure phase sequence are determined. The contribution of phonon modes to the thermal expansion is analyzed and the negative thermal expansion is shown to be dominated by negative mode Gruneisen parameters at specific points on the Brillouin zone boundaries. The elastic (Debye) theory for negative thermal expansion is shown to be irrelevant for these phenomena. Uncertainties in the calculated results are discussed in light of experimental observations & motivating further experimental studies.

O 88.6 Thu 11:45 GER 38

Molecular orbitals in the bismuth perovskites — •Kateryna Foyevtsova[1,2], Arash Khazraie[1,2], Ilya Elfimov[1,2], and George A. Sawatzky[1,2] — [1]Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada V6T 1Z1 — [2]Stewart Blusson Quantum Matter Institute, Vancouver, BC, Canada V6T 1Z4

The bismuth perovskites $SrBiO_3$ and $BaBiO_3$ become superconducting upon hole doping, with the transition temperatures as high as 30 K. The origin of the superconductivity in these compounds has remained unidentified for more than three decades. The BCS mechanism alone is not sufficient to account for such a high T_c due to the small electron-phonon coupling that is being consistently found in numerous experimental and theoretical studies. Further effects must therefore be of key importance, such as, for example, formation of bipolarons.

In this talk, we will focus on the insulating state of the pristine $SrBiO_3$. Peculiarly, this state is associated with a structural distortion whereby the Bi-O bonds disproportionate, resulting in a three-dimensional array of alternating small and large BiO_6 octahedra. This "breathing" distortion melts away with doping and is believed to be competing with superconductivity. We will show using DFT calculations that the microscopic state in the pristine bismuthates corresponds to a lattice of frozen bipolarons. More specifically, the holes, intrinsically present in the material, condense pairwise into the A_{1g}-symmetric molecular orbitals formed from the O-p_σ atomic orbitals of the small BiO_6 octahedra. This is facilitated by the strong hybridization between the O-2p states and the Bi-6s states.

O 88.7 Thu 12:00 GER 38

Ab initio calculations and strain-dependent scaling of excitons in carbon nanotubes — •Christian Wagner[1,3], Jörg Schuster[2], Michael Schreiber[3], and André Schleife[4] — [1]Center for Microtechnologies, TU Chemnitz, Germany — [2]Fraunhofer Institute ENAS, Chemnitz, Germany — [3]Institute of Physics, TU Chemnitz, Germany — [4]Department for Materials Science, UIUC, USA

Optical transitions in carbon nanotubes (CNTs) show a strong strain sensitivity, which makes them suitable for optical strain sensing at the nano-scale and for strain-tunable emitters. The origin of this effect is the band-gap change, depending on strain and chirality, which is well explored. However, there is no quantitative model for the strain dependence of optical transitions — as they are subject to strong excitonic effects due to the quasi one-dimensional structure of CNTs.

One approach towards such a model is the scaling relation of CNT excitons with respect to dielectric constant, reduced mass, and CNT radius given by Perebeinos *et al.* However, the description of screening in this model is insufficient, since for CNTs, a one-dimensional wave-vector dependent dielectric function $\epsilon(q)$ is needed instead of an effective-medium dielectric constant ϵ_0.

We achieve this by combining the scaling relation with the wave-vector dependent screening model by Deslippe *et al.* The strain-dependent scaling is fitted to electronic-structure calculations within many-body perturbation theory as a reference. This enables us to quantitatively predict the strain dependence of optical transitions for any CNT.

O 88.8 Thu 12:15 GER 38

Dzyaloshinskii-Moriya-interaction energy, where it is located? Real and reciprocal spaces views. — •Leonid Sandratskii — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Recently Dzyaloshinskii-Moriya interaction (DMI) attracted new wave of intense attention stimulated by its role in the stabilization and fast dynamics of skyrmions. Numerous approaches have been suggested for the estimation of the the DMI parameters. Many efforts are devoted to reveal the electronic properties responsible for the strength of the DMI and, in this way, to help to engineer the materials with desired DMI characteristics. Although there is full consensus with respect to the most fundamental reasons of the DMI, the SOC and broken inversion symmetry, in details the physical pictures suggested by different authors differ strongly. In particular, this concerns the role of the avoiding crossings in the electronic structure, the spatial location of the DMI energy, the role of the orbital moments. This stimulated us to perform detailed study of the DMI in CoPt bilayer focusing on the open questions. We used both the approximate calculations for spin spirals with arbitrary wave vectors and more precise but also more time and resources consuming full relativistic calculations for supercells with the magnetic structures of opposite chirality. The results of the calculations are presented and analyzed.

O 88.9 Thu 12:30 GER 38

***Ab-initio* study of the Raman spectra of strained graphene** — •Albin Hertrich, Caterina Cocchi, Pasquale Pavone, and Claudia Draxl — Department of Physics, Humboldt-Universität zu Berlin, Germany

Raman spectroscopy is an important non-destructive method for characterizing graphene-based materials. The main features of Raman spectra of pristine graphene are the first-order G-band at $\approx 1580\,\mathrm{cm}^{-1}$ and the dispersive second-order 2D-band at $\approx 2700\,\mathrm{cm}^{-1}$. In this work, we perform a systematic analysis on the effect of strain on both bands. All calculations are done using the full-potential all-electron code `exciting` [1]. Phonon properties are computed within the frozen-phonon approximation, the frequency-dependent dielectric tensor within the random-phase approximation. Raman-scattering intensities are calculated from vibrational matrix elements and derivatives of the dielectric tensor with respect to the phonon normal coordinates [2]. Under biaxial strain both Raman bands are shifted, while uniaxial strain leads to a splitting of the G-band by lifting the degeneracy of the optical in-plane Γ-point phonons. Further, we explore the effect of different types of inhomogeneous strain on the optical phonon frequencies and Raman-scattering intensities.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[2] C. Ambrosch-Draxl *et al.*, Phys. Rev. B **65**, 064501 (2002).

O 88.10 Thu 12:45 GER 38

DFT meets Landau Theory: The High Pressure Phase Transition of Lead Titanate — •Andreas Tröster — Vienna University of Technology, Institute of Material Chemistry, Getreidemarkt 9 A-1060 Wien, Austria

Landau theory (LT) coupled to infinitesimal strain is a cornerstone of the theory of structural phase transitions. At high pressures, however, this approach breaks down due to the appearance of large strains and the accompanying nonlinear elastic energy contributions. In density functional theory (DFT), on the other hand, stress and strain are easy to control, but entropic effects are difficult to incorporate since DFT is a genuine zero temperature method. Recently we have shown how to combine the strengths of these two antipodal approaches by constructing a high pressure extension of conventional LT with the help of DFT. Essential for the success of this approach is the ab initio calculation of pressure-dependent elastic constants. This theory yields a concise numerical description of the high pressure phase transition in strontium titanate, and also allows to resolve a number of severe and long-standing discrepancies between the experimental data and the theoretical description of the ferroelectric high pressure phase transition of the perovskite lead titanate, a material which is also of considerable technological interest.

O 88.11 Thu 13:00 GER 38

Ground-State and Excitation Properties of Orthorhombic MAPbI$_3$ — •Claudia Rödl and Silvana Botti — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Hybrid organic-inorganic halide perovskites are one of the most promising candidates for the next generation of photovoltaic devices with high power-conversion efficiencies. Despite the amazing progress in device fabrication, many of the fundamental properties of these materials are not yet understood. The flexibility in composition of hybrid perovskites permits to tune physical properties like band gap, dielectric constant, or optical absorption which renders them interesting also from a fundamental point of view and for applications beyond photovoltaics. The most intensively studied compound, methylammonium lead iodide (MAPbI$_3$), condenses in a low-temperature orthorhombic phase which undergoes a phase transition to a tetragonal structure at 162.2 K and transforms into a cubic high-temperature phase above 327.4 K. These phase transitions go along with a change in the optical properties. Here, we focus on the orthorhombic phase of MAPbI$_3$. We have studied the ground-state atomic structure, and in particular the orientation of the MA$^+$ ion within the inorganic cage, within density-functional theory. We investigate the one-particle excitation properties (band gap, photoemission spectrum) within the GW approximation of many-body perturbation theory. Moreover, we calculate optical and loss spectra using time-dependent density-functional theory and solving the Bethe-Salpeter equation.

O 88.12 Thu 13:15 GER 38

Structure, nonstoichiometry, and geometrical frustration of α-tetragonal boron — •Jens Kunstmann[1], Naoki Uemura[2], Hagen Eckert[1], and Koun Shirai[2] — [1]TU Dresden, Germany — [2]Osaka University, Japan

It is currently believed that boron in the α-tetragonal structure is not an elemental crystal. Here we contradict this view and resolve the structural and thermodynamic characteristics of pure α-tetragonal boron via density functional theory calculations. The conditions for stable covalent bonding are almost fulfilled at a stoichiometric composition B$_{52}$. This phase is an elemental crystals with geometrical frustration. Furthermore, our thermodynamic considerations show that small, positive deviations from the stoichiometric composition occur at finite temperatures. [Uemura, Shirai, Eckert, Kunstmann, Phys. Rev. B 93, 104101 (2016)]

O 88.13 Thu 13:30 GER 38

Magnetic response properties of thin films using Kubo's linear response formalism — •Andreas Held, Sebastian Wimmer, Sergiy Mankovsky, and Hubert Ebert — Department Chemie, Ludwig-Maximilians-Universität München

We have applied the fully relativistic spin-polarized Korringa-Kohn-Rostoker method to investigate various magnetic response properties of two-dimensional systems such as free-standing mono- and multilayers, surfaces and thin films on surfaces. Our approach is based on an implementation of Kubo's linear response formalism within the tight-binding (or screened) KKR framework that allows introducing layer-resolved response coefficients τ_{ij}^{IJ}. Extending previous work [1] focusing on the symmetric part of the electrical conductivity tensor, we are able to describe the full response tensors connected to charge and spin transport, Gilbert damping, spin-orbit torque and the Edelstein effect. An implementation of the Coherent Potential Approximation for layered systems allows the treatment of disorder effects including the Vertex Corrections to the response coefficients [2]. This can be used to study chemical disorder in alloys but also to include the effect of finite temperatures. For the latter the so-called Alloy-Analogy Model [3] is employed to treat vibrations and spin fluctuations.

[1] W.H. Butler *et al.*, *Phys. Rev. B* **52**, 13399 (1995). [2] W.H. Butler, *Phys. Rev. B* **31**, 3260 (1985); K. Palotás *et al.*, *Phys. Rev. B* **67**, 174404 (2003). [3] H. Ebert *et al.*, *Phys. Rev. B* **91**, 165132 (2015).

O 89: Oxide and Insulator Surfaces: Adsorption III

Time: Thursday 10:30–12:45 Location: TRE Phy

O 89.1 Thu 10:30 TRE Phy

Adsorption of Water on (Ca,Sr)$_3$Ru$_2$O$_7$ surfaces — •Wernfried Mayr-Schmölzer, Daniel Halwidl, Florian Mittendorfer, Ulrike Diebold, Josef Redinger, and Michael Schmid — Institute of Applied Physics, TU Vienna

Perovskite oxides are promising materials for a wide range of applications as diverse as sensors, fuel cells and catalysts. Surprisingly an atomic scale knowledge of their surface chemistry is still rather poor. Here we present a combined DFT, STM and XPS study of the first monolayer H$_2$O formation on the (001) surfaces of three Ruddelsden-Popper type compounds, Sr$_3$Ru$_2$O$_7$, Ca doped Sr$_3$Ru$_2$O$_7$ and Ca$_3$Ru$_2$O$_7$. All cleave nicely, yielding flat rocksalt-like SrO-, (Sr,Ca)O- and CaO-type terminated surfaces. Adsorbed H$_2$O monomers dissociate on all surfaces by transferring an H to an apical O while the remaining OH resides at a nearby Sr-Sr, Ca-Sr, or Ca-Ca bridge, respectively. On the SrO-type surface dimers of dissociated H$_2$O are formed, which at higher coverage combine to chains and cages[1]. The CaO-type surface is much more reactive ($\Delta E_{Ads}^{H_2O} \approx$ 0.4eV) and also shows chains of dissociated H$_2$O, but due to the different rotation and tilting of the RuO octahedra they only occur along the [010] direction. On the Ca doped SrO-type surface the dissociated H$_2$O molecule is preferably located at the dopant site and reactivity is increased by 0.1eV compared to the pure SrO-type surface. Additionally the dopant impedes dimer formation.

[1]D. Halwidl et. al., Nature Materials, 15(4), 450-455.

O 89.2 Thu 10:45 TRE Phy

Consecutive Charging of a Molecule-on-Insulator Ensemble Using Single Electron Tunnelling Methods — •Philipp Rahe[1], Ryan P. Steele[2], and Clayton C. Williams[3] — [1]Fachbereich Physik, Universität Osnabrück, Osnabrück, Germany — [2]Department of Chemistry, The University of Utah, Salt Lake City, USA — [3]Department of Physics and Astronomy, The University of Utah, Salt Lake City, USA

Redox-active molecules are attractive materials for memory elements in future electronic devices [1]. Early success [2] in fabricating molecular memory cells notwithstanding, combining and interconnecting the functionality of single molecules into devices while electrically insulating them from the environment still remains a challenge [3].

Here, we follow the bottom-up strategy to fabricate a ferrocene-on-insulator system where the molecules self-assemble into islands stable at room-temperature. The charge state of this ferrocene-on-calcite(10$\bar{1}$4) system can locally be modified at room temperature [4], where single electron tunnelling methods reveal the charging step. Kelvin probe force microscopy confirms a trapping of the charge within the island structure, and we introduce a model to explain the KPFM contrast [5]. Interestingly, our data gives evidence for charge stability even for multiple charges.

[1] J.S. Lindsey and D.F. Bocian, Acc. Chem. Res. 44, 638 (2011); [2] Z. Liu et al., Science 302, 1543 (2003); [3] J.R. Heath, Annu. Rev. Mater. Res. 39, 1 (2009); [4] P. Rahe et al., Nano Letters 16, 911 (2016); [5] J.L. Neff and P. Rahe, Phys. Rev. B 91, 085424 (2015).

O 89.3 Thu 11:00 TRE Phy

Electron Transfer between Anatase TiO$_2$ (101) and an Adsorbed O$_2$ Molecule: Direct Observation by nc-AFM — •Martin Setvin, Jan Hulva, Gareth Parkinson, Michael Schmid, and Ulrike Diebold — TU Wien

The electron transfer between the substrate and an adsorbed molecule is a key process in catalysis, photocatalysis, electrochemistry or redox chemistry. We use a low temperature q-Plus STM/AFM to study the electron transfer between the anatase TiO$_2$ (101) surface and a single adsorbed O$_2$ molecule. We can directly distinguish neutral physisorbed O$_2$ molecules in the triplet state from negatively charged

(O$_2$)$^-$ radicals, based on their different chemical reactivity towards the tip apex. Neutral O$_2$ molecules are inert, while the (O$_2$)$^-$ radicals readily form a chemical bond with the tip. By biasing the tip, we can charge and discharge the molecules at will and we show that the identical processes occur during UV illumination of the sample. Using the Kelvin-probe force spectroscopy, we investigate in detail the process of charge transfer between the substrate and the adsorbed molecule. The experiments point towards a key importance of the physisorbed O$_2$ state and its electron affinity. The AFM data are supported by area-averaged spectroscopic techniques such as temperature programmed desorption or photoelectron spectroscopy.

O 89.4 Thu 11:15 TRE Phy

Methanol adsorption and reaction on a CuWO4 monolayer on Cu(110) — •Matthias A. Blatnik, Carl Drechsel, Nassar Doudin, Falko P. Netzer, and Svetlozar Surnev — Surface and Interface Physics, Institute of Physics, University of Graz, Universitätsplatz 5, 8010 Graz, Austria

Here we investigate the chemical reactivity of CuWO4 nanolayers on Cu(110), with a coverage between 0 and 1 ML, towards adsorption and reaction of methanol (CH3OH) using a combination of high-resolution XPS and STM. Methanol has been dosed at 110 K, at which temperature it adsorbs molecularly as a multilayer. On heating to 160 K the methanol multilayer transforms into a methanol monolayer, methoxy (CH3O) and some formaldehyde (CH2O) intermediates. After heating to 260 K the methanol monolayer has fully converted into methoxy and some hydrocarbon (CHx) adsorbates, which remain stable up to 310 K. After heating to 450 K methoxy has been desorbed from most of the CuWO4 surface, except on those with coverages between 0.65 ML and 0.8 ML. The latter CuWO4 surfaces show the largest methoxy yield and degree of reduction. This is a strong indication that the oxidation reaction is promoted at the periphery of the oxide islands, which expose a large number of active under-coordinated reaction sites. This is indeed confirmed by the STM measurements, which show that the methanol oxidation reaction is initiated at the boundaries between the Cu-O and CuWO4 islands. Finally, flashing above 500 K results in the complete methoxy removal from the CuWO4 surfaces

O 89.5 Thu 11:30 TRE Phy

Adsorption properties and reactivity of single Rh atoms on Fe3O4 (001) — •Jan Hulva[1], Roland Bliem[1], Zdeněk Jakum[1], Adam Závodný[1], Michael Schmid[1], Ulrike Diebold[1], Peter Blaha[2], and Gareth S. Parkinson[1] — [1]Institute of Applied Physics, TU Wien, Wiedner Hauptstrasse 8-10, 1040 Vienna, Austria — [2]Institute of Materials Chemistry, TU Wien, Getreidemarkt 9, 1060, Vienna, Austria

Single atom catalysis operates in the smallest particle size limit of supported metal catalyst. Although It has been shown that this approach is promising for the synthesis of highly active catalysts containing only small amount of expensive metal [1], the concept still remains controversial. It has been shown that Fe3O4 (001) surface is able to stabilize single metal atoms up to relatively high temperatures [2] due to its surface reconstruction [3]. This makes it an ideal candidate for a model system for fundamental studies of the single atom catalysis.

STM shows that Rh adatoms can be adsorbed at the magnetite surface in several different configurations. This can be linked to different chemical states of Rh seen by XPS. As predicted by DFT, CO bounds strongly to Rh adatoms and dimers giving an origin to two desorption peeks in TPD at 460K and 530K. Strong interaction of CO and Rh also leads to CO2 formation by Mars-van Krevelen mechanism at these temperatures.

[1] Qiao B., Nature Chemistry, 3, (2011): 634-641. [2] Novotný Z., et al., Phys.Rev.Lett.108(2012): 216103 [3] Bliem R., et al. Science 346 (2014): 1215-1218.

O 89.6 Thu 11:45 TRE Phy

Imaging and manipulation of dissociated water on In2O3(111) — •Margareta Wagner[1], Martin Setvin[1], Steffen Seiler[2], Lynn A. Boatner[3], Michael Schmid[1], Bernd Meyer[2], and Ulrike Diebold[1] — [1]Institut für Angewandte Physik, TU Wien, Österreich — [2]Computer Chemistry Center, FAU Erlangen-Nürnberg, Deutschland — [3]Materials Science and Technology Division, ORNL, Tennessee, USA

Indium oxide is one of the most important transparent conductive oxides (TCOs), and commonly used as a contact and sensor material.

Here, the adsorption of water is investigated with low temperature STM/AFM, XPS and DFT. Above 100 K dissociative adsorption of water on In2O3(111) single crystals is observed. At room temperature the surface is saturated with three dissociated water molecules per unit cell, symmetrically arranged around the six-fold coordinated In atoms. The fully hydroxylated surface shows a (1x1) structure with respect to the clean In2O3(111) surface. This leads to a well-ordered, hydroxylated surface where the three terminal OH groups plus the three protons (forming surface OH groups) are imaged together as one bright triangle in STM. The internal structure is revealed by AFM measurements, and manipulations with the STM tip, where surface OH grouse can be individually removed.

O 89.7 Thu 12:00 TRE Phy

Water adsorption at the Zirconia Surface on Pt$_3$Zr — •Peter Lackner[1], Jan Hulva[1], Joong-Il J. Choi[1,2], Gareth Parkinson[1], Ulrike Diebold[1], and Michael Schmid[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Institute for Basic Science, KAIST, Daejeon, Republic of Korea

Oxidation of Pt$_3$Zr(0001) single crystals leads to the formation of a ZrO$_2$(111) trilayer on top of a Pt layer [1]. In scanning tunneling microscopy (STM), the ZrO$_2$ layer shows a $(\sqrt{19}\mathrm{x}\sqrt{19})\mathrm{R}23.4^\circ$ superstructure with 12 Zr atoms in every unit cell. The Zr layer is strongly buckled and the ZrO$_2$ trilayer is distorted above substrate dislocation lines, thus creating different adsorption locations.

We have employed this ZrO$_2$/Pt$_3$Zr system as a model system for water adsorption studies on zirconia, combining temperature-programmed desorption (TPD), X-ray photoelectron spectroscopy (XPS) and STM. In TPD, $\approx$ 90% of the adsorbed D$_2$O contributes to the monolayer peak at 180 K ($E_{\mathrm{ads}} = 0.5 - 0.6$ eV). According to XPS, these adsorbates are bound in molecular form. The remaining 10% are bound in the form of hydroxyls. They have higher binding energies, which leads to a tail in the TPD spectrum reaching up to 550 K.

Repeated TPD measurements lead to a decrease of the monolayer peak area and to an increase of the tail area. Thus, water changes the surface structure, creating adsorption sites with higher adsorption energies. This surface change was examined by low-temperature STM.

[1] Antlanger et al., Phys. Rev. B 86, 035451 (2012).

O 89.8 Thu 12:15 TRE Phy

Self-assembled π- π-stacked triphenylamine derivatives on bulk MgO(001) and KBr(001) — •Tim Sander[1], Maximilian Ammon[1], Natalie Hammer[2], Martin Gurrath[3], Bernd Meyer[3], Milan Kivala[2], and Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, Germany — [2]Chair of Organic Chemistry I, Department of Chemistry and Pharmacy, Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, Germany — [3]Computer-Chemie-Centrum, Friedrich-Alexander University Erlangen-Nürnberg, Germany

Well-ordered molecular self-assemblies on insulating surfaces play a key role towards the controlled formation of organic nanostructures for potential applications in nanoelectronics. On bulk insulators, the subtle influence of the often weak and unspecific molecule-surface interaction on the self-assembly is of high interest.

Here, we discuss molecular self-assemblies of halogen-substituted carbonyl-bridged triphenylamine derivatives on bulk MgO(001) and KBr(001) by means of low temperature non-contact atomic force microscopy (nc-AFM) combined with density functional theory. We observe π-π-stacked structures with comparable adsorption energies on both surfaces. Molecularly resolved nc-AFM images indicate that the intermolecular distances in the triphenylamine structures are similar to the respective lattice spacing underneath. In addition, we find that the growth direction of the π-π-stacked chains is influenced by the choice of the substrate.

O 89.9 Thu 12:30 TRE Phy

Improving the photoelectrochemical performance of cobalt ferrite by transition metal substitution: A DFT+U study — •Hamidreza Hajiyani and Rossitza Pentcheva — Fakultät für Physik and Center of Nanointegration (CENIDE), Universität Duisburg-Essen, 47057 Duisburg

Transition metal oxides are considered as promising materials for photo-anodes to convert solar energy into hydrogen fuel through water oxidation. Here we report density functional theory+U (DFT+U) calculations on the influence of transition metal mixing on the performance of cobalt ferrite (CoFe$_2$O$_4$) as anode material in the oxygen evolution reaction (OER). Our results on M$_x$Co$_{1-x}$Fe$_2$O$_4$ (111) surfaces illustrate that the overpotential during OER process can be reduced by partial substitution of Co sites with elements such as Ni. We find that this improvement is related to modification of the binding energy of the reaction intermediates during water oxidation. Analysis of spin density and electronic properties shows that substitution of nickel in cobalt ferrite varies the band gap, band edge positions and oxidation state of cations at the (111) surface.

We acknowledge support by the DFG within priority program SPP1613, project PE883/9-2 and the computational time at the Leibnitz Rechenzentrum (grant pr87ro) and at magnitUDE.

O 90: Surface Dynamics: Experiments

Time: Thursday 10:30–12:45 Location: WIL C107

O 90.1 Thu 10:30 WIL C107

Adsorption Dynamics of Methanol on Si(001) Studied by Means of Molecular Beam Techniques — •Tamam Bohamud[1], Marcel Reutzel[1], Michael Dürr[1,2], and Ulrich Höfer[1] — [1]Philipps-Universität, 35037 Marburg — [2]Justus-Liebig-Universität, 35392 Giessen

Understanding the reaction of organic molecules on semiconductor surfaces is a fundamental step on the way to hybrid structures with high functionality. For this reason, the adsorption of organic molecules with different functional groups on silicon surfaces has been studied in detail. In most cases, the adsorption dynamics are governed by a metastable intermediate state [1,2]. For methanol, such an intermediate state was also proposed but could not be observed experimentally yet.

In this contribution, we make use of molecular beam experiments to investigate the adsorption dynamics of methanol on Si(001). The initial sticking probability s_0 was measured both as a function of surface temperature and kinetic energy of the impinging molecules. It was found that s_0 decreases with increasing surface temperature, indicating adsorption via an intermediate state. The dependence of s_0 on the kinetic energy of the incoming molecules deviates from a simple non-activated adsorption behavior. This is discussed both in terms of strong coupling between intermediate and final state as well as in terms of additional reaction channels accessible at higher kinetic energy.

[1] M. Lipponer et al., Chem. Phys. Lett. 624, 69 (2015)

[2] M. Lipponer et al., Surf. Sci. 651, 118 (2016)

O 90.2 Thu 10:45 WIL C107

Surface-morphology transition between step-flow growth and step bunching — •Konrad Bellmann[1], Udo W. Pohl[1], Alexander Sabelfeld[1], Christian Kuhn[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

Epitaxially grown opto-electronic devices rely on smooth interfaces with step-flow morphology. The surface-morphology transition between step-flow growth and step bunching will be theoretically discussed by comparing two different boundary conditions to solve the differential equation for surface diffusion. Favored smooth surfaces rely on vicinal terraces which are characterized by a mean terrace width and terrace-edge conditions. An energy diffusion-barrier at the terrace edge, the Ehrlich-Schwöbel barrier, influences the adatom incorporation towards the lower terrace edge. The first approach simply considers an asymmetric equilibrium adatom-density at the edges which offers a simple analytic morphology transition relation. The second more-physical approach considers an asymmetric adatom-incorporation flux at the edges. Both approaches yield a similar qualitative behavior. However, the morphology transition does not only rely on the two adatom-incorporation rates at the edges and the surface diffusion, but also on the adatom-mean resident time on the surface. Finally, the morphology transition between step-flow growth and step bunching is experimentally confirmed by homoepitaxial growth of AlN.

O 90.3 Thu 11:00 WIL C107

On the reduction behavior of CeO2 (100) and (111) surfaces — •Johanna Hackl[1], Tomas Duchoň[2], David Nikolaus Müller[1], Daniel Marius Gottlob[3], Imtiaz Khan[1], Stefan Cramm[1], Slavomir Nemšák[1], and Claus Michael Schneider[1] — [1]Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, Germany — [2]Department of Surface and Plasma Science, Charles University in Prague, Czech Republic — [3]SPEC, CEA, CNRS, Université Paris Saclay, F-91191 Gif-sur-Yvette, France

Ceria has an ability to store and release oxygen by changing its oxidation state reversibly between CeO2 and Ce2O3. This gives ceria unique catalytic properties with many applications. DFT calculations predict a strong dependence of oxygen vacancy formation energies for different CeO2 surface orientations. Particularly the (100) surface is expected to have a lower oxygen vacancy formation energy than the (111) surface. In the present work CeO2 islands with (111) and (100) surfaces are simultaneously grown in-situ onto a Cu (111) substrate. The island formation is observed and characterized with low energy electron microscopy (LEEM) and micro-LEED. Using laterally resolved x-ray absorption spectroscopy (XAS) performed in a photoemission electron microscope (PEEM) the partial reduction of CeO2 to Ce2O3 in an H2 environment is observed in-situ and in real-time, directly comparing the reduction kinetics of the (111) and the (100) islands. Spectra of the Ce M5 edge show a more pronounced reduction state of cerium for the (100) islands. This behavior can be connected to a higher catalytic activity of CeO2 (100) for some types of the oxidizing reactions.

O 90.4 Thu 11:15 WIL C107

Surface Phase Behavior of [PPh4][Tf2N] / Cs[Tf2N]- and [PPh4][Tf2N] / Ni[Tf2N]2 Low-Temperature Molten Salt Mixtures — Patrick Schreiber[1], Marlene Scheuermeyer[2], •Radha G. Bhuin[1], Peter Wasserscheid[2], Hans-Peter Steinrück[1], and Florian Maier[1] — [1]Lehrstuhl für Physikalische Chemie II, FAU, Erlangen, Germany — [2]Lehrstuhl für Chemische Reaktionstechnik, FAU, Erlangen, Germany

We report on surface investigations using a new class of organic/inorganic molten salt mixtures based on a [PPh4][Tf2N] compound. Depending on composition, these mixtures combine low melting points with exceptionally high thermal stability, and thus, exhibit considerably enlarged reaction windows compared to conventional ionic liquids.[1] To elucidate their surface behavior, temperature-dependent angle-resolved XPS investigations were performed using our unique spectrometer DASSA (Dual Analyzer System for Surface Analysis).[2] The DASSA comprises an UHV chamber equipped with two electron analyzers for simultaneous electron detection at 0° and 80°. We follow temperature-induced changes in bulk and surface composition for mixtures of [PPh4][Tf2N]/Cs[Tf2N] and [PPh4][Tf2N]/Ni[Tf2N]2. Interestingly, the Cs-containing mixture in the liquid state favors the presence of [Cs]+ at the surface on expense of the bulky [PPh4]+ ions. RGB and HPS thank the ERC for financial support through an Advanced Investigator Grant to HPS. References: [1] Scheuermeyer et al., New J. Chem., 40, 7157, 2016. [2] Niedermaier et al., Rev. Sci. Instrum., 87, 045105, 2016.

O 90.5 Thu 11:30 WIL C107

The effect of chemical pressure on Ag+ cation substitution in CdSe nanocrystals — •Urko Petralanda, Luca De Trizio, Liberato Manna, and Sergey Artyukhin — Istituto Italiano di Tecnologia, Via Morego 30, Genova (Italy)

Cd2+ cations in CdSe nanocrystals experience, at ambient conditions, a fast and total replacement by Ag+ cations when exposed to the latter in an appropriate solvent [1,2]. A promising mechanism proposed to describe the cation exchange (CE) reactions is the so called kick-out mechanism [3,4], where the exchanged ions are considered to diffuse through interstitials. Within this framework, we use a tight binding model based on ab initio calculations to investigate the effect of chemical pressure on the CE reaction energy barrier and discuss the role played by different energy contributions.

[1] E. M. Chan, M. A. Marcus, S. Fakra, M. ElNaggar , R. A. Mathies, A. P. Alivisatos, J. Phys. Chem. A, 111, 12210 (2007). [2] L. De Trizio, L. Manna, Chem. Rev. 116, 10852 (2016). [3] U. Gösele, W. Frank, A. Seeger, Appl. Phys. 23, 361 (1980). [4] F. D. Ott, L. L. Spiegel, D. J. Norris, S. C. Erwin, Phys. Rev. Lett. 113, 156803

(2014).

O 90.6 Thu 11:45 WIL C107

Surface explosion of tartaric acid diastereomers on a Cu(111) surface in ultrahigh vacuum — •Alexandra Rieger and Karl-Heinz Ernst — Nanoscale Materials Science, Swiss Federal Laboratories for Materials Testing and Research (EMPA), Überlandstrasse 129, CH-8600 Dübendorf, Switzerland

Tartaric acid (TA) comes as three diastereomers: the two enantiomers L-TA and D-TA as well as the achiral meso form m-TA. We have studied the adsorption of m-TA, L-TA and the racemic mixture of L- and D-TA on a Cu(111) and on a Pd(110) surface. Using thermally desorption spectroscopy (TDS), we have investigated the thermally induced auto-catalytic decomposition reaction, the so-called surface explosion, which leads to decomposition into carbon dioxide, water and hydrogen within a very narrow temperature interval. This allows identification of structural differences in the monolayer of the isomers. X-ray photoelectron spectroscopy was used in order to identify the adsorption mode as a function of coverage. Using low-energy electron diffraction (LEED), we have investigated how the molecules self-assemble on a Cu(111) and on a Pd(110) surface.

O 90.7 Thu 12:00 WIL C107

Photodesorption of CO from Si(100) — •Michael Lackner, Daniel Lucassen, and Eckart Hasselbrink — Universität Duisburg-Essen, Fakultät für Chemie, 45141 Essen

Velocity distributions of photodesorbed molecules can provide substantial insights into the desorption dynamics.

CO adsorbed on Si(100) is desorbed by a pulsed UV laser (266/355 nm). Time of flight spectra of these desorbed CO molecules are measured with a mass spectrometer, yielding velocity distributions. We observe at least two desorption channels. The yield in these solely depends on photon wavelength.

Furthermore cross sections were determined by a similar measurement setup. Here, the total signal decays double exponentially and depends on photon exposure.

O 90.8 Thu 12:15 WIL C107

Kinetic controlled hierarchical self-assemblies of all-trans-retinoic acid on Au(111) — •Chao Li and yongfeng Wang — Key laboratory for the physics and cemistry of nanodevices, Department of Electronics, Peking University, Beijing 100871, China

Kinetic controlled hierarchical self-assemblies of all-trans-retinoic acid on Au(111) are investigated by low-temperature scanning tunneling microscopy (STM) in ultra-high vacuum. The dominant molecular hierarchical superstructure can be selectively controlled to dimer, tetramer, or pentamer patterns, which are stabilized by hydrogen bonds and vdW interactions.

O 90.9 Thu 12:30 WIL C107

A test experiment to determine the long term behaviour of surface work functions — •Matthias Wecker and KATRIN Collaboration — Karlsruhe Institute of Technology (KIT), ITeP/TLK, Postfach 3640, 76021 Karlsruhe

The **Ka**rlsruhe **Tri**tium **N**eutrino (KATRIN) experiment aims to determine the effective mass of neutrinos with a sensitivity of 200 meV/c^2 (90% C.L.). This requires the precise measurement of the β-spectrum from tritium-decay close to the endpoint at 18.6 keV. The energy is analysed with the Main Spectrometer, a electrostatic high-pass filter with a filter width of 0.93 eV. The filter voltage of 18.6 kV has to be known with 60 mV accuracy. Thus, the plasma potential in the windowless gaseous tritium source (WGTS), where the β-electrons are produced, has to be known with the same precision. The rear end of the WGTS is electrically terminated by the Rear Wall, a gold-coated stainless steel disk. Superconducting solenoids around the beam-pipes produce a strong magnetic field (3.6 - 6 T) that guides the β-electrons to the spectrometer. The field also connects the plasma in the WGTS with the Rear Wall. Thus, inhomogeneities and fluctuations in the potential of the Rear Wall directly translate into an uncertainty of the WGTS potential, thus limiting the ultimate sensitivity of KATRIN. Exposure to ambient air before its subsequent operation in vacuum can lead to such changes of the work function. This talk introduces a new experiment at KIT for the in-situ determination of the work function. Initial results will be presented. We acknowledge the support of KSETA, the BMBF (05A14VK2) and the Helmholtz Association.

O 91: Nanostructures at Surfaces: Molecular Systems I

Time: Thursday 10:30–13:00 Location: REC/PHY C213

O 91.1 Thu 10:30 REC/PHY C213

Synthesis of highly ordered arrays of organic nanowires on a magnetic surface alloy — •Jens Brede[1], Mikel Abadia[1], Celia Rogero[1,2], Ignacio Piquero-Zulaica[1], Maxim Ilyn[1], and J. Enrique Ortega[1,2,3] — [1]Centro de Física de Materiales CFM–MPC(CSiC-UPV/EHU), Paseo Manuel Lardizabal 5, E-20018 San Sebastián, Spain — [2]Donostia International Physics Center, Paseo Manuel Lardizabal 4, E-20018 San Sebastián, Spain — [3]Departamento Física Aplicada I, Universidad del País Vasco, E-20018 San Sebastián, Spain

The transfer of well-established *in-situ* methods for growing covalently bonded macromolecules with atomic precision onto magnetic substrates presents a viable route toward studying emergent intrinsic magnetic properties in these novel structures as well as their magnetic coupling to the underlying substrate. Here, we present a multi-technique characterization of the polymerization of 4,4-dibromoterphenyl precursors into ordered arrays of poly (p-phenylene) chains on top of the bimetallic GdAu$_2$ surface alloy. The activation temperature for bromine scission and subsequent homocoupling of molecular precursors was followed by temperature dependent XPS. Structural characterizations of the highly ordered molecular and polymeric phases were performed by LEED and STM. The electronic structures of the valence band of the different phases were determined with ARPES and magnetic ordering in the GdAu$_2$ alloy was established by XMCD during all stages of the reaction.

O 91.2 Thu 10:45 REC/PHY C213

Light-Induced Translation of Motorized Molecules on a Surface — •Alex Saywell[1,2], Anne Bakker[1], Johannes Mielke[1], Takashi Kumagai[1], Martin Wolf[1], Victor García-López[3], Pinn-Tsong Chiang[3], James M. Tour[3], and Leonhard Grill[1,4] — [1]Department of Physical Chemistry, Fritz-Haber-Institute of the Max-Planck Society, 14195 Berlin, Germany. — [2]School of Physics & Astronomy, The University of Nottingham, United Kingdom. — [3]Rice University, Houston, Texas 77005, United States. — [4]Department of Physical Chemistry, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria.

A key component of molecular nanotechnology are molecular machines that can perform controlled work. The motion of such machines should be triggered remotely in order to address a large number of molecules at the same time, with light being an attractive stimulus as a single source. Here, we report the photo-induced translation of molecular machines across a surface by characterizing single molecules before and after illumination. Illumination of molecules containing a motor unit results in an enhancement in the diffusion of the molecules. The effect vanishes if an incompatible photon energy is used or if the motor unit is removed from the molecule, revealing that the enhanced motion is due to the presence of the wavelength-sensitive motor in each molecule.

O 91.3 Thu 11:00 REC/PHY C213

Charge switching in multi-ferrocene molecules observed — •Martin Ondráček, Pavel Jelínek, Jan Berger, Oleksandr Stetsovych, and Martin Švec — Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

The ability to switch between different redox states makes ferrocene molecules an attractive subject of research aiming to nano-scale electronics. Linking several ferrocene units into multi-ferrocene molecules expands the potential functionality, due to the interaction among the individual ferrocene sub-units and the possibility to switch their charge state in a coordinated manner. Our study shows how the charge of bis- and tetra-ferrocene molecules on NaCl substrate can be detected and controlled by an atomic force microscope (AFM). Here, I focus on theoretical explanation of the main features observed in the AFM and electrostatic force spectroscopy (EFM) with these molecules. Especially notable are sharp boundary-like features characterized by increased frequency shift as well as an increased energy dissipation signal. We interpret them in terms of charge transfer among the ferrocene centers facilitated by the AFM tip. Using a modified version of an earlier written simulator [1], we back our interpretation with a model that encompasses the AFM cantilever dynamics and electrons hopping among the AFM tip and ferrocene centers. We supplement our empirical model with DFT-based calculations of the geometry and electronic structure of the molecules on NaCl.

[1] M. Ondráček, P. Hapala, P. Jelínek, Nanotechnology **27**, 274005 (2016).

O 91.4 Thu 11:15 REC/PHY C213

Electric-field effect on the formation of single-molecule contacts — •Jonathan Brand, Nicolas Néel, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau

Pristine and C_{60}-terminated tips of an atomic force microscope are used to form contacts to single C_{60} molecules adsorbed on Pb(111) and Cu(111). A pronounced variation of the point of contact with the electric potential difference across the junction is inferred from bias-dependent force spectroscopy. The conventional approach to describing forces in atom-scaled junctions by a superposition of van der Waals, electrostatic, and Lennard-Jones forces with a rigid junction geometry fails. Rather, the experimental observations may be rationalized by considering voltage-dependent relaxations of the electrodes.

Financial support by the Deutsche Forschungsgemeinschaft through Grant No. KR 2912/10-1 is acknowledged.

O 91.5 Thu 11:30 REC/PHY C213

Control of charge states within a single molecule — •Jan Berger[1], Oleksandr Stestovych[1], Martin Ondráček[1], Martin Švec[1], Irena G. Stará[2], Ivo Starý[2], and Pavel Jelínek[1] — [1]Insitute of Physics, ASCR, Prague, Czech republic — [2]Institute of Organic Chemistry and Biochemistry ASCR, Prague, Czech republic

The field of molecular electronics aims at using a single molecule as building block for electronic devices. Ferrocene-based molecules are extremely appealing as they offer prospects of having a built-in charging functionality. They are known of being stable under redox states and therefore promising as candidates for quantum cellular automata units. Previous works demonstrated charging single metal adatoms [1], molecules or their clusters on insulating films [2] as well as charging of large self-assembled islands of molecules by STM or nc-AFM. [3]

Here we will present experimental evidence of controlling multiple charge states on a single 3,6,3',6'-tetraferrocene-9,9'bis-fluorenylidene, deposited on thin insulating NaCl film, by means of nc-AFM. We succeed to control the multiple charge states within a single molecule including reversible transitions between them. The induced charged states have prominent fingerprints in both the frequency shift and dissipation channels. Moreover, we demonstrate that the charge states can be modified by presence of neighboring charged molecules.

[1]J. Repp et al., Science 305, 493 (2004) [2]W. Steurer et al., Nature Comm. 6:8353 (2015). [3]P. Rahe et al., Nano Letters 2, 16 (2016)

O 91.6 Thu 11:45 REC/PHY C213

Revealing an atomic nodal plane by LT-UHV-STM investigations on single benzylnaphthoic diimides — •René Ebeling[1], Shigeru Tsukamoto[2], Vasile Caciuc[2], Nicolae Atodiresei[2], Stefan Blügel[2], Rainer Waser[1], and Silvia Karthäuser[1] — [1]Forschungszentrum Jülich GmbH - (PGI-7), Jülich, Germany — [2]Forschungszentrum Jülich GmbH - (PGI-1/IAS-1), Jülich, Germany

The LT-UHV-STM investigations presented here demonstrate the adsorption behavior and the exact geometry of single target molecules in orbital resolution on atomically flat surfaces of Pt(111). The conformation and the orbital symmetry of single molecules have been deduced. For this purpose N,N'-dibenzyl-naphthoic diimide (BNI), which consists of a large π-conjugated backbone and two phenyl-rings each connected with a methylene-linker to the central part, have been studied. According to the high resolution STM images, the naphthoic diimide backbone of the molecule adsorbs flat on the substrate while the two benzyl groups build one line together with the backbone and the atomic nodal plane can be identified located at the C atoms of the phenyl rings. That points to phenyl groups standing vertically with their phenyl plane on the substrate. The orbital symmetry of the HOMO and the LUMO identified by STM was compared to DFT based calculations on BNI in the gas phase and tunneling transmission calculations which take the 3-dimensional structure of the molecule into account. These calculations agree with the measurements and provide further evidence for the supposed structure of BNI on Pt(111).

O 91.7 Thu 12:00 REC/PHY C213

Formation of metallofullerene magnetic arrays: theoretical perspectives. — •Stanislav Avdoshenko and Alexey Popov — Institute for Solid State Research, IFW, Dresden

Modeling of formation and properties self-assembled monolayer (SAM) is a very challenging task, especially if highly functional-ligands are concerned. It is true, for instance, in the case of endohedral metallofullerene (EMF) based SAM - promising single molecular magnets (SMMs) grids in-making. Properties of such SMM grids would be a function of SAM architecture (attachment types and crowding effects) and innercluster dynamics under these geometrical constrains. Electronic structure complexity of EMFs and structural mobility of ligands in SAMs brings a dual issue. On the one hand, a minimal level of theory to address the magnetic properties of the systems would require "complete active space"- quality methods. On the other hand, while the system dynamic can be approached by less computationally demanding semiclassical or even classical approaches, such methods are unable to give a reliable magneto-physics of the SMM unit. In our report, we will offer a set of concepts to deal with this problem by extensive development of the multiscale methods (MSM), in which the whole system is divided into the regions described with different levels of theory accordingly to its complexity.

O 91.8 Thu 12:15 REC/PHY C213

Metal-coordinated molecular chains on gold — •Sujoy Karan and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Choosing right precursors (molecules) is a prerequisite for getting desired polymerized structures, be it a graphene nanoribbon or other molecular networks, on surfaces. When metal atoms are incorporated into those structures, the bondings may change to form completely different networks. We show that metal coordination may not only change the structures of the networks but can also have different physical properties.

O 91.9 Thu 12:30 REC/PHY C213

Tuning the adsorption and self-assembly of terpyridine derivatives: From metal to bulk insulator surfaces — •Tuan Anh Pham[1], Yi Liu[1], Manh Thuong Nguyen[2], and Sabine Maier[1] — [1]Department of Physics, University Erlangen-Nürnberg, Erwin-Rommel-Str. 1, 91058 Erlangen, Germany — [2]Center for Computational Physics, Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan St., Hanoi, Vietnam

Controlling and understanding the on-surface self-assembly of organic molecules are of utmost importance for the effective usage of molecular systems in potential applications. On metal surfaces, it is well-known that the structure of the on-surface self-assembly is strongly dependent on the subtle balance between molecule-molecule and molecule-substrate interactions. On bulk insulators, however, the role of the molecule-substrate interaction on the structure formation is widely unexplored.

Herein, we report the self-assembly of terpyridine derivatives, on both, metal (Au and Cu) and bulk insulator surfaces (KBr), by a combination of high-resolution non contact atomic force microscopy at low temperatures and density functional theory. We achieved to selectively tune the dimensionality of the molecular structures depending on the choice of the substrate: monomeric species on Cu(111), linear chains on Au(111), and two-dimensional networks on KBr. Interestingly, we found that the substrate may induce the rotation of pyridine rings around the C-C bond axis in the terpyridine units and thus, generating the formation of H-bonds stabilizing the self-assembled networks.

O 91.10 Thu 12:45 REC/PHY C213

Metal coordination of tri-cyano-lophine on surfaces — •Bodong Zhang[1], Li Jiang[1], Yuanyuan Guo[1], Guillaume Médard[2], Simon Nadal[2], Bernhard Kuster[2], Francesco Allegretti[1], Joachim Reichert[1], Anthoula C. Papageorgiou[1], and Johannes V. Barth[1] — [1]Chair of Molecular Nanoscience & Chemical Physics of Interfaces (E20), Department of Physics, Technical University of Munich, DE — [2]Chair of Proteomics and Bioanalytics, Technical University of Munich, DE

Lophine (2,4,5-triphenylimidazole) and its derivatives are of interest due to their large potential in chemiluminescence, fluorescence, and bioanalytics. To expand the application of lophine derivatives, they have been decorated with various functional groups, such as -H, -OH, -NO_2, -CN. Cyano groups are known to direct the fabrication of well defined metal coordination structures on surfaces through their interaction with metal atoms.

Here, we study the self-assembly and metal directed assembly of a tri-cyano-lophine on Ag(111), Au(111) and Cu(111) surfaces with scanning tunneling microscopy and X-ray photoelectron spectroscopy. On Ag and Au, well-ordered phases are stabilized by dipolar coupling and attractive interactions between cyano groups and phenyl rings. Addition of Co/Fe atoms leads to three-fold coordination of the terminal cyano groups. However, on Cu a different well-ordered phase forms, exhibiting hydrogen bonding of the C≡N· · · H-N type. Annealing leads to complete Cu adatom coordination of a terminal cyano group and a deprotonated N atom of the imidazole moiety.

O 92: Gerhard Ertl Young Investigator Award

Time: Thursday 10:30–13:00 Location: TRE Ma

O 92.1 Thu 10:30 TRE Ma

Controlling the magnetic state of individual single atom magnets — •Fabian D. Natterer[1,2], Kai Yang[1,3], William Paul[1], Philip Wilke[1,4], Taeyoung Choi[1], Thomas Greber[1,5], Andreas J. Heinrich[1,6], and Christopher P. Lutz[1] — [1]IBM Almaden Research Center, San Jose, USA — [2]EPFL, Lausanne, Switzerland — [3]University of Chinese Academy of Sciences, Beijing, China — [4]University of Göttingen, Germany — [5]University of Zürich, Switzerland — [6]Ewha Womans University, Seoul, Republic of Korea

The possibility of data storage in single atom magnets represents the natural limits of a thought experiment for miniaturization in magnetic storage media. Up to now, the magnetic bit size was reduced to clusters containing few atoms, but a recent investigation showing magnetic remanence in ensembles of single holmium atoms on magnesium oxide (MgO) presented the prospect of data storage at the atomic limit. However, it was unclear how the magnetic state of a selected rare earth magnet could be controlled. We demonstrate here the reading and writing of individual Ho atoms on MgO. The Ho atoms independently retain their magnetic state over several hours. A selected Ho bit is read by tunnel magnetoresistance and written by current pulses using a scanning tunneling microscope. Using STM enabled electron spin resonance, we unambiguously prove the magnetic origin of the Ho states and reveal a large Ho magnetic moment of $(10.1 \pm 0.1)\ \mu_B$. The long lifetime of the magnetic state, combined with electrical reading and writing shows that the programming of single atom magnets is possible.

O 92.2 Thu 11:00 TRE Ma

Fascinating two-dimensional oxide quasicrystals — •Stefan Förster[1], Sebastian Schenk[1], Klaus Meinel[1], Eva Maria Zollner[1], Rene Hammer[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

When approaching the two-dimensional limit, oxides are known to exhibit strong variations in their structures and properties as compared to the respective bulk materials[1]. One of the best examples are the two-dimensional oxide quasicrystals (OQCs), which have been discovered for reduced $BaTiO_3$ on Pt(111) [2]. We report here on a second OQC derived from $SrTiO_3$ on Pt(111) as well as on approximant structures for both OQC systems, in which selected motifs of the OQC are periodically repeated. Those approximants differ drastically in their complexity. For $BaTiO_3$ a simple approximant structure is observed, which contains six of the building blocks (tiles) of the OQC in the unit cell and which has been structurally fully resolved recently [3]. For $SrTiO_3$ the more complex approximant contains a patch of 36 tiles in the unit cell. This approximant very closely resembles the ideal OQC. Our studies unravel OQCs as best-controlled QC model systems for addressing the fundamental questions related to the driving forces for aperiodic structure formation.

[1] F. Netzer, S. Fortunelli (Eds.), Oxide Materials at the two-dimensional limit, Springer (2016) [2] S. Förster K. Meinel, R. Hammer, M. Trautmann, W. Widdra, Nature 502, 215 (2013) [3] S. Förster et al., Phys. Rev. Lett. 117, 095501 (2016)

O 92.3 Thu 11:30 TRE Ma

Tuning the electrocatalytically active site: atomic ensemble effects and surface strain — •Maria Escudero-Escribano — Technical University of Denmark, Department of Physics, Fysikvej, 2800 Kgs. Lyngby (Denmark)

In order to improve the kinetics of the oxygen reduction reaction (ORR), we can modify the geometric structure (1) and/or alter the electronic properties of the surface atoms (2,3) of the catalyst.

We used a self-ordered molecular pattern, cyanide-modified Pt(111), to study the ORR (1) and to decorate surfaces at the atomic scale (4,5). My electrochemical scanning tunneling microscopy images provided an atomically resolved visualization of the honeycomb structure in the presence of cations (4). Interestingly, CN groups block the adsorption of spectator anions in the electrolyte, while allowing the adsorption of oxygen. As a consequence, CN-Pt(111) presents a 25-fold enhancement over Pt(111) (1).

In addition, we have studied novel Pt-lanthanide alloys for ORR. A Pt overlayer is formed onto the bulk alloys by acid leaching. Our surface-sensitive X-ray diffraction measurements on Gd/Pt(111) show the formation of a crystalline Pt overlayer under compressive strain (6). The ORR activity versus the lattice parameter follows a volcano relation (2). We use the lanthanide contraction to control surface strain effects and tailor the activity, stability and reactivity of Pt.

(1) Nature Chem. 2010, 2, 880; (2) Science 2016, 352, 73; (3) J. Am. Chem. Soc. 2012, 130, 16476; (4) ChemPhysChem 2011, 12, 2230; (5) J. Phys. Chem. C 2009, 113, 12340; (6) Nano Energy 2016.

O 92.4 Thu 12:00 TRE Ma

Towards Accurate Electronic Structure Predictions for Hybrid Interfaces — •David A. Egger — Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel

A highly relevant physical quantity for nanostructured molecule-metal interfaces is the energy level alignment of the molecular electronic states with respect to the Fermi level of the metal. Typical density functional theory (DFT) calculations, especially those using local and semi-local functionals, often underestimate level alignment and lead to inaccurate descriptions of electronic structure and charge transport properties of interfaces. Here, we introduce an efficient theoretical method that is based on DFT, but in contrast to common approximations fulfills physically motivated criteria for exchange-correlation interactions relevant for surfaces and interfaces. To this end, we combine the optimally-tuned range-separated hybrid (OT-RSH) functional with a DFT-derived image-charge model to accurately determine level alignment at molecule-metal interfaces in a non-empirical but system-dependent manner.[1,2] We apply our fully self-consistent approach to several physisorbed and chemisorbed molecule-metal interface systems. For both the level alignment and work-function changes, we find that our calculated results are in very good agreement with reference data from photoemission spectroscopy. Our findings indicate new ways of accurate and efficient electronic structure predictions for hybrid interfaces. [1] Egger, D. A.; Liu, Z.-F.; Neaton, J. B.; Kronik, L.: Nano. Lett. 15, 2448 (2015). [2] Liu, Z.-F.; Egger, D. A.; Refaely-Abramson, S.; Kronik, L.; Neaton, J. B.: under review.

O 92.5 Thu 12:30 TRE Ma

Structural Lubricity under Ambient Conditions — •Mehmet Z. Baykara — Department of Mechanical Engineering, Bilkent University, Ankara, Turkey — UNAM - Institute of Materials Science and Nanotechnology, Bilkent University, Ankara, Turkey

Despite its fundamental importance, physical mechanisms that govern friction are poorly understood. While a state of ultra-low friction, termed structural lubricity, is expected for any clean, atomically flat interface consisting of two different materials with incommensurate structures, associated predictions could only be quantitatively confirmed under ultra-high vacuum (UHV) conditions so far. In this contribution, we report structurally lubric sliding under ambient conditions at mesoscopic (4,000-130,000 nm^2) interfaces formed by gold islands on graphite, in excellent agreement with theory [1]. Ab initio calculations reveal that the gold-graphite interface is expected to remain largely free from contaminant molecules, leading to structurally lubric sliding. The experiments reported here demonstrate the potential for practical lubrication schemes for micro- and nano-electromechanical systems that would mainly rely on an atomic-scale structural mismatch between the slider and substrate components.

[1]: E. Cihan, S. Ipek, E. Durgun, M.Z. Baykara, Nature Communications 7, 12055 (2016).

O 93: Heterogeneous Catalysis: Experiment

Time: Thursday 15:00–17:00 Location: TRE Phy

Invited Talk O 93.1 Thu 15:00 TRE Phy

Oxygen and Oxide Cluster Functionalized Graphene for Model Catalytic Studies — •Zdenek Dohnalek — Pacific Northwest National Laboratory, Richland, WA, USA

Well-defined, monodispersed catalysts supported on oxidized carbon nanotubes and nanosheets are a promising class of new materials for heterogeneous catalysis. We have chosen graphene (Gr) supported on Ru(0001) as a surface science model and employed scanning tunneling microscopy to investigate its functionalization with oxygen atoms (AOs) and ceria and titania nanoclusters. On Ru(0001), Gr forms a Moiré structure with a periodicity of 3 nm with three distinct regions: C ring atop Ru, on HCP and FCC. At room temperature, AOs are found preferentially within the FCC regions. At 400 - 500 K, the AOs move primarily within the FCC regions or away from the metastable HCP regions. The high-resolution time-lapse data is used to assign the AO adsorption configuration to the on-top terminally-bound groups rather than the expected bridge-bonded epoxy species. For ceria and titania nanoclusters we find that they are anchored at the intrinsic defects in Gr. The thermal evolution of the cluster size distribution suggests that the sintering proceeds via diffusion and aggregation of entire clusters. To follow the cluster redox properties we examined their oxygen storage and release in an oxygen atmosphere at elevated temperature (550 - 700 K). Under oxidizing conditions, oxygen intercalation under the Gr layer is observed for ceria but not titania. Time-dependent studies demonstrate that the intercalation starts in the vicinity of the ceria clusters and extends until a completely intercalated layer is observed.

Invited Talk O 93.2 Thu 15:30 TRE Phy

Oxide model interfaces from ultrahigh vacuum conditions to liquid environments — •Jörg Libuda — Friedrich-Alexander-Universität Erlangen-Nürnberg

Oxide-based hybrid interfaces are at the heart of many functional materials: Organic films on oxides find applications in molecular electronics and solar energy conversion; metal nanoparticles on oxides are used in heterogeneous catalysis and electrocatalysis. Studies on atomically-defined model hybrid interfaces can provide detailed insights into their chemical and physical functionalities.

Model electrocatalyst are prepared by deposition of active metals on ordered oxide films. Surface science studies of such systems in UHV provide a detailed understanding of electronic metal-support interactions, reaction mechanisms and catalytic activities. Recently, we showed that UHV-born model systems may preserve their atomic structure when used as electrocatalysts in liquid environments. This allows us to explore electrocatalytic reactions at complex atomically-defined model interfaces.

Model organic-oxide hybrid interfaces are prepared by anchoring of organic molecules, e.g. porphyrines, on ordered oxide surfaces. Exemplifying anchoring reactions with carboxylates, we explore the molecular orientation, metalation and the formation kinetics. Strong structure dependencies are observed for the film stability which are rationalized on the basis of the cation arrangement at the surface. Finally, we discuss the role of water and hydroxyl groups in molecular anchoring, both under UHV conditions and in liquid environments.

O 93.3 Thu 16:00 TRE Phy

In operando study on MnOx thin films during electrocatalytic water oxidation using soft x-ray absorption and emission spectroscopy — •Maryam N. Shaker[1,2], Marc F. Tesch[1], Shannon A. Bonke[3], Alexandr Simonov[3], Leone Spiccia[3], and Emad F. Aziz[1,2] — [1]Helmholtz Zentrum Berlin — [2]Freie Universität Berlin — [3]School of Chemistry, Monash University, Clayton, VIC, 3800, Australia

Manganese oxides (MnOx) are promising candidates to act as catalysts for the water oxidation half reaction, which is mandatory to produce hydrogen from water. To systematically understand what drives the catalytic efficiency of MnOx a comprehensive knowledge about its electronic structure is necessary. A powerful tool to study the electronic structure of transitions metal oxides is soft X-ray spectroscopy. However, such studies are usually restricted to ex situ measurements unable to unambiguously identify structural and electronic changes of the material occurring at working conditions, i.e. applying a potential. Here, we present an in operando study using X-ray absorption spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS) at the Mn L-edge of electrodeposited MnOx films while applying potentials in a systematic fashion. Clear, potential dependent spectral changes related to variations in the Mn oxidation state were observed. The XAS spectra taken in operando are compared to ex situ XAS measurements and will be discussed with respect to in operando RIXS measurements revealing distinct changes in the structure of the occupied valence state, which play a key role for all catalytic reactions.

O 93.4 Thu 16:15 TRE Phy

Reactivity of quasi one-dimensional CoO_2 nanostructures on Ir(100) — Pascal Ferstl[1], M. Alif Arman[2], Jan Knudsen[2], Edvin Lundgren[2], Lutz Hammer[1], and •M. Alexander Schneider[1] — [1]Lst. f. Festkörperphysik, FAU Erlangen-Nürnberg, Germany — [2]Division of Synchrotron Radiation Research, Lund University, Sweden

In this study we analyze the catalytic properties of quasi one-dimensional CoO_2 nanostructures grown on the Ir(100) surface [1], exemplified by the oxidation of hydrogen and CO. Due to the long range order of the system before and after the reactions it was possible to quantify the structural changes by means of full dynamical LEED analyses. Combining this detailed structural information with data obtained by HR-XPS, STM and TDS we were able to follow the processes during the reactions in situ on the atomic scale.

We thus identified the relevant species during the different stages of the two oxidation reactions. Further the observed structural changes hint at the importance of defects like grain boundaries for the reaction kinetics. In summary, the cobalt oxide nanostructures enable both reactions at temperatures lowered by 150 K – 200 K compared to the oxygen covered Ir(100)-(2×1)O surface [2] and therefore show high catalytic activity.

[1] P. Ferstl, et al., Phys. Rev. Lett. **117**, 046101 (2016); [2] P. Ferstl, et al., Phys. Rev. B **93**, 235406 (2016)

O 93.5 Thu 16:30 TRE Phy

Strong Metal-Support Interaction and Catalytic Edge-Effects for Controlling Electrical Transport Edge-Effects in Nanowires — •Alex Lord[1], Philip Davies[2], Jon Evans[1], and Steve Wilks[1] — [1]Centre for Nanohealth, Institute of Life Sciences 2, Singleton Campus, Swansea University, Singleton Park, Swansea SA2 8PP, UK — [2]Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Park Place, Cardiff, CF10 3AT, United Kingdom

Semiconductor nanowires grown by techniques catalyzed with metal nanoparticles present a bottom-up solution for new technological devices. Here, I will discuss a strong metal-support interaction (SMSI) that encapsulates the Au growth particle adding material to the edge-region of the interface between the catalyst and the ZnO nanowire. The electron microscopy evidence shows the process occurs at room temperature over a long time period and in ambient benign conditions. It is shown by directly correlating atomic-resolution electron microscopy to electrical transport measurements that the nature of the SMSI-diffused ZnO material at the interface edge creates a channel affecting the quantum-mechanical tunneling electron-transport. The results are confirmed by using the enhanced catalytic activity of the Au-ZnO interface edge to etch away the ZnO at the edge-region undercutting the metal nanoparticle. The microscopy analysis and transport measurements show this removes the support edge-region and eliminates the quantum-mechanical tunneling path. This work correlates catalytic edge-effects with electrical transport edge-effects found in metal-semiconductor electrical contacts.

O 93.6 Thu 16:45 TRE Phy

Electronic properties of Au nanoparticles on CeO_2 in the water-gas shift (WGS) reaction using operando X-ray absorption spectroscopy — •Joachim Bansmann, Gabriela Kucerova, Ali Abdel-Mageed, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Small Au nanoparticles (NPs) on ceria surfaces are important catalysts in the CO oxidation and water-gas shift (WGS) reaction. The activity and deactivation during time on stream (TOS) of those catalysts strongly depends on the nature (oxidic and/or reductive) of pre-treatments. Here, we will concentrate on the oxidation state and the size of the Au nanoparticles after different pretreatments and during reaction using ex-situ characterization techniques (e.g. XPS) as well as operando methods such as XANES/EXAFS and diffuse IR spectroscopy (DRIFTS). Reductive pretreatments lead to metallic Au particles, whereas oxidic pretreatments results in partially oxidized Au NPs (depending on the temperature).

Employing operando X-ray absorption spectroscopy, we followed the changes in chemical state and size of the Au particle during the water-gas shift reaction at 180°C. The results are discussed in comparison with the activity and deactivation of these catalysts considering also effects such as blocking of active sites by formation of carbonates and formates. Finally, we compare our findings with results obtained in the CO oxidation [1] using similar Au/CeO_2 catalysts.

[1] A. Abd El-Moemen et al., J. Catal. 341 (2016) 160

O 94: Graphene: Electronic Properties, Structure and Substrate Interaction II

Time: Thursday 15:00–18:15 Location: TRE Ma

O 94.1 Thu 15:00 TRE Ma

Microscopic investigations of graphene grown on copper foil — •Philip Schädlich[1], Florian Speck[1], Julia Krone[1], Patrick Herlinger[2], Pranoti Kshirsagar[2], Martina Wanke[1], Jurgen Smet[2], and Thomas Seyller[1] — [1]Professur für Technische Physik, TU Chemnitz, Reichenhainer Straße 70, D-09126 Chemnitz, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

Graphene grown by CVD on polycrystalline copper foil is investigated by PEEM, LEEM, LEED and STM. LEED indicates that the flakes consist of rotated domains as well as twisted bilayer areas. The twist between two graphene layers grown on top of each other leads to the formation of periodic Moiré superstructures, which were observed by STM. In addition, the formation of surface facets on the copper foil gives rise to a stripe pattern in PEEM and LEEM, and a displaced LEED pattern, which can be attributed to the inclined terraces of the faceted surface by dark field LEEM. Inclination angles between facets have been determined by energy dependent LEED and are comparable with literature reports [1, 2]. AFM and STM confirm the results of the faceted surface obtained by LEEM.

[1] S. Nie, et al., New J. Phys. **14**, 093028 (2012).
[2] J. Kraus, et al., Carbon **64**, 377 (2013).

O 94.2 Thu 15:15 TRE Ma

Local electronic properties of the graphene-protected giant Rashba-split $BiAg_2$ surface — •Julia Tesch[1], Milan Jubitz[1], Elena Voloshina[2], Yuriy Dedkov[1], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Institut für Chemie, Humboldt-Universität zu Berlin, 10099 Berlin, Germany

In search of future spintronic devices, combined systems of graphene and strongly Rashba-split surfaces, such as the heavy post-transition and noble metal surface alloy $BiAg_2$, have become of particular interest.

Following a detailed discussion of the challenging yet well reproducible sample fabrication technique that allows us to fine tune the properties of the resulting system, we present a comprehensive study of the gr/$BiAg_2$ structure by means of scanning tunnelling microscopy as well as spectroscopy supported by density functional theory calculations. Besides the persistent relativistic nature of graphene charge carriers upon adsorption, we report on a downward shift of the preserved $BiAg_2$ surface state. This peculiar phenomenon can be explained by an inward relaxation of Bi atoms into the underlying thick Ag layer and thus a subsequent delocalisation of the surface state wavefunction. Despite the close proximity of the giant Rashba-split surface to graphene, no spin splitting has been observed in graphene in both experiment and theory, while the spin-texture of $BiAg_2$ remains intact protected by graphene adsorption making this system a promising candidate for spintronic applications.

O 94.3 Thu 15:30 TRE Ma

Controlling intramolecular hydrogen-transfer by electrostatic doping using gate-tunable STM — •Shai Mangel[1], Christian Dette[1], Katharina Polyudov[1], Paul Punke[1], Roberto Urcuyo[1], Marko Burghard[1], Soon Jung Jung[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, D-70569 Stuttgart — [2]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Electron transport properties can be controlled by intramolecular reactions that reshape the electronic configuration without changing the conformation. A prominent example is tautomerization, i.e. the interconversion between two isomers due to migration of hydrogen, which can be induced by STM. Several methods to control the tautomerization reaction were developed, such as depositing adatoms or using thermal and photoinduced excitation. However, those methods are usually limited in their spatial range and not always reversible. In this work, we demonstrate a global control of the electron density surrounding H_2-phthalocyanine on graphene/SiO_2/Si. By using a gate-tunable STM, we electrostatically doped the graphene substrate altering the chemical potential in the molecules surrounding, which results in up to 60% decrease of the tautomeric switching rate. This reduction is assigned to an increase in the energetic barrier of the tautomerization reaction. Understanding and controlling the electric field-effect on molecules via modification of the chemical potential of graphene is critical for designing future molecular electronic devices.

O 94.4 Thu 15:45 TRE Ma

Structure of pristine and hBN-embedded graphene quantum dots on Ir(111) — •Jiaqi Cai[1], Caio Silva[1,2], Wouter Jolie[2], Ferdinand Farwick zum Hagen[2], Christoph Schlueter[3], Tien-Lin Lee[3], and Carsten Busse[1,2] — [1]Institut für Materialphysik, Münster, Germany — [2]II. Physikalisches Institut, Köln, Germany — [3]Diamond Light Source Ltd, Didcot, United Kingdom

Nanometer-sized graphene flakes (graphene quantum dots, GQDs) provide a playground for the confinement of Dirac electrons [1]. On Ir(111), these GQDs are dome-shaped, with their edges bend towards and strongly bond to Ir surface atoms [2]. We prepare GQDs with an average size of 2 nm, and explore the details of the varying graphene-substrate interaction with the x-ray standing wave technique. We precisely measure the bond distances of the C atoms at the edges as well as in the interior of the GQDs.

In order to stabilize these graphene nanostructures and to reach a well-defined edge termination, we embedded the GQDs in hexagonal boron nitride (hBN). We investigate the structural changes caused by the embedding, especially at the graphene-hBN interface, where peculiar electronic effects, such as half-metallicity are predicted [3]. The GQDs edges remain strongly bonded to the substrate, and the interface is comprised of both N-C and B-C bonds.

[1] W. Jolie et al., Phys. Rev. B 89, 155435 (2014).
[2] P. Lacovig et al., Phys. Rev. Lett. 103, 166101 (2009).
[3] S. Dutta et al., Phys. Rev. Lett. 102, 096601 (2009).

O 94.5 Thu 16:00 TRE Ma

Investigation of Graphene using Simultaneous Scanning Tunneling/Atomic Force Microscopy — •Majid Fazeli Jadidi and Hakan Özgür Özer — Istanbul Technical University, Istanbul, Turkey

We investigated graphene layers grown on Cu foils using simultaneous Scanning Tunneling Microscopy/Atomic Force Microscopy (STM/AFM). Atomic resolution images of the surface were obtained in many channels such as STM topography, oscillation amplitude, force, tunnel barrier height and phase shift. The simultaneous acquisition of multiple channels allows us to compare images at every pixel, which in turn sheds light on the contrast mechanisms in probe microscopy. In HOPG or multilayer graphene, due to the shift between two successive layers, 3 atoms of the hexagon have an atom underneath (alpha (A) site) whereas the other 3 don't have (beta (B) site). Hence, three main atomic structures at the surface are A and B atoms and hollow sites. In STM images B atoms appear higher due to the dominance of their electronic structure over A site atoms. In the oscillation amplitude images which is a measure of the interaction stiffness[1], the brighter spots match with the A sites. The oscillation amplitude throughout the entire image is well below the free amplitude which suggests a very high positive interaction stiffness. This observation is supported also by the Force-distance spectroscopy which is simultaneously acquired with all such acquisition channels.

[1] A. Oral, R. A. Grimble, H. Ö. Özer, P. M. Hoffmann, and J. B. Pethica, Appl. Phys. Lett. 79, 1915 (2001).

O 94.6 Thu 16:15 TRE Ma

Strong electron-phonon coupling in the σ band of graphene — Federico Mazzola[1], Thomas Frederiksen[2], Thiagarajan Balasubramanian[3], Philip Hofmann[4], •Bo Hellsing[5], and Justin W. Wells[1] — [1]Department of Physics, Norwegian University of Science and Technology (NTNU), Trondheim, Norway — [2]Donostia International Physics Center (DIPC) – UPV/EHU, San Sebastián, Spain — [3]MAX IV Laboratory, Lund, Sweden — [4]Department of Physics, Aarhus University, Denmark — [5]Department of Physics, University of Gothenburg, Sweden

First-principles studies of the electron-phonon coupling in graphene predict a high coupling strength for the σ band with values of the dimensionless mass-enhancement parameter λ up to 0.9. Near the top of the σ band λ is found to be ≈ 0.7. This value is consistent with the observed kink in the σ band dispersion near the $\bar{\Gamma}$-point in the Brillion zone. The calculations show that the electron-phonon coupling is driven primarily by the optical LO and TO phonon modes in graphene. The photoemission intensity from the σ band is strongly suppressed near the $\bar{\Gamma}$-point due to sublattice interference effects. These effects are removed by taking data in the neighbouring Brioullin zone. By this we have been able to disentangle the influence of sublattice interference and electron-phonon coupling. A rigorous analysis of the experimentally determined complex self-energy further supports the assignment of the observed kink to strong electron-phonon coupling and yields $\lambda \approx 0.6$, in excellent agreement with the calculations.

O 94.7 Thu 16:30 TRE Ma

Imaging Anisotropic Carrier Dynamics in Graphene — •Sven Aeschlimann[1], Mariana Chavez-Cervantes[1], Hubertus Bromberger[1], Razvan Krause[1], Ameer Al-Temimy[2], Camilla Coletti[2], Andrea Cavalleri[1,3], and Isabella Gierz[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg, Germany — [2]Center for Nanotechnology @ NEST, Istituto Italiano di Tecnologia, Pisa, Italy — [3]Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, United Kingdom

Photo-excitation of graphene transfers electrons from the valence band to the conduction band in a direct interband transition. The initial distribution of holes and electrons is known to be anisotropic with nodes along the direction of the light polarization. We use time- and angle-resolved photoemission spectroscopy to image the initially anisotropic carrier distribution on constant energy cuts through the Dirac cone and follow its relaxation as a function of pump-probe time delay. We find that ultrafast collinear electron-electron scattering rapidly redistributes the energy among the carriers and establishes a momentum-dependent electronic temperature on time scales short compared to our experimental resolution. Momentum relaxation occurs mainly through optical phonon emission within approximately 100 femtoseconds determined from the time it takes for the electron distribution to become isotropic. Our measurements provide a complete picture of the ultrafast thermalization dynamics in photo-excited graphene.

O 94.8 Thu 16:45 TRE Ma

Quantifying electronic band interactions in van der Waals materials using angle-resolved reflected-electron spectroscopy — •Johannes Jobst[1,2], Alexander J. H. van der Torren[1], Eugene E. Krasovskii[3], Jesse Balgley[2], Cory R. Dean[2], Rudolf M. Tromp[4,1], and Sense Jan van der Molen[1] — [1]Leiden Institute of Physics, Leiden University, The Netherlands — [2]Department of Physics, Columbia University, New York, USA — [3]Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian/Donostia, Spain — [4]IBM T.J. Watson Research Center, Yorktown Heights, USA

High electron mobility is one of graphene's key properties, exploited for applications and fundamental research alike. Highest mobility values are found in heterostructures of graphene and hexagonal boron nitride, which consequently are widely used. However, surprisingly little is known about the interaction between the electronic states of these layered systems. Rather pragmatically, it is assumed that these do not couple significantly. Here we study the unoccupied band structure of graphite, boron nitride and their heterostructures using angle- resolved reflected-electron spectroscopy. We demonstrate that graphene and boron nitride bands do not interact over a wide energy range, despite their very similar dispersions. The method we use can be generally applied to study interactions in van der Waals systems, that is, artificial stacks of layered materials. With this we can quantitatively understand the 'chemistry of layers' by which novel materials are created via electronic coupling between the layers they are composed of.

O 94.9 Thu 17:00 TRE Ma

Magneto-optic effects of graphene at the carbon 1s edge on metallic substrates - theory and experiment — •Dominik Legut[1], Peter M. Oppeneer[2], Christine Jansing[3], Markus Gilbert[3], Andreas Gaupp[3], Hans-Christoph Mertins[3], Andrey Sokolov[4], Suk-Ho Choi[5], Hud Wahab[6], and Heiko Timmers[6] — [1]IT4Innovations Center, VSB-TU Ostrava, 17.listopadu 15, CZ 70833 Ostrava, Czech Republic — [2]Dept. of Physics and Astronomy, Box 530, S-751 21 Uppsala, Sweden — [3]FH Münster, Stegerwaldstr. 39, D-48565 Steinfurt, Germany — [4]HZB, Albert Einstein Str. 15, D-12489 Berlin, Germany — [5]Dept. of Applied Physics, Kyung Hee University, Korea — [6]Univ. of New South Wales Canberra, Australia

The optical properties at the carbon 1s of the free standing graphene utilizing the electronic structure models are calculated from first principles. For its better description the core-hole quasiparticle is taken into account. One can model it by the so-called Slater transition state employing the supercell calculation with partial hole on one of the carbon atoms with the electron charge distributed over the valence states. Another approach is to solve Bethe-Salpeter equations for the many-body electronic effects. The latter approach clearly identify the excitonic features of π- and σ-excitations of graphene. Next, optical response of the graphene on metallic substrate (Cu, Ni, and Co) is calculated and the degree of the hybridization between the p_z and d-states is determined, together with the identification of the magnetic moments. Next, using multilayerd optical code the T-MOKE and XMCD spectra are determined and compared with recently recorded data.

O 94.10 Thu 17:15 TRE Ma

Bottom-up synthesis of graphene nanomembranes with tunable porosity — •Christof Neumann[1], Michael Mohn[2], Matthias Füser[3], David Kaiser[1], Ute Kaiser[2], Andreas Terfort[3], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm — [3]Institute of Inorganic and Analytical Chemistry, Goethe University Frankfurt, 60348 Frankfurt

The potential of 2D materials like carbon or graphene nanomembranes [1] for separation or ultrafiltration applications is based on the unique features of these novel nanomaterials having pore sizes suitable for molecular sieving and negligible thicknesses compared to the molecular mean free paths or even below. Here we present a versatile method for tuning the properties of graphene nanomembranes by conversion of 4-(1H-pyrrol-1-yl)thiophenol, 4-(2,5-dimethyl-1H-pyrrol-1-yl)thiophenol and 4-(pyrimidin-2-yl)phenylthiol self-assembled monolayers (SAMs) on polycrystalline copper foils into carbon nanomembranes (CNMs) via electron induced crosslinking and their further pyrolytic transformation into the nanoporous graphene monolayers. We characterize the resulting SAMs, CNMs and graphene-nanomembranes by different complementary techniques including X-ray photoelectron (XPS) and Raman spectroscopy, atomic force (AFM), helium ion (HIM) and high-resolution transmission electron microscopy (HRTEM) as well as by electric transport measurements. [1] A. Turchanin and A. Gölzhäuser, Adv. Mater. 28, 5075 (2016)

O 94.11 Thu 17:30 TRE Ma

tracking electron dynamics in graphene and TMDCs —

•Cephise Cacho — Artemis - Central Laser Facility, Didcot, UK

Novel quantum materials such as graphene and transition metal dichalcogenides (TMDC) are attracting vast interest particularly for their application in spintronic and optoelectronic devices. Their properties are intrinsically governed by the large momentum electrons (at the Brillouin zone K-point). In order to eject such electrons in vacuum and observe their dynamics, a high energy (>20 eV) photon source is required as well as ultrashort pulse duration. High Harmonic Generation source [1] combined to an Angle-Resolved PhotoEmission Spectroscopy (ARPES) end-station is a powerful tool to observe such electron dynamics. After an introduction on ARPES and experimental concepts, I will present an overview of recent time-resolved ARPES studies [2-6] performed at the Artemis facility.

Single-layers of MoS2, WS2 and bulk WSe2 were resonantly pumped across the band gap at the K point. Monitoring the valence/conduction bands population reveals the band dynamics during excitation. Furthermore the intervalley scattering is explored by exciting the surface with circularly polarized light.

References 1. F. Frassetto et al., Optics Express 19, 19169 (2011) 2. E. Pomarico et al., arXiv:1607.02314 (2016) 3. A. Grubišić Čabo et al., Nano Lett. 15, 5883 (2015) 4. S. Ulstrup et al., ACS Nano 10, 6315 (2016) 5. S. Ulstrup et al., arXiv:1608.06023 (2016) 6. R. Bertoni et al., arXiv:1606.03218 (2016)

O 94.12 Thu 17:45 TRE Ma

Phase diagram of a graphene bilayer in the zero-energy Landau level — •Angelika Knothe[1,2] and Thierry Jolicoeur[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — [2]Laboratoire de Physique Théorique et Modèles Statistiques (LPTMS), Université Paris-Sud, 91405 Orsay, France

We theoretically investigate the ground state structure of bilayer graphene (BLG) in the quantum Hall regime. In BLG, the zero energy states carry, besides the real spin, two pseudospin degrees of freedom: a valley isospin and a Landau level (n = 0, n = 1) isospin. This peculiar property leads to an octet of states that is eightfold degenerate in the absence of any symmetry breaking and can be treated in the frame of quantum Hall ferromagnetism. If this SU(8) symmetry is indeed broken, an extraordinary rich phase structure emerges, with each phase characterized by a different spin and isospin configuration. Recent experiments have revealed a plethora of transitions upon variation of the strength of an applied magnetic or electric field. We start from a four-band model Hamiltonian for Bernal stacked BLG and take into account both, intrinsic symmetry breaking effects, as well as the influence of externally applied fields. Using a Hartree-Fock treatment, we study the ground state spin and isospin phases as a function of external magnetic and electric field strengths. For the different filling factors of the zero energy multiplet we predict the number of phases, as well as the nature and the properties of the respective phase transitions.

[1] Angelika Knothe and Thierry Jolicœur, arXiv:1609.04983

O 94.13 Thu 18:00 TRE Ma

Graphene-multiferroic interfaces for spintronics applications — •Zeila Zanolli — Institute for Theoretical Solid State Physics, RWTH Aachen University and ETSF, D-52056 Aachen, Germany.

Graphene and magnetoelectric multiferroics are promising materials for spintronic devices with high performance and low energy consumption. A very long spin diffusion length and high carrier mobility make graphene attractive for spintronics. The coupling between ferroelectricity and magnetism, which characterises magnetoelectrics, opens the way towards unique device architectures. In this work[1], we combine the features of both materials by investigating the interface between graphene and BaMnO$_3$, a magnetoelectric multiferroic. We show that electron charge is transferred across the interface and magnetization is induced in the graphene sheet due to the strong interaction between C and Mn. Depending on the relative orientation of graphene and BaMnO$_3$, a quasi-half-metal or a magnetic semiconductor can be obtained. A remarkably large proximity induced spin splitting of the Dirac cones (∼300 meV) is achieved. We also show how doping with acceptors can make the high-mobility region of the electronic bands experimentally accessible. This suggests a series of possible applications in spintronics (e.g. spin filters, spin injectors) for hybrid organic-multiferroic materials and reveals hybrid organic-multiferroics as a new class of materials that may exhibit exotic phenomena such as the quantum anomalous Hall effect and a Rashba spin-orbit induced topological gap.

[1] Z. Zanolli, Scientific Reports, 6, 31346 (2016)

O 95: Metal Substrates: Adsorption of Atoms and Inorganic Molecules

Time: Thursday 15:00–18:15 Location: WIL A317

Invited Talk O 95.1 Thu 15:00 WIL A317

Visualizing surface X-ray diffraction: the active phase of CO oxidation model catalysts — •Johan Gustafson — Synchrotron Radiation Research, Lund University, Lund, Sweden

Surface X-Day Diffraction (SXRD) is a very powerful surface characterization tool, especially for in-situ investigations. As a diffraction tool, it is closely related to Low-Energy Electron Diffraction (LEED), but is much less used due to the need for intense synchrotrons and the complexity to record and interpret the diffraction data.

The use of large 2D detectors provide the means to facilitate both the collection and the interpretation of the data. As a larger part of reciprocal space is probed simultaneously, larger datasets can be aqcuired in realistic time frames, which enables a more comprehensible visualization of the data, similar to a LEED-pattern. In addition, significantly more information can be obtained from time-resolved measurements.

We have used SXRD with 2D detectors to establish the most active phase of Pd(100) and Rh(111) during catalytic CO oxidation, a subject that has been under debate for about 15 years. In contrast to what is often assumed, these model catalysts behave quite differently, and while the most active phase of rhodium is metallic, for Pd it is a thin oxide film. Some of the conclusions we draw would not have been possible without 2D detectors.

O 95.2 Thu 15:30 WIL A317

Site-specific adsorption of heavy-metal atoms on corrugated graphene: A challenge for first-principles theory — •Georg S. Michelitsch and Karsten Reuter — Technische Universität München

Single, heavy-metal atoms are an appealing ultimate unit in the quest for an ever more miniaturized information storage. Adsorption on corrugated single-layer graphene could thereby protect the magnetic encoding and act as a template for self-assembly. Quantitative first-principles calculations would be a much desired source for independent insight into the geometric, electronic and magnetic properties of such systems. Unfortunately, they are challenged by the prerequisite to accurately describe the localized spin structure on the heavy-metal adsorbate simultaneously with the Moiré superstructure of the extended support. To this end we present systematic density-functional theory (DFT) calculations addressing the adsorption of Dy atoms on corrugated graphene. We compare treatments on the screened hybrid functional with the Hubbard-corrected (DFT+U) level, and discuss approaches to reach electronic self-consistency in this delicate system. The calculations reveal intricate consequenes of minor changes in electronic level alignment and state occupation on the preferred adsorption site. This calls for judicious choice and scrutiny of the employed U value in the numerically more efficient DFT+U approach.

O 95.3 Thu 15:45 WIL A317

Adsorption on PtRu surface alloys and stepped surface: A computational study — •David Mahlberg[1], Julia M. Fischer[2], Sung Sakong[1], Tanglaw Roman[1], Jürgen Behm[1], and Axel Gross[1] — [1]Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany — [2]Australian Institute for Bioengineering and Nanotechnology, TheUniversity of Queensland, St Lucia, QLD 4072, Australia

Bimetallic surface alloys offer the possibility to tailor their reactivity through modifying their composition and/or structure. We have performed a computational study based on density functional theory adressing the adsorption of water on PtRu/Pt(111) surface alloys [1] and the hydrogen adsorption on Pt monolayer islands on Ru(0001) and on stepped Ru(10$\bar{1}$9) surfaces decorated with atomic Pt rows.

We discuss the reactivity of bimetallic alloys using the concept of the ligand and geometric strain effects. It turns out that the Ru atoms interact more strongly than Pt with the adsorbed water molecules thus influences the adsorption geometries of both water monomers and ice-like water layers. The results with respect to hydrogen adsorption indicate that the influence of the surface imperfections on the adsorption properties extends up to two atomic rows away from the edges and steps, in good agreement with recent temperature programmed desorption and spectroscopy experiments [2].
[1] J.M. Fischer, D. Mahlberg, T. Roman, and Axel Groß, Proc. R. Soc. A **472**, 20160618 (2016). [2] H. Hartmann, T. Diemant, J. Bansmann, and R. J. Behm, PCCP **14**, 10919 (2012)

O 95.4 Thu 16:00 WIL A317

DFT study of water at the stoichiometric and defected Fe(110) surfaces — •Tomasz Ossowski[1], Juarez L.F. Da Silva[1,2], and Adam Kiejna[1] — [1]Institute of Experimental Physics, University of Wrocław, Poland — [2]Instituto de Química de São Carlos, Universidade de São Paulo, Brazil

Water adsorption on iron surfaces is important in understanding of corrosion and reduction of iron oxides by hydrogen. Density functional theory (DFT) with van der Waals correction is applied to study molecular water adsorption on stoichiometric and defected Fe(110) surfaces. Structural and electronic properties of the H_2O/Fe(110) system, and a role of the vacancies are analysed. Results show that vacancy prefers sites at the topmost atomic layer, without energy barrier for its diffusion from the interior. The vacancies cause decreasing of the work function and local change the geometry with larger effects for higher vacancy density. At stoichiometric surface water adsorbs flat on top the Fe atoms with the H-O-H plane parallel to the surface, with binding energy of about 0.3 eV/molecule. Moreover, the adsorption energy of flat lying water is degenerated for few different orientation. It suggests possibility of H_2O rotation around direction perpendicular to the surface. At the defected surface, H_2O prefers sites near the vacancy. The binding of water to defected surface is by more than 0.2 eV stronger than to the stoichiometric one. Moreover, the adsorption of H_2O at stoichiometric region of the defected surface is by about 0.2 eV less preferable. It means that water is stronger bound to defected Fe(110) surface and vacancy can be considered as an adsorption centre for H_2O.

O 95.5 Thu 16:15 WIL A317

Transition Metal Complexes as Functional Units on Metal Surfaces - Structure, Properties and Reactivity from Density Functional Theory — •Wolfgang Hieringer — Theoretical Chemistry, University of Erlangen-Nürnberg

Transition metal coordination compounds adsorbed on metal surfaces have received increasing attention in recent years. Not only do they appear as intermediates in on-surface synthesis schemes, e.g. in Ullman coupling reactions, but they may also serve as linking units in the formation of nanostructured networks and coordination polymers, as catalytic centers, or as functional units that tune the electronic properties of the surface. Transition metal complexes also play a central role as precursors in coating processes such as atomic layer deposition. I will present results from density functional theory calculations which aim at a better understanding of the basic properties and reactivity of transition metal complexes adsorbed on metal surfaces. We had shown before that the direct, coordinative interaction of the metal substrate with an adsorbed coordination compound can strongly alter the electronic properties of the central metal. In this contribution, I will discuss how the chemical bond between an adsorbed transition metal center and coordinating ligands can be influenced by the presence of a metal surface. I will analyze the electronic structure of the adsorbed complexes in terms of molecule-substrate charge transfer effects and hybridization of the molecular states with the surface.

O 95.6 Thu 16:30 WIL A317

LT-STM study of the structural and electronic properties of triazatruxene molecules on Ag(111) — •Anja Bauer[1], Florian Singer[1], Philipp Erler[1], Markus Maier[2], Rainer Winter[2], Yuriy Dedkov[1], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Fachbereich Chemie, Universität Konstanz, 78457 Konstanz, Germany

The opportunity of tuning the electrical and spin dependent properties of molecules is of great interest since this could enable the fabrication of molecule-based functional devices. Besides the stabilization and controlled manipulation of the charge and spin states, it is important to learn about the structural properties like the adsorption geometry and the orientation of the molecules on different substrates.
We investigated triazatruxene (TAT) molecules on Ag(111) by low temperature scanning tunneling microscopy (STM) and spectroscopy (STS). Coverages up to one monolayer (ML) were deposited by means of electrospray ionization (ESI) in ultra high vacuum. Sub-monolayer coverages feature the molecules lying flat on the Ag(111) surface with characteristic distances in between them and exhibiting three different types of appearances, possibly due to the interaction with the substrate. By further increasing the coverage they grow in highly ordered structures depending on the density of TAT molecules. STS and time resolved current measurements at individual molecules reveal characteristic excitations beyond a certain threshold energy showing a telegraph noise behaviour with the period depending both on the voltage and the current.

O 95.7 Thu 16:45 WIL A317

Zn on Au(111) - Surface alloy formation and interaction with Oxygen — •Konstantin M. Schüttler and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Methanol is a promising molecule for chemical energy storage, e.g., when using H_2 from renewable sources for its synthesis. Au/ZnO was found to be a highly active catalyst for the synthesis of "Green Methanol" from CO_2/H_2 as a "Solar Fuel", suitable also for the specific operation conditions resulting from that application[1]. Previously, CuZn alloys have been used as model systems for the industrially used Cu/ZnO catalysts[2]. For Au/ZnO this approach is similarly plausible.
In order to gain more insight into the formation and nature of active sites, the formation, structure, electronic and chemical properties of bimetallic Zn/Au(111) surfaces serving as structurally well-defined 2D model catalysts were studied. The reactivity of Zn surface atoms, which may be crucial for the catalytic performance of ZnO supported MeOH synthesis catalysts, was studied by exposing Zn/Au(111) to oxygen. Also, the influence of temperature on Zn growth behavior was studied both by varying the Zn deposition temperature and by subsequent annealing. Resulting consequences of these findings on the structure of realistic Au/ZnO catalysts are discussed.
[1] Y. Hartadi et al., ChemSusChem 8 (2015), 456
[2] J. Nakamura et al., Catal. Lett. 31 (1995), 325

O 95.8 Thu 17:00 WIL A317

Oxidation of the Zr(0001) Surface — Peter Lackner[1], Wen Ma[2], Bilge Yildiz[2], Ulrike Diebold[1], and •Michael Schmid[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Dept. of Nuclear Science & Engineering, Massachusetts Institute of Technology, USA

The first stages of oxidation of Zr(0001) were studied by scanning tunneling microscopy (STM) and x-ray photoelectron spectroscopy (XPS). Dosing oxygen at room-temperature does not lead to ordered structures. Upon annealing to $\approx 550\,^\circ\mathrm{C}$, we observe two types of ordered phases. The first one shows a hexagonal lattice with an in-plane lattice parameter of 331 pm, significantly smaller than bulklike $ZrO_2(111)$ (≈ 361 pm) and the ultrathin $ZrO_2(111)$ films obtained by oxidation of Zr alloys (≈ 350 pm, Refs. [1,2]). The second phase exhibits a moiré structure perfectly fitting a $ZrO_2(100)$ lattice on the Zr substrate. Previous studies of ultrathin ZrO_2 films created by reactive deposition of Zr [3] and oxidation of Zr alloys [1,2] have always resulted in the non-polar $ZrO_2(111)$ orientation, which has the lowest surface energy [4]. To our knowledge, this is the first atomic-scale observation of a $ZrO_2(100)$ surface, opening new possibilities for studying this technologically important material.
[1] Antlanger et al., Phys. Rev. B 86, 035451 (2012).
[2] Choi et al., J. Phys.: Condens. Matter 26, 225003 (2014).
[3] Meinel et al., Phys. Rev. B 74, 235444 (2006) and Refs. therein.
[4] Christensen & Carter, Phys. Rev. B 58, 8050 (1998).

O 95.9 Thu 17:15 WIL A317

The chemical properties of PtCu/Ru(0001) monolayer surface alloys — •Thomas Diemant and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, Albert-Einstein-Allee 47, D-89081 Ulm

Bimetallic catalysts are well known for their unusual catalytic properties, which often excel those of the respective individual components with respect to activity, selectivity or long term stability. Studies of the adsorption / reaction properties of bimetallic model surfaces with defined structure and composition can contribute significantly to an improved understanding of the microscopic origin of this effect.

We studied the chemical properties of structurally well-defined CuPt monolayer surface alloys by temperature programmed desorption (TPD) and IR measurements using CO as probe molecule. These surface alloys were created by sequential deposition of Cu and Pt on a Ru(0001) surface; their structural properties were clarified already before by our group using scanning tunnelling microscopy (STM) with chemical contrast [1]. We studied the change of the chemical properties (CO adsorption) of the alloy layers as a function of the alloy composition. We will correlate our findings to the results of structural characterization and compare to a previous study of similar type on the CO adsorption on PdCu/Ru(0001) monolayer surface alloys [2].

[1] A. Engstfeld et al., Surf. Sci. 643 (2016) 65. [2] T. Hager et al., Surf. Sci. 558 (2004) 181.

O 95.10 Thu 17:30 WIL A317

Crystallographic Structure of the Oxidized Rh(100) Surface — •Tilman Kisslinger, Pascal Ferstl, M. Alexander Schneider, and Lutz Hammer — Lehrstuhl für Festkörperphysik, Universität Erlangen–Nürnberg, D–91058 Erlangen, Germany

In this study we combine quantitative LEED–IV, STM and DFT calculations to reinvestigate the adsorption behavior of oxygen on the Rh(100) surface in the coverage regime up to 0.67 ML.
In this range three distinct phases exist: A (2×2)–O [1], a (2×2)–2O [2] and a (3×1)–2O structure [3]. The proposed models of these phases are verified by low R–factors between 0.07 and 0.10. For the (2×2)–O phase we corroborate the hollow site adsorption with additional 13 parameters determined. In case of the (2×2)–2O structure the clockwise-/ anticlockwise reconstruction of the substrate is confirmed. However, contrary to [2] our LEED analysis correctly accounts for all symmetry elements observed in experiment. It turned out that this does not change the structural parameters significantly, but alters the interpretation of the underlying physical processes. Instead of statistically disordered domains a statistical occupation of adjacent threefold coordinated sites by oxygen is the result of our structure determination ($R_P = 0.098$). Regarding the (3×1)–2O phase the proposed model by Gustafson *et al.* is validated with structural parameters similar to those of the $Pt_{75}Rh_{25}(100)$–(3×1)–2O structure [4].
[1]: Oed *et al.*, Surf. Sci. **207**, 55 (1988) [2]: Baraldi *et al.*, Phys. Rev. Let. **82**, 4874 (1999) [3]: Gustafson *et al.*, J. Phys. Cond. Mat. **24**, 225006 (2012) [4]: Sporn *et al.*, Surf. Sci. **416**, 384 (1998)

O 95.11 Thu 17:45 WIL A317

Solvation in molecularly thin water films and their growth — •Barbara A J Lechner[1,2], Sabine Maier[3], Youngsoon Kim[4], Heon Kang[4], and Miquel Salmeron[1] — [1]Materials Sciences Division, Lawrence Berkeley Lab, Berkeley, CA — [2]Department of Chemistry, Technical University of Munich — [3]Department of Physics, Friedrich-Alexander University of Erlangen-Nürnberg — [4]Department of Chemistry, Seoul National University, Seoul, Korea

The first water layer on hexagonal single crystal surfaces typically forms rotated hexagons, pentagons and heptagons of molecules in addition to strongly bound hexagonal rings commensurate with the substrate. Furthermore, the water monolayer does not expose any dangling hydrogen bonds in a vacuum environment. The growth of the entropically favorable proton-disordered ice, however, requires flipping some of the molecules in the first layer to expose dangling bonds. Using scanning tunneling microscopy (STM) we studied this transition from the first layer to water multilayers on Pt(111) and Ru(0001). We observed that a second layer initially forms an amorphous structure when grown on the crystalline monolayer. To facilitate the growth of ice in a bulk-like hexagonal arrangement, the first wetting layer needs to rearrange into a purely hexagonal structure commensurate with the surface. Ammonia (NH3) molecules can adsorb to certain water molecules in the monolayer on Pt(111), specifically those that are slightly elevated from the surface and weakly bound to the metal. Ammonia molecules thus detect locations in the wetting layer where a water molecule can change its orientation relatively easily to flip up a hydrogen atom.

O 95.12 Thu 18:00 WIL A317

Field emission microscopy study of nonlinear dynamics during NO2 hydrogenation — •Cédric Barroo[1], Yannick De Decker[1], Pierre Gaspard[1], Norbert Kruse[1], and Thierry Visart de Bocarmé[2] — [1]Universiteé libre de Bruxelles, Brussels, Belgium — [2]Washington State University, Pullman WA, USA

Field emission microscopy (FEM) is a technique that enables to probe reactions and their dynamics at the scale of a single nanoparticle. This study reports on the observation and analysis of various nonlinear behaviors during the catalytic hydrogenation of NO2 on Pt. A tip-sample is used to study reactions during the ongoing reactive processes and down to 10nm2. By changing a control parameter, it is possible to observe different behaviors, among which self-sustained periodic oscillations, and to determine the type of bifurcation leading to the emergence of the oscillations. In the case of periodic oscillations, the robustness is quantified via Fourier transform and temporal autocorrelation functions analyses. We also show how the dynamical attractor and the phase space dynamics can be reconstructed from experimental time series, and we prove that the periodic oscillations can be linked to a limit cycle. Experiments at high temporal resolutions show the presence of propagating processes at the surface of the catalyst, and the propagation of chemical waves on a single facet of the nanocrystal is also observed. These waves take the form of target patterns with a velocity in the order of a few μm/s, in good agreement with previous studies of catalytic reactions at the mesoscale. The experiments prove the robustness of nonlinear behaviors down to the nanoscale.

O 96: Metallic Nanowires on Semiconductor Surfaces

Time: Thursday 15:00–17:45 Location: WIL C107

O 96.1 Thu 15:00 WIL C107

Femtosecond electronic response of photo-excited in situ grown Indium wires — •Mariana Chavez-Cervantes[1], Sven Aeschlimann[1], Hubertus Bromberger[1], Razvan Krause[1], Andrea Cavalleri[1,2], and Isabella Gierz[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, United Kingdom

Strong electronic correlations in one-dimensional wires lead to a metal-to-insulator transition at low temperatures. The low-temperature insulating phase is characterized by a complex order parameter with amplitude (size of the band gap) and phase. Photo-doping with femtosecond laser pulses excites carriers across the band gap and leads to an instantaneous reduction of the amplitude of the order parameter followed by amplitude and possibly phase oscillations. We have grown one-dimensional indium wires in situ on a Si(111) substrate and characterized them with low-energy electron diffraction (LEED) and angle-resolved photoemission spectroscopy (ARPES). At room temperature the system exhibits three one-dimensional metallic bands that undergo a complex metal-to-insulator transition at T=110K. We excited the indium wires with intense femtosecond pulses at 1.5eV and probed the response of the electronic structure with time-resolved ARPES at extreme ultraviolet wavelengths. We analyze the dynamics of the complex order parameter and the energy-dependence of the photo-excited population life time.

O 96.2 Thu 15:15 WIL C107

Ginzburg-Landau-Langevin theory for the phase transition in In/Si(111) — •Yasemin Ergün and Eric Jeckelmann — Appelstraße 2, 30167 Hannover

We investigate thermal fluctuations and collective excitations in quasi-one-dimensional charge-density-wave systems using the Ginzburg-Landau (GL) theory. Starting from a microscopic Su-Schrieffer-Heeger-like model for In/Si(111), we generalized the GL theory for grand canonical Peierls transitions. The equilibrium properties and the non-equilibrium dynamics are simulated using the Langevin approach. We calculated the phonon spectrum for the Landau-Langevin theory. We discuss our theoretical results in relation to doping and spectroscopy experiments for In/Si(111). Extending this approach for local fluctuations within a two-dimensional Ginzburg-Landau-Langevin is computationally expensive. We developed a frequency filter for smoothing fluctuations included in the linear response spectrum by finite simulation size and time. Support from the DFG through the Research Unit FOR 1700 is gratefully acknowledged.

O 96.3 Thu 15:30 WIL C107

Pinning of topological solitons at extrinsic defects in a quasi one-dimensional charge density wave — •Samad Razzaq[1], Stefan Wippermann[1], Taehwan Kim[2], and Hanwoong Yeom[2] — [1]Max Planck Inst fuer Eisenforschung GmbH — [2]IBS Center for Artificial Low Dimensional Electronic Systems , University of Pohang

Quasi one-dimensional (1D) electronic systems are known to exhibit exotic physical phenomena, such as, e.g., Jahn Teller distortions, charge density wave (CDW) formation and non-Fermi liquid behavior. Solitonic excitations of the charge density wave ordered ground state and associated topological edge states in atomic wires are presently the focus of increasing attention. We carried out a combined ab initio and scanning tunneling microscopy (STM) study of solitonic and non-solitonic phase defects in the In/Si(111) atomic wire array. While free solitons move too fast to be imaged directly in STM, they can become trapped at extrinsic defects within the wire. We discuss the detailed atomistic structure of the responsible extrinsic defects and trapped solitons. Our study highlights the key role of coupled theory-experimental investigations in order to understand also the elusive fast moving solitons. S. W. gratefully acknowledges financial support from the German Research Foundation (DFG), grant No. FOR1700.

O 96.4 Thu 15:45 WIL C107

Ultrafast Peierls Transition in In/Si(111) Nanowires Probed by trARPES — •C. W. Nicholson[1], A. Lücke[2], M. Puppin[1], L. Rettig[1], R. Ernstorfer[1], W. Gero Schmidt[2], and M. Wolf[1] — [1]Fritz-Haber-Institut, Berlin — [2]Universität Paderborn

Quasi-1D metals on semiconducting substrates, of which In/Si(111) is one of the most interesting and intensively studied systems, promise not only novel 1D physics, but also control over electronic properties and dimensionality. In/Si(111) undergoes a structural transition from a (4x1) to an (8x2) unit cell at around 120 K, concomitant with a metal-to-insulator transition. A recent combined DFT and Raman study [1] points strongly to a Peierls-like scenario, whereby a combination of shear and rotary distortions leads to the opening of band gaps at specific points in the band structure.

Here we investigate the momentum resolved changes of the electronic structure during the ultrafast photoinduced Peierls transition using high-harmonic-driven trARPES with 50 fs time resolution. Starting from the (8x2) phase, we track the evolution of states both above and below the Fermi level following pulsed excitation and observe the transition from (8x2) to (4x1) phases on a 500 fs time scale. By comparison to complementary DFT calculations we analyse the contributions from the expected shear and rotary distortions to the transient electronic band structure. The observation of coherent phonon oscillations at 2.4 THz provides further insights into the many-body interactions in the system.

[1] E. Jeckelmann et al. Phys. Rev. B, 93, 241407(R) (2016)

O 96.5 Thu 16:00 WIL C107

Tuning of 1D Plasmon properties on Si(hhk)-Au by adsorbates — •Zamin Mamiyev, Timo Lichtenstein, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany

Gold-induced atomic wires on Si(hhk) surfaces possess intriguing properties of collective electron excitations which are strongly responsive to the electronic state and also to structural motifs. The modification and control of plasmonic excitations in metallic nanowires are of particular interest due to their fundamental and technological importance. In this work, the effect of O$_2$ and H$_2$ adsorption on the plasmons in arrays of single [Si(557)-Au] and double chains of gold [Si(553)-Au] have been examined by Electron Energy Loss Spectroscopy with high resolution both in energy and momentum. Theoretical results show that oxygen and hydrogen atoms bind preferably not to the Au chains directly, but to adjacent Si-honeycomb chains (Si-HC) and Si-adatom rows (The latter exist only in Si(557)-Au). The Si-HC turns out to be mostly responsible for the plasmonic changes. While atomic H reduces the plasmon frequency on Si(553)-Au, as predicted theoretically, adsorbed oxygen leaves it unchanged, whereas a frequency increase is found to be induced by oxygen in Si(557)-Au, indicating an enhanced electron density in the partially filled surface band(s). Comparing the oxygen results on Si(553)-Au and Si(557)-Au, both the structural motifs (double vs. single chain), as well as electronic distribution across the terraces play a role. These effects still need further detailed consideration in order to separate them clearly.

O 96.6 Thu 16:15 WIL C107

Analysis of the electronic and atomic structure of Pb/Si(557) by polarization dependent two-photon photoemission — •Abdul Samad Syed[1], Vesna Miksic-Trontl[1], Manuel Ligges[1], Ping Zhou[1], Herbert Pfnür[2], Christoph Tegenkamp[2], and Uwe Bovensiepen[1] — [1]Universität Duisburg-Essen, Fakultät für Physik und Zentrum für Nanointegration (Cenide), 47048 Duisburg — [2]Leibniz-Universität Hannover, Institut für Festkörperphysik, Appelstrasse 2, 30167 Hannover

The local structure of atomic wires Pb/Si(557) is determined (i) by the macroscopic quasi one dimensional symmetry imposed by the vicinal cut substrate and (ii) local arrangement of Pb atoms on the Si terraces. We analyze the electronic structure by angle-resolved two-photon photoemission (2PPE) as a function of light polarization and find a dichroism in the 2PPE intensity for opposite electron momenta along the terraces k_x and $-k_x$. Considering earlier work [1] on Pb/Si(111) which concluded on the coexistence of the H3 and T4 symmetry in the $\sqrt{3}\times\sqrt{3}$ reconstruction, the observed polarization dependent dichroism suggests a combination of three and six fold symmetry of the Pb arrangement on Si(557) in agreement with a compressed structure along the Si terrace.

Funding by the DFG through FOR 1700 is gratefully acknowledged.

[1] A. Baumann, E. Speiser, S. Chandola, J. Räthel, P. Kratzer, S. Sakong, C. Tegenkamp, N. Esser (2016).

O 96.7 Thu 16:30 WIL C107

Spin correlations in the Si(553)-Au nanowire system — •Bernd Hafke[1], Tim Frigge[1], Tobias Witte[1], Boris Krenzer[1], Julian Aulbach[2], Ralph Claessen[2], Jörg Schäfer[2], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — [2]Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), 97074 Würzburg

Deposition of 0.5 ML Au on Si(553) at 650 °C results in the formation of Au double-strand chains per Si terrace with a twofold periodicity along the wire. These metallic wires are structurally terminated by Si step edge atoms, which exhibit a three-fold periodicity of half-filled dangling bonds of the Si atoms along the steps. Theory predicts an antiferromagnetic spin ordering of every third Si step edge atom [1]. The long-range interaction of the two-fold and three-fold periodicity is investigated by spot-profile analysis in LEED at a sample temperature of 80 K. The strict two-fold periodicity of the Au atoms is not correlated between adjacent wires as concluded from the streak like intensity in LEED. In contrast, the threefold ordering of the Si spins exhibit a clear ordering perpendicular to the Au wires. A modification of the structure model [2] explains the structural correlation between adjacent Si step edge atoms. The resulting frustrated structure indicates the formation of a 2D spin-liquid in this system [2].

[1] S. C. Erwin and F. J. Himpsel, Nature Commun. **1**, 58 (2010).

[2] B. Hafke, *et al.* PRB **94**, 161403(R) (2016).

O 96.8 Thu 16:45 WIL C107

The electronic structure of rare earth silicide nanowires on Si(001) — •Stephan Appelfeller, Martin Franz, Hans-Ferdinand Jirschik, and Mario Dähne — Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin

Trivalent rare earths are known to form silicide nanowires on Si(001). Based on the chemical similarity of the rare earths and the similar appearance of the nanowires in scanning tunneling microscopy, it is generally assumed that the nanowires have the same atomic structure for all rare earths. On the other hand, angle resolved photoemission spectroscopy (ARPES) studies of Gd and Dy silicide nanowires disagree with each other in the observed band structure, even though both studies indicate an one-dimensional dispersion [1,2]. Here, we report on ARPES experiments on Y and Tb silicide nanowires. Their electronic structure is quasi-one-dimensional, showing only small oscillations of the Fermi contours. Furthermore, the disagreement in the literature data is resolved by the observation of strong matrix element effects in our data, in which all the bands described in the literature are observed indicating that the nanowires have the same electronic properties and, consequently, also the same atomic structure.

This work was supported by the DFG (FOR1700, project E2). We kindly acknowledge the support of K. Horn and coworkers, C. Papp, and of BESSY II (HZB Berlin), where the photoemission experiments were carried out at the beamline UE56/2 PGM-1.

[1] H. W. Yeom et al., Phys. Rev. Lett. **95**, 205504 (2005).
[2] M. Wanke et al., Phys. Rev. B **83**, 205417 (2011).

O 96.9 Thu 17:00 WIL C107

Strain induced quasi-one dimensional structure of rare earth silicides on Si substrates — Frederic Timmer[1], Robert Oelke[1], Christof Dues[2], Simone Sanna[2], Wolf Gero Schmidt[2], Martin Franz[3], Stephan Appelfeller[3], Mario Dähne[3], and •Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Germany — [2]Lehrstuhl für Theoretische Physik, Universität Paderborn, Germany — [3]Institut für Festkörperphysik, Technische Universität Berlin, Germany

One dimensional (1D) systems have attracted a lot of attention since their physical properties are distinctively different from structures of higher dimensionality. Recently, a new class of quasi-1D systems based on rare earth silicides has attracted attention. Here, we report on combined studies on quasi-1D structures by scanning tunneling microscopy (STM), spot profile analysis of low-energy electron diffraction (SPA-LEED) and density functional theory (DFT).

Depositing rare earth elements as Dy or Tb at elevated temperature on Si(111), a $2\sqrt{3} \times \sqrt{3}$ superstructure is observed. This structure is attributed to the formation of periodically arranged Si vacancies in different silicide layers. The complex structure of this superstructure with buckled surface layer, $\sqrt{3} \times \sqrt{3}$ superstructure in the first subsurface layer $2\sqrt{3} \times \sqrt{3}$ superstructure in the second subsurface layer can only be analyzed applying the different techniques used here. The anisotropic character of this structure is emphasized by the formation of periodically arranged domain boundaries. The width of the silicide domains formed in two domains is roughly two unit cells.

O 96.10 Thu 17:15 WIL C107

Infrared Spectroscopy of Charge Carrier Excitation in Metallic Nanowires on the Atomic Scale — Annemarie Pucci and •Fabian Hötzel — Kirchhoff Institute for Physics, Heidelberg University, Germany

Atomic chains, as for example gold superstructures on vicinal silicon surfaces, may show infrared resonances that can be attributed to plasmonic excitations in nanowires of a finite length of the order of 100 nm. The appearance of the resonances clearly indicates the metallic character of the atomic chains. The quantitative analysis of the spectral weight and the resonance position yields the data on the nanowire conductivity and complementary information on the electronic band structure. Conductivity changes upon doping can be directly seen in the infrared spectra. Furthermore, as we have recently found out, the plasmonic resonances are sensitive to the changes of the polarization of the silicon step edges with temperature.

O 96.11 Thu 17:30 WIL C107

Functionalization of Si(553)-Au surface with hydrogen and small organic molecules — •Julian Plaickner[1], Sandhya Chandola[1], Eugen Speiser[1], Svetlana Suchkova[1], Norbert Esser[1], and Simone Sanna[2] — [1]Schwarzschildstrasse 8, 12489 Berlin — [2]Warburger Str. 100, 33098 Paderborn

Atomic metallic chains deposited on vicinal Si substrates form templates for the growth of hybrid molecule-solid nanostructures. The advantage of these structures is the possibility to vary the substrate geometry and the metallic element. We investigate the adsorption of toluene-3,4-dithiol molecules on hydrogen-passivated Si(553)-Au surfaces as model system/process. Hydrogen is able to drive a reversible metal-insulator transition on the Si(553)-Au surface and is also changing the adsorption geometry of organic molecules, extending the functionalization possibilities of the surface in organic electronics and biosensing.

We are using a set of polarization-sensitive optical techniques, such as Raman Spectroscopy (RS), Reflection Anisotropy Spectroscopy (RAS) and Infrared Spectroscopic Ellipsometry (IRSE). Our approach consists in establishing a direct connection between optical spectra and surface structure via ab-initio calculations. Optical fingerprints allow us to gain information on structural and electronic properties of the system.

The plan for the future is the realization of highly ordered molecular array geometries and the understanding of charge transfer between molecules and atomic wires. This will open possibilities for further functionalization through modification of terminal groups of molecules.

O 97: Nanostructures at Surfaces: Molecular Systems II

Time: Thursday 15:00–18:30 Location: REC/PHY C213

Invited Talk O 97.1 Thu 15:00 REC/PHY C213

The challenge of atomic resolution in liquid and ambient conditions with AFM — •Alfred J. Weymouth — University of Regensburg, Germany

Since the invention of the atomic force microscope, there has been substantial drive to image in ambient and liquid environments. One challenge in these environments is atomic resolution. Keeping surfaces clean in vacuum, combined with cryogenic temperatures to lower both the instrumental noise and thermal drift, makes force microscopy easier. We have had great success with stiff sensors and frequency-modulation AFM. With these techniques, we are returning to the challenge of imaging samples in device- and biologically-relevant conditions.

We demonstrated atomic resolution with the qPlus sensor on KBr [1], and followed this with investigations on graphitic surfaces [2]. In order to better understand our data of HOPG we conducted a parallel investigation in UHV. We have also started to study biological samples: Working with Daniel Müller's group, we imaged a protein membrane in a liquid drop. More recently, we have imaged mica with atomic resolution in a liquid cell in a variety of solutions.

[1] Wastl et. al., Phys. Rev. B, 87, 245415 (2013)
[2] Wastl et. al., ACS Nano, 8, 5233 (2014)

Invited Talk O 97.2 Thu 15:30 REC/PHY C213

Single-molecule magnets: The influence of the surface — •Katharina Diller — Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

A prerequisite for using magnetic nanostructures in data storage applications is magnetic remanence, i.e., magnetization after removal of an external magnetic field. Single-molecule magnets are metal-organic compounds which (below a certain blocking temperature) possess this property. However, the interaction with the environment often leads to fast relaxation of the magnetization, a problem especially prevalent for single-molecule magnets adsorbed on metal supports. Using the example of terbium phthalocyanine double decker ($TbPc_2$) molecules we will discuss the influence of the surface on the magnetic and electronic properties of the adsorbates. The $TbPc_2$ molecules are either deposited by molecular beam epitaxy onto the substrate of choice or are directly created by on-surface metallation, which allows us to selectively probe different scenarios. Using a combination of scanning tunnelling microscopy and X-ray absorption spectroscopy, we show how different decoupling layers enhance the magnetic remanence of $TbPc_2$ and discuss which other factors influence the system.

O 97.3 Thu 16:00 REC/PHY C213

Self-assembly of cyano and pyridil functionalized molecules on epitaxial h-BN and metal supports — •Domenik M. Zimmermann[1], Knud Seufert[1], Jiri Klivar[2], Gael Amans[2], Irena G. Stará[2], Ivo Starý[2], Luka Dordević[3], Tomas Marangoni[3], Davide Bonifazi[3], Johannes V. Barth[1], and Willi Auwärter[1] — [1]E20, Technische Universität München, Germany — [2]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Czech Republic — [3]Department of Chemical and Pharmaceutical Sciences, University of Trieste, Italy

Functionality at the nanoscale is based on both, intrinsic properties of the basic building blocks like molecules or atoms and their modification due to interaction with the environment.

One such building block is helicene, an ortho-condensed polycyclic aromatic compound. Di-cyano, di-benzo functionalized helicenes feature a large in-plane dipole moment, favoring the formation of 1D chains along the high symmetry directions of a Ag(111) surface. In contrast the molecules assemble into large two-dimensional islands upon adsorption on h-BN/Cu(111). Another example is pyrene. Pyridil functionalized derivatives have shown distinct self-assembled structures, including arrays and kagome heterostructures[1]. On h-

BN/Cu(111) these architectures can be electronically decoupled. Scanning tunneling spectroscopy is used to address their electronic properties to pave the way for potential optoelectronic applications.

[1] T. Kaposi et al., ACS Nano 10, 7665 (2016).

O 97.4 Thu 16:15 REC/PHY C213

A comparative temperature-programmed XPS study of surface-assisted Ullmann coupling on Au(111) vs. Ag(111) — •Massimo Fritton[1,2], David Duncan[1], Peter Deimel[1], Atena Rastgoo Lahrood[1,2], Francesco Allegretti[1], Wolfgang M. Heckl[1,2,3], and Markus Lackinger[1,2,3] — [1]Departement of Physics, TU München, James-Franck-Str. 1 — [2]Center for NanoScience (CeNS), Schellingstr. 4 — [3]Deutsches Museum, Museumsinsel 1

The intention of our study is to compare the kinetics of thermally activated Ullmann coupling of 1,3,5-Tris(4-bromophenyl)benzene on Au(111) vs. more reactive Ag(111) under ultrahigh vacuum conditions. Two aspects are studied here: activation by cleavage of halogen substituents as well as formation and conversion of reaction intermediates, i.e. organometallic networks. Therefore, we use temperature-programmed XPS (TP-XPS) in combination with STM. TP-XPS allows us to track the progression of dehalogenation, vs. temperature while heating due to chemical shifts of the Br 3d line. On Ag(111) debromination starts at 250 K and is completed at 300 K, while on Au(111) the dehalogenation occurs at higher temperature and over a more extended temperature range between 330 K and 460 K. STM images on both surfaces endorse the spectroscopic data. On Ag(111) the organometallic intermediates can easily be distinguished by the increased bond length and a bright feature corresponding to the C-Ag-C linkages. In contrast on Au(111) annealing directly leads to the covalent network formation.

O 97.5 Thu 16:30 REC/PHY C213

Host-guest chemistry in carbonyl functionalized pores of covalent structures on Au(111) — •Yi Liu[1], Christian Steiner[1], Maximilian Ammon[1], Natalie Hammer[2], Julian Gebhardt[3], Andreas Görling[3], Milan Kivala[2], and Sabine Maier[1] — [1]Department of Physics, University of Erlangen-Nürnberg, Erlangen, Germany — [2]Chair of Organic Chemistry I, Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Erlangen, Germany — [3]Chair of Theoretical Chemistry, Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Erlangen, Germany

Host-guest chemistry in nanoporous supramolecular networks physisorbed on solid surfaces is a rapidly expanding field owing to potential applications in separation technology, catalysis, and sensor devices. However, most structures rely on non-covalent interaction forces, which results in a lack of thermal stability and weak intermolecular transport.

We report on the host-guest interaction between atoms and molecules with carbonyl-functionalized pores in covalent networks. The covalent structures are obtained by on-surface synthesis of halogen-substituted carbonyl-bridged triphenylamines on Au(111). The templating effect of the pores was investigated by low-temperature scanning tunneling microscopy in combination with density-functional theory. We found that trimesic acid and halogen atoms can be trapped at specific sites in the pores through hydrogen bonds or van der Waals interaction, respectively. Interestingly, we observed that iodine-iodine interactions are preferred over iodine-carbonyl interactions.

O 97.6 Thu 16:45 REC/PHY C213

Electronic structure of one- and two-dimensional polymers fabricated in a hierarchical on-surface synthesis on Au(111) — Christian Steiner[1], Maximilian Ammon[1], Zechao Yang[1], Julian Gebhardt[2], Alexander Heidenreich[3], Natalie Hammer[3], Andreas Görling[2], Milan Kivala[3], and •Sabine Maier[1] — [1]Department of Physics, University of Erlangen-Nürnberg, Erlangen, Germany — [2]Chair of Theoretical Chemistry, Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Erlangen, Germany — [3]Chair of Organic Chemistry I, Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Erlangen, Germany

The fabrication of nanostructures in a bottom-up approach from specific molecular precursors offers the opportunity to create tailored materials for applications in nanoelectronics. However, the formation of defect-free 2D covalent networks remains a challenge and makes it difficult to unveil their electronic structure.

Here, we report on the hierarchical on-surface synthesis of nearly defect-free 1D and 2D covalent architectures on Au(111), which were investigated by low-temperature scanning tunneling microscopy in combination with density-functional theory. The carbonyl-bridged triphenylamine precursors formed six-membered macrocycles and 1D chains as intermediates in a Ullmann-type coupling reaction that were subsequently interlinked to 2D networks. We observed a reduction of the electronic band gap from the monomer to the 1D and 2D structures. The significant drop of the gap from the monomer to the polymer confirms an effective conjugation along the building blocks.

O 97.7 Thu 17:00 REC/PHY C213

Growth of Tm-based organometallic nanostructures on Gr/Ir(111) — •Stefan Kraus[1], Felix Huttmann[1], Nico Rothenbach[2], Katharina Ollefs[2], Lucas M. Arruda[3], Wolfgang Kuch[3], Heiko Wende[2], and Thomas Michely[1] — [1]Universität zu Köln, Germany — [2]Universität Duisburg-Essen, Germany — [3]Freie Universität Berlin, Germany

Organometallic compounds containing rare earth elements are of interest in molecular spintronics owing to the robust magnetic moment of the $4f$ ion. Here, we combine the lanthanide Tm with the organic molecule cyclooctatetraene (Cot) for the growth of organometallic nanostructures on Gr/Ir(111), obtaining three distinct phases (1)–(3). Synthesis on the undoped substrate yields (1) a disperse phase of repulsively interacting adsorbates. Based on its punctiform appearance it is presumed to consist of TmCot monomers which are stabilized by charge transfer into the substrate leading to a Coulomb repulsion between them. When surpassing a coverage of about 2% ML, (2) an island-forming “coffee bean” phase condenses out of (1) and coexists with it. Formation of (1) and (2) is inhibited by n doping of graphene via intercalation as further charge transfer is suppressed. Rather, synthesis on the doped substrate results in the formation of (3) sandwich-molecular wires growing in islands. Tuning the Tm/Cot ratio during growth controlls the achievable wire length, in some islands exceeding 100 Tm ions per wire. Magnetic anisotropy from the action of the Cot ligand field on the Tm ion and the differing Tm separations in each phase are expected to yield a rich spectrum of magnetic properties.

O 97.8 Thu 17:15 REC/PHY C213

Trimethylsilyl protected alkyne precursors on metal surfaces — •Liding Zhang[1], Yi-Qi Zhang[1], Zhi Chen[2], Mateusz Paszkiewicz[1], Tao Lin[1], Mario Ruben[2], Johannes Barth[1], and Florian Klappenberger[1] — [1]TU München, Physik E20, Garching, Deutschland — [2]Karsruher Institut für Technologie, Institute of Nanotechnology, Eggenstein-Leopoldshafen, Deutschland

We report on the application of trimethylsilyl(TMS) terminated alkyne precursors for opening new pathways for fabricating novel 1-D and 2-D carbon nano- materials on metal surfaces.

The commonly employed organic molecular beam epitaxy limits the weight of employed precursors as with increased weight, the temperature for evaporation can rise above the temperature required for intermolecular reactions. The chemical inertness of TMS protection groups inhibits intermolecular reactions and thus allows the evaporation of larger and heavier alkyne precursors.

All utilized TMS-protected alkyne precursors were successfully evaporated onto Cu, Au and Ag surfaces. Investigations with low temperature STM imaging show dense packed self-assembled supramolecular islands. Thermal annealing triggers TMS group cleave off and a subsequent two step reaction pathway reminiscent of on-surface Glaser coupling, allowing the formation of covalently bonded structures with varying degrees of structural regularity.

O 97.9 Thu 17:30 REC/PHY C213

Trimethylsilyl protected alkyne precursors on metal surfaces — •Liding Zhang[1], Yi-Qi Zhang[1], Zhi Chen[2], Mateusz Paszkiewicz[1], Tao Lin[1], Mario Ruben[2], Johannes Barth[1], and Florian Klappenberger[1] — [1]TU München, Physik E20, Garching, Deutschland — [2]Karsruher Institut für Technologie, Institute of Nanotechnology, Eggenstein-Leopoldshafen, Deutschland

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All utilized TMS-protected alkyne precursors were successfully evaporated onto Cu, Au and Ag surfaces. Investigations with low temperature STM imaging show dense packed self-assembled supramolecular islands. Thermal annealing shows TMS groups exhibiting different levels of inertness on different metal surfaces and triggers TMS group cleave off and a subsequent two step reaction pathway reminiscent of on-surface Glaser coupling, allowing the formation of covalently bonded structures with varying degrees of structural regularity.

O 97.10 Thu 17:45 REC/PHY C213

Solution-free synthesis of diboronic acid-derived COF monolayers on surfaces — •Saskia Spitzer[1,2], Atena Rastgoo[1,2], Viktoria Ritter[1,2], Wolfgang Heckl[1,2,3], and Markus Lackinger[1,2,3] — [1]Department of Physics, Tech. Univ. Munich, James-Franck-Str. 1, 85748 Garching — [2]Center for NanoScience (CeNS), Schellingstr. 4, 80799 Munich — [3]Deutsches Museum, Museumsinsel 1, 80538 Munich

Currently, surface-supported highly stable two-dimensional covalent organic frameworks (COF) with the highest structural qualities are achieved through condensation reactions as boronic acid dehydration. [1,2] The presence of water during the polymerization as equilibrium regulating agent induces bond reversibility. We combined this established approach with the merits of a solvent-free monomer deposition from the vapor phase. Thermal sublimation of larger diboronic acid monomers, due to their high reactivity, required an additional protection-deprotection-approach. The resulting networks were characterized on different length scales by a combination of light microscopy and Scanning Tunneling Microscopy, thus verifying the preparation protocol.

[1] J. F. Dienstmaier et al., ACS Nano, 5, 9737-9745 (2011)

[2] C. Z. Guan et al., Chem. Commun., 48, 2943-2945 (2012)

O 97.11 Thu 18:00 REC/PHY C213

The role of intrinsic vs. extrinsic adatoms for the formation of metal-organic structures from triphenylenehexamine: A comparative STM study on Ag(111) vs. Cu (111) — •Matthias Lischka[1], Renhao Dong[2], Massimo Fritton[1], Wolfgang M. Heckl[1,3], Xinliang Feng[2], and Markus Lackinger[1,3] — [1]Department of Physics, TU München, James-Franck-Str. 1, 85748 Garching — [2]Department of Chemistry and Food Chemistry, and Center for Advancing Electronics TU Dresden, 01062 Dresden — [3]Deutsches Museum, Museumsinsel 1, 80538 München

The thermally activated formation of metal-organic structures of triphenylenehexamine (THA) is comparatively studied on Ag(111) and Cu(111) under ultra high vacuum conditions. The structural characterization of each phase is carried out by high resulotion scanning tunneling microscopy. On both pristine surfaces THA is initially partly deprotonated and directly forms metal-organic structures. On Ag(111) densely packed structures were observed, whereas on Cu(111) Cu-adatom coordinated hexamers were found. Upon progressive heating on Ag(111) no further structural change was observed until the desorption of THA. On Cu(111), however, further heating drives deprotonation of THA and results in a conversion of the Cu-adatom coordinated hexamers into trimers. A profound change was found on Ag(111) after additional deposition of Ni-atoms: moderate heating leads to porous networks that collapse into a more densely packed structure after annealing at higher temperatures.

O 97.12 Thu 18:15 REC/PHY C213

On-surface indene-formation by methyl bromide cleavage — •Frank Eisenhut[1], Dmitry Skidin[1], Justus Krüger[1], Thomas Lehmann[1], Andreas Viertel[2], Seddigheh Nikkipar[1], Dmitry A. Ryndyk[1], Stefan Hecht[2], Francesca Moresco[1], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science, Max Bergmann Center of Biomaterials, and Center for Advancing Electronics Dresden, TU Dresden, 01069 Dresden, Germany, — [2]Department of Chemistry & IRIS Adlershof, Humboldt-Universität zu Berlin, Brook-Taylor-Straße 2, 12489 Berlin, Germany, — [3]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01069 Dresden, Germany.

Manufacturing molecules with predefined structural and electronic properties is one of the central tasks in surface science nowadays. We investigate the thermal induced cyclization of dibromo-diphenyl-pyrene on Au(111) using scanning tunneling microscopy (STM) and spectroscopy.

We show that precursor molecules self-assemble on Au(111) and form by annealing intermediate structures assembled in characteristic dimers or tetramers. By further annealing the surface, we can cleave methyl bromide groups and synthetize diindeno-pyrene molecules, as shown by high resolution STM images and dI/dV maps of the electronic orbitals. Density functional theory (DFT) and electron scattering quantum chemistry (ESQC) calculations confirm the experimental results.

O 98: Nanostructures at Surfaces: 1D Systems

Time: Thursday 15:00–16:00 Location: WIL C307

Invited Talk O 98.1 Thu 15:00 WIL C307

Spin-charge transport phenomena on the atomic scale — •Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

Low dimensional metallic structures, e.g. quantum wires and films on surfaces, reveal fascinating phenomena of condensed matter physics. Among others, 2D-superconductvity, formation of charge density waves and topologically protected edge states were realized lately with atomic precision and directly probed by electronic transport. Generally, the surface science approach benefits from the fact that the low dimensional systems can be comprehensively characterized and manipulated in view of their atomic structure and electronic bands. This is a prerequisite to understand electronic transport on the atomic scale. In this talk I will introduce the technique of surface sensitive transport and highlight some recent examples of our group from seemingly different fields, e.g. spintronic, correlated materials and mesoscopic physics. Besides epitaxial Bi-semimetal films with magnetic impurities the talk covers spin-orbit density wave driven metal-insulator transitions in Pb-wires as well as ballistic transmittance of electrons in graphene nanostructures.

Invited Talk O 98.2 Thu 15:30 WIL C307

Electronic properties of functional organic materials at surfaces — •Petra Tegeder — Ruprecht-Karls-Universität Heidelberg, Physikalisch-Chemisches Institut

For improvement and optimization of the performance of organic molecule-based devices, comprehensive insight into the physical and chemical properties of the organic material at surfaces is necessary.

I will present two case studies in which we investigated the electronic properties of organic/inorganic hybrid systems, namely graphene nanoribbons (GNRs) on gold surfaces and photochromic molecular switches on silicon. The GNRs are generated using a bottom-up approach based on a thermally activated and surface-assisted reaction of suitable precursor molecules. We studied the effect of N-doping on the energy level alignment. Additionally, we identified excitonic states in GNRs on gold surfaces. Incorporating photochromic molecules into organic/inorganic hybrid materials can lead to photoresponsive systems. In such systems, the second-order nonlinear optical (NLO) properties can be controlled via external stimulation with light at an appropriate wavelength, which we could demonstrate.

O 99: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VII

Time: Thursday 16:00–18:30 Location: GER 38

Invited Talk O 99.1 Thu 16:00 GER 38
Spectacular success of DFT in predicting novel topological phases — •Arun Bansil — Northeastern Univ, Boston USA

The revolutionary discovery of topological insulators has turned out to be the proverbial tip of the much larger iceberg of exotic phases of quantum matter driven by spin-orbit coupling effects. The consideration of electronic states protected by time-reversal, crystalline and particle-hole symmetries has led to the prediction of many novel materials that can support Weyl, Dirac and Majorana fermions, and to new types of topological crystalline and Kondo insulators, and quantum spin Hall insulators with large band gaps. The first-principles DFT-based band theory paradigm has been a key player not only in this discovery process but also in identifying salient characteristics of topological states, enabling direct and sharpened confrontation between theory and experiment. [1] I will discuss our recent theoretical work aimed at predicting topological materials and identify cases where the materials have been realized successfully. [2-10] I will also comment on the potential of topological materials as next generation platforms for manipulating spin and charge transport and other applications.

[1] Bansil, Lin and Das, Rev. Mod. Phys. 88, 021004 (2016). [2] Chang et al, Sci. Adv. 2, e1600295 (2016). [3] Huang et al., PNAS 113, 1180 (2016). [4] Zheng et al., ACS Nano 10, 1378 (2016). [5] Xu et al., Science 349, 613 (2015). [6] Zeljkovic et al., Nat. Mat. 14, 318 (2015). [7] He et al., Nat. Mat. 14, 577 (2015). [8] Xu et al., Nat. Phys. 11, 748 (2015). [9] Crisostomo et al., Nano Lett. 15, 6568 (2015). [10] Xu et al., Sci. Adv. 1, e1501092 (2015).

O 99.2 Thu 16:30 GER 38
Interlayer excitons and Band Alignment in MoS_2/hBN/WSe_2 van der Waals Heterostructures — •Simone Latini — Technical University of Denmark, Copenhagen, Denmark

Van der Waals Heterostructures (vdWHs) are a unique platform for the realization of novel (opto)-electronic devices with embedded multifunctionality. Combining two-dimensional (2D) semiconductors with misaligned band edges can lead to the formation of photo-excited electrons and holes localized in distinct layers, which result into interlayer excitons. Understanding the energetics behind the formation of interlayer excitons is the first step towards the engineering of charge separation processes in photovoltaic devices and photodetectors. The contribution of our work is then twofold. (I) We calculate, for the first time, the interlayer exciton binding energies in complex vdWHs, specifically MoS_2/hBN/WSe_2 heterostructures, using a first-principles approach. The binding energy is of extreme technological importance as it is a measure of how strongly the electron-hole pair is bound and hence how easily it can be separated. (II) We obtain accurate electronic band edges at the interface between the layers of the vdWHs, a task which could not yet be accomplished with any available state of the art technique. Importantly, the accuracy of our calculated exciton binding energies and band edges is confirmed by a striking agreement with experimental data on photoluminesce of interlayer excitons in MoS_2/hBN/WSe_2 heterostructures.

O 99.3 Thu 16:45 GER 38
Trionic effects in graphene nanoribbons and further nanomaterials — •Thorsten Deilmann and Kristian Sommer Thygesen — Center for Atomic-Scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Among low-dimensional materials armchair-edged graphene nanoribbons are very promising candidates with optical properties which are dominates by excitons. In the presence of additional charges, trions (i.e. charged excitons) can occur in the optical spectrum. With our recently developed first-principle many-body approach [1], we predict strongly bound trions in nanoribbons with decreasing binding energies of 660 to 140 meV for widths of 3.6 to 14.6 Å. We determine their optical spectra and identify several trions by their real-space wave functions.
[1] Phys. Rev. Lett. **116**, 196084.

O 99.4 Thu 17:00 GER 38
Interface Structure Prediction using the Ab Initio Random Structure Searching Method — •Georg Schusteritsch and Chris Pickard — Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, U.K.

First-principles structure prediction of bulk materials is now routinely performed, however the field of predicting the atomic structure of interfaces is still in its infancy. A detailed understanding of and ability to predict the atomic structure of interfaces is however of crucial importance for many technologies. Interfaces are very hard to predict due to the complicated geometries, crystal orientations and possible non-stoichiometric conditions involved and provide a major challenge to structure prediction. We present here the ab initio random structure searching (AIRSS) method and how it can be used to predict the structure of interfaces. Our method relies on generating random structures in the vicinity of the interface and relaxing them within the framework of density functional theory. The method is simple, requiring only a small set of parameters, and can be efficiently run on modern parallel computer architectures. We focus here on the prediction of grain boundaries, but application to heterostructure interfaces is straightforward. Examples for several grain boundary defects in technologically important materials will be presented: In particular grain boundaries in graphene, the prototypical two-dimensional material will be discussed, alongside with examples of grain boundaries in transition metal oxides, such as SrTiO3 and TiO2.

O 99.5 Thu 17:15 GER 38
Predicting new materials and their properties with supercomputers: the example of perovskites — •Silvana Botti[1] and Miguel A.L. Marques[2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Can new materials with optimized properties be designed using supercomputers?

I will try to convince you through the example of the search of new perovskites that first-principles calculations can efficiently speed up the discovery of new materials.

Theoretical approaches based and going beyond density functional theory ally today accuracy and efficiency, and are therefore suitable tools for understanding the physics not only of simple perfect crystals, but also of nanostructured materials, doped semiconductors, interfaces, alloys, etc. As a result, ab initio simulations of spectroscopic properties can finally account for the complexity of "real" experimental samples, allowing accurate comparison of calculated and measured structural and excitation properties. The powerful combination of theoretical spectroscopy with high-throughput calculations, structural prediction and machine learning can therefore provide a precious guide to experimentalists in the search of new materials.

O 99.6 Thu 17:30 GER 38
Spectral property prediction with artificial neural networks — •Annika Stuke[1], Milica Todorovic[1], Kunal Ghosh[2], Aki Vehtari[2], and Patrick Rinke[1] — [1]Department of Applied Physics, Aalto University, Finland — [2]Helsinki Institute of Information Technology, Department of Computer Science, Aalto University, Finland

The ability to efficiently design new and advanced optoelectronic materials is hampered by the lack of suitable methods to rapidly and accurately identify yet-to-be-synthesized materials that meet a desired application. To overcome such design challenges, a machine learning model based on a deep multi-task artificial neural network (ANN) is presented that can predict spectral properties of small organic molecules. The ANN is trained and validated on data generated by accurate state-of-the art quantum chemistry computations for diverse subsets of the GDB-13 and GDB-17 datasets [1,2]. The molecules are represented by a simple, easily attainable numerical description based on nuclear charges and cartesian coordinates and are mapped onto multiple excited-state properties simultaneously using a deep ANN trained by gradient descent and error backpropagation [3]. This on-demand prediction model can be used to infer spectral properties of various candidate molecules in an early screening stage for new optoelectronic materials at negligible computational cost, thereby completely bypassing conventional laborious approaches towards materials discovery.

[1] L. C. Blum et al., J. Am. Chem. Soc. 2009, 131, 8732, [2] R. Ramakrishnan et al., Scientific Data 2014, 1, 140022, [3] G. Montavon et al., New J. Phys. 2013, 15, 095003

O 99.7 Thu 17:45 GER 38

Machine-Learning Based Interatomic Potential for Amorphous Carbon — •Volker Deringer and Gábor Csányi — University of Cambridge, Cambridge, UK

Machine-learning based interatomic potentials are currently of growing interest in the solid-state theory communities, as they enable materials simulations with close-to DFT accuracy but at much lower computational cost. Here, we present such an interatomic Gaussian approximation potential (GAP) model for liquid and amorphous carbon. We first discuss the maximum accuracy that any finite-range potential can achieve in carbon structures; then, we show how a hierarchical set of two-, three-, and many-body structural descriptors can be used to fit a GAP that indeed reaches the target accuracy. The new potential yields accurate energetic and structural properties over a wide range of densities; it also correctly captures the structure of the liquid phases, at variance with state-of-the-art empirical potentials. Exemplary applications to surfaces of "diamond-like" tetrahedral amorphous carbon (ta-C) will be presented, including simulations of high-temperature surface reconstructions ("graphitization"). The method appears to be promising for realistic and accurate simulations of nanoscale amorphous carbon structures.

O 99.8 Thu 18:00 GER 38

High-throughput computational search for new high mobility transparent (semi)conducting materials — •Geoffroy Hautier[1], Joel Varley[2], Anna Miglio[1], David Waroquiers[1], Viet-Anh Ha[1], and Gian-Marco Rignanese[1] — [1]Université catholique de Louvain, Louvain-la-Neuve, Belgium — [2]Lawrence Livermore National Laboratory

Transparent conducting oxides (TCMs) are large band gap materials (to favor transparency) doped with electrons (n-type) or holes (p-type). TCMs are essential to many technologies from solar cell to transparent electronics and there is currently a large effort towards the discovery of new TCMs. I will present the results of a high-throughput computational search for new TCMs especially directed at p-type materials. Focusing on low effective masses (leading to high mobility), large band gaps and dopability, I will show how thousands of compounds can be screened using various ab initio techniques (from density functional theory to GW) to find new potential high performance TCMs. I will discuss several unsuspected compounds with promising electronic structures and when available link our findings to experimental results. Beyond the description of those novel TCM candidates, I will chemically rationalize our findings, highlighting several design strategies towards the development of future high mobility TCMs.

O 99.9 Thu 18:15 GER 38

Cross-validation in the cluster expansion method — •Axel Hübner, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

The cluster expansion technique allows the construction of model Hamiltonians for an efficient evaluation of the total energy of alloys. This technique relies on a fit to a small set of *ab-initio* calculations for selected atomic configurations. Key aspects to maximize the predictive performance of the model are the selection of a set of basis functions, i.e. clusters, and of configurations. To achieve this, the cross-validation technique is typically used [1]. In this work, an analytical formula for the calculation of the leave-many-out cross-validation score (CV) is derived. This formula exhibits numerical instabilities, whose analytical properties yield a criterion for structure selection in cluster expansions. Moreover, a relation between the noise in the data and the CV is outlined. This leads to a tool which allows us to estimate, for a given noise level, the size of the ab-initio data set upon which no improvements of the model are obtained. These results are exemplified for a cluster expansion of the thermoelectric clathrate alloy $Ba_8Al_xSi_{46-x}$, calculated with the `CELL` package [2].

[1] A. van d. Walle *et al.*, Journal of Phase Equilibria 23 (2002), Aug., Nr. 4

[2] M. Troppenz *et al.*, submitted (2016); S. Rigamonti *et al.*, in preparation.

O 100: Electronic Structure of Surfaces: Spectroscopy, Surface States II

Time: Thursday 16:00–18:30 Location: WIL C307

O 100.1 Thu 16:00 WIL C307

Existence of Topological Nontrivial Surface States in Strained Transition Metals: W, Ta, Mo, and Nb — Danny Thonig[1], Tomáš Rauch[2], Hossein Mirhosseini[3], •Jürgen Henk[2], Ingrid Mertig[2,3], Henry Wortelen[4], Bernd Engelkamp[4], Anke B. Schmidt[4], and Markus Donath[4] — [1]University Uppsala, Sweden — [2]Martin Luther University Halle-Wittenberg — [3]Max Planck Institute of Microstructure Physics, Halle — [4]Westfälische Wilhelms-Universität, Münster

We show that a series of transition metals with strained body-centered cubic lattice—W, Ta, Nb, and Mo—hosts surface states that are topologically protected by mirror symmetry and, thus, exhibits nonzero topological invariants. These findings, reported in [1], extend the class of topologically nontrivial systems by topological crystalline transition metals. The investigation is based on calculations of the electronic structures and of topological invariants. The signatures of a Dirac-type surface state in W(110), e. g., the linear dispersion and the spin texture, are verified. To further support our prediction, we investigate Ta(110) both theoretically and experimentally by spin-resolved inverse photoemission: unoccupied topologically nontrivial surface states are observed.

[1] D. Thonig *et al.*, Phys. Rev. B **94** (2016) 155132.

O 100.2 Thu 16:15 WIL C307

Asymmetric Rashba band topology of Fe films — •Sanjoy Kr Mahatha[1], Paolo Moras[1], Gustav Bihlmayer[2], Polina M Sheverdyaeva[1], and Carlo Carbone[1] — [1]Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, 34149 Trieste, Italy — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The control and manipulation of the electron spin in a two-dimensional system without the need to apply an external magnetic field is a key topic in condensed matter research aiming at future spintronic devices. In this regard, heterostructures where heavy metal and ferromagnetic layers brought in contact, are attracting increasing interest since the Rashba effect and exchange interaction can together control the electron transport. Electronic spin bands in ferromagnetic metal exhibit exchange energy splitting, while the Rashba spin-orbit effect shifts the spin-polarized bands in k||. The combination of these effects has been realized at the interface of a Fe thin film grown on a W(110) substrate. We find an asymmetry in the band dispersion of Fe quantum well states along structurally equivalent directions, resulting from exchange and spin-orbit effects at the interface and propagating in the whole film.

O 100.3 Thu 16:30 WIL C307

One and two-photon photoemission from the giant Rashba system Bi/Ag(111) — •Philipp Rosenzweig, Sebastian Otto, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Time- and angle-resolved, mono- and bichromatic two-photon photoemission (2PPE) with different photon energies $h\nu$ ranging from 1.51 eV to 4.89 eV is used to study the electronic structure of the $(\sqrt{3}\times\sqrt{3})R30^\circ$ substitutional surface alloy Bi/Ag(111). Various unoccupied band structure features are found, such as a surface state dispersing downwards from around 1.1 eV above the Fermi level as well as two image-potential states with binding energies of 0.69 eV and 0.18 eV. The spin-split sp_z surface state [1] is also identified as an initial state in 2PPE and in one-photon photoemission at $h\nu = 6.2\,\mathrm{eV}$. In addition, circular dichroism is employed as an indirect probe of the unconventional spin structure [2] of this giant Rashba system.

[1] C. R. Ast et al., Phys. Rev. Lett. **98**, 186807 (2007).

[2] S. N. P. Wissing et al., Phys. Rev. Lett. **113**, 116402 (2014).

O 100.4 Thu 16:45 WIL C307

Multiple Dirac cones at the surface of the topological metal LaBi — •Jayita Nayak[1], Shu-Chun Wu[1], Nitesh Kumar[1], Chandra Shekhar[1], Sanjay Singh[1], Jörg Fink[1,2], Emile E. D. Rienks[2,3], Gerhard H. Fecher[1], Stuart S. P. Parkin[4], Binghai Yan[1,5], and Claudia Felser[1] — [1]Max Planck Institut CPFS, Dresden, Germany — [2]Leibniz Institut fur Festkorper- und Werkstoffforschung IFW Dresden, Dresden, Germany — [3]Institute of Solid State Physics, Dresden University of Technology, Dresden, Germany — [4]Max Planck Institute for Microstructure Physics, Halle, Germany — [5]Max Planck Institute for Physics of Complex Systems, Dresden, Germany

The rare-earth monopnictide LaBi, LaSb exhibits very large, unusual magnetoresistance which stimulates the interest in directly observing any topological surface states. Although band inversions have been postulated to induce a topological phase in LaBi but there were no experimental evidence for topological surface states in this compound. By using angle-resolved photoemission spectroscopy (ARPES) and ab initio calculations, we have revealed the existence of topological surface states of LaBi through the observation of three Dirac cones: two coexist at the corners and one appears at the center of the Brillouin zone. The odd number of surface Dirac cones is a direct proof of the topological nature of LaBi compound. Our results afford insight of the topological surface states of LaBi and semi-metallicity and related magneto-transport properties.

O 100.5 Thu 17:00 WIL C307

Reconstruction-induced trefoil knot Fermi contour of Au(111) — •Maciej Dendzik, Marco Bianchi, Matteo Michiardi, Charlotte Sanders, and Philip Hofmann — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark

Using angle-resolved photoemission spectroscopy (ARPES), we study the effect of the so-called herringbone reconstruction of Au(111) on the dispersion of the free electron-like surface state [1]. While earlier ARPES investigations have only reported a minor interplay of the surface state dispersion and the underlying reconstruction, we show that the uniaxial lattice distortion and the thereby changed reciprocal lattice for the first atomic layer leads to distinct surface state dispersions around the first order reciprocal lattice points of the three domains, creating a constant energy surface resembling a trefoil knot. The findings resolve the long-standing discrepancy between, on one hand, the reconstruction-induced surface state modifications reported in scanning tunnelling microscopy and first principle calculations and, on the other hand, their conspicuous absence in photoemission.

[1] M. Dendzik *et al.*, Phys. Rev. B (Rapid Communication) **94**, 201401 (2016).

O 100.6 Thu 17:15 WIL C307

Strain–induced surface state shift on Ag(111) and Ag/Fe(110) — •Schmitt Martin, Kemmer Jeannette, and Bode Matthias — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The surface electronic properties of both, pristine Ag(111) as well as Ag films grown on various substrates, are well studied. Especially the spectroscopic fingerprint of the *L*-gap Shockley-type surface state (SS) is commonly used for calibration purposes. While the SS onset is energetically located at $E_{\mathrm{SS}} = -65\,\mathrm{meV}$ on pristine Ag(111), a depopulation was observed on strongly miscut Ag(111) crystals [1]. Furthermore, thin Ag films grown on Si(111) indicated that the SS onset may also be influenced by strain that occurs around dislocation lines [2,3].

We have investigated in the electronic properties of Ag(111) around screw dislocations found on a pristine single crystal by low temperature scanning tunneling spectroscopy. While the expected electronic properties are confirmed on terraces, strain–induced spatial variations of the SS onset are observed at certain locations around screw dislocations. The structure–electronic property relationship identified on Ag(111) will be used to qualitatively explain the SS pinning of the Ag/Fe(110) epitaxial system.

[1] K. Morgenstern *et al.*, Phys. Rev. Lett. **89**, 226801 (2002).
[2] Neuhold and Horn, Phys. Rev. Lett. **78**, 1327 (1997).
[3] K. Sawa *et al.*, Phys. Rev. Lett. **104**, 016806 (2010).

O 100.7 Thu 17:30 WIL C307

Manipulation of two-dimensional states at the XTiO$_3$ surface (X=Sr, Ba, Ca) — •Stefan Muff[1,2], Mauro Fanciulli[1,2], Nicolas Pilet[2], Andrew Weber[1,2], Zoran Ristic[2], Zhiming Wang[2], Nicholas Plumb[2], Milan Radovic[2,3], and Hugo Dil[1,2] — [1]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland — [2]Swiss Light Source, Paul Scherrer Institut, Switzerland — [3]SwissFEL, Paul Scherrer Institut, Switzerland

The discovery of a two dimensional electron gas (2DEG) at the surfaces of clean SrTiO$_3$ and KTaO$_3$ triggered research into possibilities to manipulate its characteristics in a controlled manner, using the wide range of physical properties as ferroelectricity, superconductivity, and giant magneto resistance observed in this class of materials. A more direct way to influence the properties of the 2DEG is by chemical or lattice strain and by changes of the atomic structure of the sample surface. In this work we grow films of different perovskites by the help of pulsed laser deposition and studied the formation and properties of the 2DEG by UV ARPES.

We will show the existence of two dimensional states at the surface of of BaTiO$_3$ and CaTiO$_3$ films, whose properties are closely related, but different, to the states present on SrTiO$_3$ and KTaO$_3$. The growth of films with variable thicknesses and combinations of different perovskites, as well as the variation of surface geometry, gives us the ability to directly manipulate the properties of the two-dimensional as well as the three dimensional surface-related states.

O 100.8 Thu 17:45 WIL C307

Quantum well states and their coupling to phonons in thin multilayer Pb films on Si(111) — •Maedeh Zahedifar and Peter Kratzer — University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

The relaxation of electrons in metals far away from equilibrium constitutes a field of research that has attracted considerable attention recently. Moreover, thin metallic films on semiconductor substrates lend themselves to the study of quantum size effects in metals. In our work, we attempt to develop a sound basis for the investigation of electronic relaxation processes in atomically thin Pb layers by working with the $\sqrt{3}\times\sqrt{3}$ model for film thicknesses between 3 and 6 ML. Density functional theory calculations with the projector augmented-wave method using the software package VASP [1] are employed to obtain both the electronic and the phononic two-dimensional band structure of these films. Subsequently, the strength of the electronic-phonon coupling is investigated for some representative (either occupied or unoccupied) quantum well states in the four-layer and five-layer Pb films. The results are compared to experimental data of the energetic position, dispersion and lifetime broadening of quantum well states.

[1]G. Kresse and D. Joubert, Phys. Rev. B, 59, (1999).

O 100.9 Thu 18:00 WIL C307

Double photoemission of Pb in its normal state — Yuri Aliaev, Ilya Kostanovskiy, Jürgen Kirschner, and •Frank O. Schumann — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

We investigated double photomemission (DPE) from a polycrystalline Pb surface at room temperature. The valence consists of 6s and 6p states which are separated by an energy gap of 3.1 eV. This allows to investigate the electron-electron interaction of states with different orbital symmetry without hybridisation. The low-lying 5d core levels can be excited with a laboratory light source. Hence, core-valence-valence Auger-Photoelectron coincidences can be detected. The measured DPE intensity is dominated by the emission of 5d photoelectrons and the resulting Auger electron. The Auger electron line shape has mainly contributions due the 6p electrons rather than 6s electrons. From the sum energy spectra we find that the effective Coulomb interaction U_{eff} is to close to zero. The DPE intensity directly from the valence band is an order of magnitude smaller than the core-assisted emission. This is consistent with the small value of U_{eff}.[1,2] We discuss the experimental prospect of Cooper pair emission upon photon absorption which has been predicted theoretically.[3]

[1] B.D. Napitu and J. Berakdar, Phys. Rev. B 81, 195108 (2010).
[2] F.O. Schumann et al., Phys. Rev. B 93, 235128 (2016).
[3] K.A. Kouzakov and J. Berakdar, Phys. Rev. Lett. 91, 257007 (2003).

O 100.10 Thu 18:15 WIL C307

Double photoemission from transition metal surfaces — •Ilya Kostanovskiy, Yuri Aliaev, Gianluca Di Filippo, Jürgen Kirschner, and Frank O. Schumann — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

The evolution of the 4p photoemission spectra for the 4th group transition metals exhibits large line width. This is assigned to the breakdown of the one-electron picture and electron-electron interaction.[1] Photoemission from the 4p level is accompanied by the Auger decay resulting in the final state with two holes in the 4d level. The process of the Auger-photoelectron double photoemission (DPE) can be studies via coincidence photoemission technique. Recent studies of the DPE spectra of Pd and Ag revealed clear evidence of the attosecond dynamics of the 4p photoemission process.[2]

We studied the DPE process involving the 3d and 4p levels from Cd, In, Sn and Sb surfaces. In contrast to the Pd case, the 4d state of these materials is not part of the valence band but a core level. We measured 2D energy distributions of DPE process and plotted the sum energy shape of the Auger-photoelectron pairs. We discuss the 2D energy distributions in terms of ultrafast electron dynamics of the Auger-photoelectron pair emission. The sum energy plots of the 4p and 3d DPE spectrum are very similar despite the very different timescales.

[1] M. Ohno and G. Wendin, Solid State Commun. 39, 875 (1981).
[2] I. Kostanovskiy et al., J. Phys. Condens. Matter 28, 15601 (2016).

O 101: Heterogeneous Catalysis: Theory I

Time: Thursday 17:00–18:30 Location: TRE Phy

Invited Talk O 101.1 Thu 17:00 TRE Phy
Density Functional Theory in Surface Science and Catalysis - Successes and Limitations — •Felix Studt — Karlsruher Institut für Technologie, Institut für Katalyseforschung und -technologie

Theoretical calculation employing density functional theory (DFT) are being widely used to investigate reactions of atoms and molecules on solid surfaces as they occur e.g. in heterogeneously catalyzed reactions. When coupled with a kinetic analysis of the reaction mechanism, reaction rates can be calculated from this data giving insight into the catalytic performance of materials. The success of theoretical calculations will depend on the errors associated with the level of DFT and the approximations used in the models employed for the surface reaction. Herein I will show some examples of how DFT can be used to understand heterogeneously catalyzed reactions and how close one can mimic experimental observations. The complexity associated with surface models for heterogeneously catalyzed reactions can be a challenge requiring sophisticated models and current limitations of theory will be exemplified for the hydrogenation of CO to various products. Finally, the errors of DFT will be addressed and I will show how one can use tools to learn about errors as well as error propagation and what this means for trends that are predicted with DFT.

O 101.2 Thu 17:30 TRE Phy
Computational Screening of MXenes as potential Two-dimensional Materials for Hydrogen Evolution Reaction — •Mohnish Pandey and Kristian S. Thygesen — Center for Atomic-scale Materials Design, Technical University of Denmark, 2830 Kgs. Lyngby, Denmark

We explore a new class of 2D materials commonly known as MXenes which are primarily carbides and nitrides of transition metals.[1] The stability of bare and functionalized MXenes is assessed via heat of formation. The possibilities of hydrogen evolution from these compounds are explored using the free energy of hydrogen adsorption at equilibrium coverages as activity descriptor.[2] Using a set of criteria, we propose a list of MXenes which can potentially be used as hydrogen evolving catalysts.
[1] M. Naguib, V.N. Mochalin, M.W. Barsoum, and Y. Gogotsi. Adv. Mater., **26**, 92–1005 (2014) [2] M. Pandey, A. Vojvodic, K. S. Thygesen, K. W. Jacobsen, J. Phys. Chem. Lett., **6**, 1577-1585 (2015)

O 101.3 Thu 17:45 TRE Phy
Oxygen Activation and Methanol Oxidation on Nanoporous Gold — •Wilke Dononelli[1], Lyudmila Moskaleva[2], and Thorsten Klüner[1] — [1]Institut für Chemie, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany — [2]Institut für Angewandte und Physikalische Chemie, Universität Bremen, 28359 Bremen, Germany

Au-based catalysts can be used for fuel cells, the synthesis of esters or the selective oxidation of alcohols. There is a high interest in this gold based catalysts because the selectivity of gold to partial oxidation products is higher than the selectivity of other metal catalysts. Especially Nanoporous gold (np-Au) has recently attracted considerable interest due to its potential use in catalysis. This Au-based catalyst can be used for the selective oxidation of methanol. The bottleneck of this oxidation reaction is the activation of oxygen on the surface.For this study, a kinked au(321) surface introduced by Moskaleva represents one of the reactive surfaces of the nanoporous gold. It consists of (111) terraces and zigzag-shaped steps, which may be favourable as possible adsorption positions for methanol in partial oxidation reactions. The aim of our work is the elucidation of the detailed mechanisms for total and partial oxidation of methanol on this model surface. So far we analysed the process of the oxygen activation and were able to present a theoretical mechanism that explains the first steps of this oxidation process, where first a methoxy species and in a next step formaldehyde is formed. These catalytic surface reactions are analysed using the PBE functional implemented in VASP.

O 101.4 Thu 18:00 TRE Phy
Ligands Effects on the Structure of Gold Clusters at Finite Temperature — •Diego Guedes-Sobrinho[1], Juarez L. F. Da Silva[1], Weiqi Wang[2], and Luca M. Ghiringhelli[2] — [1]University of São Paulo, São Carlos, Brazil — [2]Fritz-Haber-Institut der MPG, Berlin, Germany

Due to their catalytic properties and consequent importance for *green energy* transformation, gold clusters have been the focus of a large number of experimental and theoretical studies. However, an atomistic understanding of temperature and ligands effects on their structure is far from satisfactory. In this work, we investigate the structural stability and electronic aspects of Au_{13} – an example of flexible clusters at finite T [Beret *et al.* Faraday Discuss. **152**, 153 (2011)] – passivated by $(\mathrm{CO})_n$ ($n = 1, 6, 10$). We use replica-exchange *ab initio* molecular-dynamics, for an unbiased statistical sampling of the phase space. The energy and forces are described via the PBE exchange-correlation functional, including many-body dispersion interactions [A. Tkatchenko *et al.*, JCP **138**, 074106 (2013)], as implemented in the all-electron FHI-aims package. For $(\mathrm{CO})_n/\mathrm{Au}_{13}$, we find an electron-density displacement from Au and C atoms to O, which is more pronounced for $n = 10$. At this high CO coverage and in the temperature range $300 - 700$ K, cationic Au clusters with compact (high average coordination) structures are prefered. In comparison, pristine Au_{13} clusters show a preference for more open (low average coordination) configurations in the same temperature range.

O 101.5 Thu 18:15 TRE Phy
Complex Reaction Networks of Oxygen Activation on Ag Clusters with Multi-Spin States at Finite Temperature — •Weiqi Wang, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

To understand the process of the oxygen activation on (noble) metal clusters such as Ag_4, Ag_8, it is critical to take finite temperature effects into account. Transient structures, having their spin ground states different from those of stable structures, could be crucial in promoting the activation of oxygen. The appearance of those transient structures, however, introduces extra complexity into the reaction network. In this work, the reaction network of oxygen adsorption on silver clusters are studied at finite-temperature and different spin states. By estimating the transition matrices, the Markov state models (MSM) are established, based on the trajectories at parallel temperatures obtained from replica-exchange (first-principles) molecular dynamics (REMD). Reaction pathways are then analyzed by transition-path theory (TPT) based on the converged sampling on MSM. The MSMs and the reaction pathways are embedded in 2-dimensions by using the non-linear dimensionality reduction method Sketch-Map. In addition, 2-dimensional free energy plots are also calculated by the Boltzmann-reweighting method multi-state Bennet acceptance ratio (MBAR). We show that the adsorption and activation of oxygen benefits from the transient geometries, with spin states different from the ground state, that are available at finite temperature. This work was supported by the UNI-CAT cluster of excellence (DFG).

O 102: New Methods: Theory

Time: Thursday 17:45–18:30 Location: WIL C107

O 102.1 Thu 17:45 WIL C107

A generalized 'dipole correction' for charged surfaces in the repeated slab approach — •Christoph Freysoldt, Arpit Mishra, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The charging of surfaces plays an important role in electrochemistry, electronic sensors, field evaporation in atom probe tomography, and many other situations. *Ab initio* calculations are hampered by the problem that appropriate electrostatic boundary conditions must be taken into account. We will demonstrate that the commonly used dipole correction for neutral asymmetric slabs, that takes care of differences in the work function on either side of the slab, can be generalized to charged surfaces. This allows for simulations of strong electric fields where linear-response-based extrapolation schemes may not be appropriate. We show how flat-band or band-bending conditions can be realized, and discuss how to meaningfully define a potential reference level for total energies. Last, we will highlight the importance of *mechanical* boundary conditions for charged slab calculations.

O 102.2 Thu 18:00 WIL C107

Revised Chen's derivative rule for STM calculations — Gábor Mándi[1] and •Krisztián Palotás[1,2] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia

Chen's derivative rule for electron tunneling [1] is revised [2] for the purpose of computationally efficient calculations of scanning tunneling microscopy (STM). New features include (i) the weighting of tunneling matrix elements of different tip-orbital characters by an arbitrary energy-independent choice or based on first-principles data, (ii) arbitrary tip geometrical orientations, and (iii) the possibility of quantitative analysis of tip-orbital interference contributions. The model is applied to two functionalized surfaces where quantum interference effects play an important role in the STM imaging and the Tersoff-Hamann model fails to describe the correct STM contrast under certain conditions: N-doped graphene [3] and a magnetic Mn_2H complex on the Ag(111) surface [4]. For both studied surfaces, the importance of interference between s and p_z tip orbitals is highlighted that cause a significant contrast change in the STM images [2].

[1] C. J. Chen, Phys. Rev. B 42, 8841 (1990)
[2] G. Mándi, K. Palotás, Phys. Rev. B 91, 165406 (2015)
[3] M. Telychko et al., ACS Nano 8, 7318 (2014)
[4] T. Sachse et al., New J. Phys. 16, 063021 (2014)

O 102.3 Thu 18:15 WIL C107

Modeling Tip enhanced Raman spectrum influenced by an external electric field — •Otto Hauler, Kai Braun, Dai Zhang, and Alfred J. Meixner — Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen

Within the last years Scanning Tunneling Microscopy (STM) gets more and more attraction in Tip enhanced Raman Spectroscopy (TERS). Various groups showed strongly increased optical resolution by using STM as feedback mechanism to keep the tip in close proximity to the surface. Despite the increased sensitivity a STM also allows for direct manipulation of the molecules in the gap via the bias voltage. In this contribution we present a theoretical model to calculate TERS-spectra of molecules in an external DC electric field. An increasing bias voltage leads to significant changes of certain Raman bands, while others are only weakly affected. We will discuss the influence of the bias voltage on TERS of a self-assembling monolayer and propose a quantum chemical model to improve the understanding of the underlying phenomenon. In details we will discuss the influence of different parameters, e.g. the molecular orientation on the metal surface, the illumination geometry, and the electric field strength due to the bias voltage, on the Raman spectrum. Furthermore we will compare the theoretical results with experimentally obtained spectra.

O 103: Annual Meeting of the Surface Science Division

Time: Thursday 19:00–19:30 Location: HSZ 01

Topics: Report of the Chairman; Presentation of the Gerhard Ertl Young Investigator Award; Miscellaneous

O 104: Post-Deadline Session

Time: Thursday 19:30–20:30 Location: HSZ 01

Contributed Post-Deadline Talks

O 105: Overview Talk: Melissa Hines

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

Invited Talk O 105.1 Fri 9:30 TRE Phy

The Surface Chemistry of Anatase (001) and Rutile (110) in Solution: Atomically Flat Surfaces and Near-Ideal Organic Monolayers — •Melissa Hines — Cornell University, Ithaca NY, USA

The surface chemistry of TiO2 – a sustainable, earth-abundant, nontoxic metal oxide – has garnered attention due to many high-profile applications, including dye-sensitized solar cells and photoactivated H2O purification; however, relatively little is known about the surface chemistry of TiO2 in technologically relevant environments, such as air and solution. This ignorance is perhaps best illustrated by our recent discovery that rutile surfaces under ambient conditions are not terminated by a H2O film as long assumed, but rather by a tightly bound, self-assembled monolayer of bicarbonate formed by the catalytic reaction of CO2 and H2O. We have developed solution processes to produce atomically flat rutile (110) and heteroepitaxial anatase (001), both with the size and quality necessary for characterization by STM and IR spectroscopy. Using these, we have prepared, imaged, and analyzed a variety of near-atomically-perfect, self-assembled monolayers from solution. The structure and photoreactivity of these monolayers provides insight into their function. For example, strong π-π interactions between phenyl rings in benzoate monolayers induce intramolecular rotations that destroy the extended π conjugation between the phenyl and carboxylate groups, presumably disrupting electron transport. STM also shows that anatase surfaces prepared in solution are very different from those prepared in UHV.

O 106: Electronic Structure of Surfaces: Spectroscopy, Surface States III

Time: Friday 10:30–13:00 Location: WIL C107

O 106.1 Fri 10:30 WIL C107

ARXPS investigations on surface composition and electronic structure of oxygen- and sulfur-functionalized ionic liquids — •Bettina Heller[1], Claudia Kolbeck[1], Inga Niedermaier[1], Sabine Dommer[2], Nicola Taccardi[3], Jürgen Schatz[2], Peter Wasserscheid[3], Hans-Peter Steinrück[1], and Florian Maier[1] — [1]Lehrstuhl für Physikalische Chemie II, FAU Erlangen-Nürnberg, Germany — [2]Lehrstuhl für Organische Chemie I, FAU Erlangen-Nürnberg, Germany — [3]Lehrstuhl für Chemische Reaktionstechnik, FAU Erlangen-Nürnberg, Germany

Angle-resolved X-ray photoelectron spectroscopy (ARXPS) is a powerful technique to investigate electronic and surface properties of ionic liquids (ILs).[1] This study focuses on sulfur- and oxygen-functionalized ILs, such as thioether and alkoxy ILs, which have the potential of forming carbene complexes used in e.g. catalysis.

With our new Dual Analyzer System for Surface Analysis (DASSA), we simultaneously record ARXPS measurements at 0° (bulk sensitive) and 80° emission (surface sensitive).[2] These spectra provide information on the electronic structure -by means of chemical shifts- and on surface orientation effects.

Imidazolium ILs with ether- and methoxy-sidechains have a random surface orientation in contrast to their non-functionalized ILs counterparts. Regarding the functionalization with sulfur as a thiouronium, a change in the electronic structure of the imidazolium ring is observed.

[1] H.-P. Steinrück, Phys. Chem. Chem. Phys. 2012, 14, 5010.

[2] I. Niedermaier et al., Rev. Sci. Instrum. 2016, 87, 045105.

O 106.2 Fri 10:45 WIL C107

Circular Dichroism in Soft X-ray Photoelectron Diffraction — •Katerina Medjanik[1,2], Gunnar Öhrwall[2], Olena Fedchenko[1], Sergey Chernov[1], Anna Zaporozhchenko-Zymaková[1], Andreas Oelsner[3], Benedikt Schönhense[4], Hans- Joachim Elmers[1], and Gerd Schönhense[1] — [1]Univ. Mainz — [2]MAX IV Lund — [3]Surface Concept GmbH Mainz — [4]Imperial College London

The interference patterns in the angular distribution of electrons from core levels due to *photoelectron diffraction (PED)* give valuable information on the short-range order around the emitter atom. For circularly polarized excitation, the *PED* patterns contain sizeable *circular dichroism in the angular distribution (CDAD)*, originating from the interference of final-state partial waves with different quantum numbers m_l [1]. Since a large region in k-space is observed simultaneously, momentum microscopy is ideal for the study of *CDAD* in *PED*. ToF (time-of-flight) energy discrimination [2] provides simple means for the selection of the desired core level even at very high photon pulse rates (here 100 MHz). We report first results for W(110) and Ir(111) taken at beamline I1011 at MAX II, Lund, Sweden. The diffraction patterns reveal pronounced dichroism in 4f core-level emission. The asymmetry maps A_{CDAD} (k_x,k_y,hv) vary strongly with photon energy between hv=300 and 1000 eV. Funded by BMBF (05K13UM2). [1] Fecher et al., JESRP **122**, 157 (2002); [2] Schönhense et al., JESRP **200**, 94 (2015).

O 106.3 Fri 11:00 WIL C107

Bulk-Sensitive Band Mapping of Mo in the *Tender* X-ray Range — •Dmitry Vasilyev[1], Katerina Medjanik[1], Martin Ellguth[1], Sergey Babenkov[1], Anna Zaporozhchenko-Zymaková[1], Christian Tusche[2], Arndt Quer[3], Florian Diekmann[3], Sebastian Rohlf[3], Matthias Kalläne[3], Kai Rossnagel[3], Yves Acremann[4], Dmytro Kutnyakhov[5], Wilfried Wurth[5], Jens Viefhaus[5], Hans-Joachim Elmers[1], and Gerd Schönhense[1] — [1]Univ. Mainz — [2]FZ Jülich — [3]Univ. Kiel — [4]ETH Zurich — [5]DESY Hamburg

Recent experiments and calculations have demonstrated that ARPES can still be performed in the X-ray range [1]. Intrinsic and extrinsic effects pose limits to the performance of this new approach: the cross section drops rapidly with increasing photon energy, direct transitions are suppressed by inelastic scattering, and the photon momentum causes a sizeable shift of the emission pattern. With increasing kinetic energy the emission angles shrink so that classical ARPES reaches its limits of angular resolution, and the required energy resolution (towards 10^5) is at the technical limit of present instruments. Here, we demonstrate that momentum-microscopy with parallel ToF energy analysis indeed opens the range beyond soft X-rays (i.e., the *tender* X-ray regime) for high-resolution bulk band mapping. Sharp k-patterns with pronounced high contrast have been measured (even for fully oxidized surfaces) up to kinetic energies of 1700 eV at the high-brilliance beamline P04 (PETRA III) for the medium-Z bcc metal Mo. [1] Gray et al., Nat. Mat. **10**, 759 (2011).

O 106.4 Fri 11:15 WIL C107

Oxygen-2p valence band dispersion of two-dimensional oxide quasicrystal — •Cheng-Tien Chiang[1,2], Martin Ellguth[2,3], Florian O. Schumann[1], Christian Tusche[2,4], Stefan Förster[1], Richard Kraska[1], Jürgen Kirschner[2,1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany — [3]Institut für Physik, Johannes-Gutenberg-Universität Mainz, Mainz, Germany — [4]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Jülich, Germany

Valence bands of ultrathin $BaTiO_3$-derived oxide quasicrystal (OQC) on Pt(111) [1] are investigated by angle-resolved photoelectron spectroscopy using the momentum microscope [2]. At around 4 and 6 eV below the Fermi level we observe valence states with flat dispersion as a function of the momentum parallel to the surface, whereas a strongly dispersive feature from 4.6 to 6 eV is discovered along the $[\overline{1}\overline{1}0]$ direction. By comparison with the bulk $BaTiO_3$ band structure we attribute these states to the O-2p valence bands of OQC and discuss their characteristic dispersion.

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, Nature **502**, 215 (2013) [2] C. Tusche, A. Krasyuk, and J. Kirschner, Ultramicroscopy **159**, 520 (2015)

O 106.5 Fri 11:30 WIL C107

Non-contact and non-destructive surface analytical tool - The Kelvin Probe: Basics to recent advances — •Subrahmanyam Aryasomayajula — Department of Physics, Indian Institute of Technology Madras, Chennai 600036 India

The surface of metals and semiconductors pose unique challenges in their understanding. Most of the surface analytical tools do modify the surfaces. The Kelvin probe is a most powerful non-contact and non-destructive analytical tool for surface engineering of the metal and semiconductor surfaces; the surface remains virgin even after the measurement. The Kelvin probe technique measures the surface workfunction (which is sensitive to the surface preparation). The technique has the unique advantage to follow the real time changes that are taking place on the surface. The Kelvin probe technique is so versatile, it is being employed in several areas: electronic behavior of surfaces of metals and semiconductors,tribology, inter-facial phenomena, adhesion, corrosion,electro-chromic behavior, surface defects and morphology and bacterial bio-film adherence etc,. The present work describes the basics and explores new areas like the failure analyses of corrosion in bio-medical implants (semiconductor - bio-fluid interactions).

O 106.6 Fri 11:45 WIL C107

spectroscopic imaging STM study on Dirac line node material ZrSiS — •qingyu he — max-planck-institute for solid state research, stuttgart, germany

3D Dirac semi-metals have attracted wide interest in recent condensed matter research. The related Dirac line node materials come into focus due to properties such as unconventional magneto-transport and their potential to host topologically nontrivial phases. The non-symmorphic material ZrSiS is one of the first discovered materials of this new family, hosting a nodal line and an unconventional surface state. [1]

Spectroscopic imaging scanning tunneling microscopy (SI-STM) has been a highly valuable technique to study the electronic structure with high energy resolution. In this presentation, we report the investigation of ZrSiS by SI-STM at the atomic scale, in combination with DFT calculations. Firstly, we succeeded in visualizing the signature of the bulk Dirac line node both in real and momentum space, adding key evidences confirming the nodal line and highlighting its exceptional properties. Secondly, an unconventional surface state related to the breaking of non-symmorphic symmetry was observed and its dispersion relation was mapped. Finally, we also discovered the spectroscopic signatures of a type-II Dirac fermion hosted by the surface state.

Our result has impact beyond ZrSiS, providing crucial insights into the Dirac line node materials and non-symmorphic crystals as well.

[1] Schoop, L. M. et al. Dirac cone protected by non-symmorphic symmetry and three-dimensional Dirac line node in ZrSiS. Nat. Commun. 7:11696

O 106.7 Fri 12:00 WIL C107

ERO modelling of surface morphology effect on metals erosion at PSI-2 facility — •Alina Eksaeva[1,2], Evgeny Marenkov[2], Dmitry Borodin[1], Arkadi Kreter[1], Daisuke Nishijima[3], Andreas Kirschner[1], Tobias Schlummer[1], Juri Romazanov[1], Albrecht Pospieszczyk[1], and Stephan Ertmer[1] — [1]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung, 52425 Jülich, Germany — [2]National Research Nuclear University MEPhI, 31, Kashirskoe sh., 115409, Moscow, Russia — [3]Center for Energy Research, University of California at San Diego, 9500 Gilman Dr., La Jolla, CA 92093-0417, USA

Linear plasma device PSI-2 with its continuous plasma operation is an excellent test bed for the investigation of plasma-facing material erosion including delicate effects like e.g. nano- and micro-scale surface structures and roughness. However, numerical modelling is indispensable for the correct interpretation of experiments. The 3D Monte-Carlo code ERO is a powerful and versatile tool for describing the erosion and local transport of impurities taking into account the particular geometry. The aim of this work is to incorporate the effect of surface morphology into the ERO modelling first based on free parameters matched with the experiments. Several experiments have already been carried out in PSI-2 facility to investigate the evolving surface morphology of tungsten (W) and chromium (Cr) and provide a consistent set of data for the interpretation with the ERO code. Generally, ERO simulation results are in a good agreement with the experiments.

O 106.8 Fri 12:15 WIL C107

ERO modelling of surface morphology effect on metal erosion at PSI-2 linear plasma facility — •Alina Eksaeva[1,2], Dmitry Borodin[1], Arkadi Kreter[1], Daisuke Nishijima[3], Tobias Schlummer[1], Albrecht Pospieszczyk[1], Stephan Ertmer[1], Andreas Kirschner[1], Juri Romazanov[1], and Evgeny Marenkov[2] — [1]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung, 52425 Jülich, Germany — [2]National Research Nuclear University MEPhI, 31, Kashirskoe sh., 115409, Moscow, Russia — [3]Center for Energy Research, University of California at San Diego, 9500 Gilman Dr., La Jolla, CA 92093-0417, USA

Linear plasma device PSI-2 with its continuous plasma operation is an excellent test bed for the investigation of plasma-facing material erosion including delicate effects like e.g. nano- and micro-scale surface structures and roughness. However, numerical modelling is indispensable for the correct interpretation of experiments. The 3D Monte-Carlo code ERO is a powerful and versatile tool for describing the erosion and local transport of impurities taking into account the particular geometry. Several experiments have already been carried out at PSI-2 facility to investigate the evolving surface morphology of tungsten (W) and chromium (Cr) and utilizing various measurement technics provide a consistent set of data for the interpretation with the ERO code. The aim of this work is to incorporate the effect of surface morphology into the ERO modelling based on free parameters matched with the experiments. This approach allows to reproduce the qualitative effects observed and understand their interplay.

O 106.9 Fri 12:30 WIL C107

Untersuchung der Rückhaltemechanismen von Wasserstoff in Beryllium Wolfram Verbindungen — •Michael Eichler, Timo Dittmar und Christian Linsmeier — Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, 52425 Jülich, Germany

In den experimentellen Fusionsreaktoren JET und zukünftig auch ITER besteht die erste Wand im Hauptraum aus Beryllium (Be). In Bereichen der höchsten Wärmelasten (Divertor) wird zusätzlich Wolfram (W) verwendet. Als Brennstoff werden die Wasserstoffisotope Deuterium (D) und Tritium (T) eingesetzt. Durch den Kontakt der Reaktorwand mit den D- und T-Ionen wird unter anderem das Oberflächenmaterial erodiert und an anderen Stellen deponiert. Dadurch entstehen Be-W Verbindungen. Da das radioaktive T während des Reaktorbetriebs in der Wand eingelagert wird, ist die Untersuchung des Wasserstoffinventars, insbesondere der Rückhaltemechanismen in Be-W Legierungen von besonderem Interesse. Dazu wird das Ultra Hoch Vakuum Experiment namens ARTOSS vorgestellt, welches verschiedene Oberflächenanalytiken vereint und somit die in situ Präparation und Analyse entsprechender Materialien unter wohldefinierten Bedingungen ermöglicht. Der Ionenbeschuss im Reaktor wird mit einer Ionenquelle simuliert. Mit Spannungen bis maximal 20 kV werden D und Wasserstoffionen in Be-W Verbindungen implantiert. Ausserdem werden erste Untersuchungen mittels Röntgenphotoelektronenspektroskopie (XPS), thermischer Desorptionsspektroskopie (TDS) und nuklearer Resonanzanalyse (NRA) gezeigt.

O 106.10 Fri 12:45 WIL C107

First-principles calculations on the surface and bulk electronic structure of TaAs — •Minkyu Shim[1], Jae Hyun Bae[1,2], Jisoon Ihm[1,3], and Cheol-Hwan Park[1] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, South Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, South Korea — [3]Department of Physics, Pohang University of Science and Technology, Pohang 37673, South Korea

Weyl semimetals are a new class of materials whose low-energy electronic excitations are described by the Weyl equation. In this presentation, we discuss the electronic structure of one of the most commonly-known Weyl semimetals, TaAs [1,2], obtained through first-principle calculations. We analyze both the bulk and Fermi arc states of this material. Our work presents a comprehensive understanding of the topological surface states of TaAs, which would be helpful for future experimental studies. The first two authors contributed equally to this work.

(The first two authors contributed equally to this work.)

[1] H. Weng, C. Fang, Z. Fang, B. A. Bernevig and X. Dai, Phys. Rev. X 5, 011029 (2015). [2] S.-M. Huang, S.-Y. Xu, I. Belopolski, C.-C. Lee, G. Chang, B. Wang, N. Alidoust, G. Bian, M. Neupane, C. Zhang, S. Jia, A. Bansil, H. Lin and M. Z. Hasan, Nat. Commun. 6, 7373 (2015)

O 107: Heterogeneous Catalysis: Theory II

Time: Friday 10:30–13:00 Location: TRE Phy

O 107.1 Fri 10:30 TRE Phy

Catalytic activity of high index platinum surfaces — •Gabriele Tomaschun and Thorsten Klüner — IfC, CvO Universität Oldenburg, 26111 Oldenburg

The key challenges of the catalysis are to investigate and improve efficient and environmentally friendly processes. This can be realized by changing the composition of the chemical process or by tuning the shape of the catalyst itself. [1] The Pt nanoparticles as catalysts for instance show different catalytic reactivity by varying the surface shape and structure. [2] It has been established, that the higher density of atomic steps and kinks leads to more active sites on the surface. This might lead to an increasing reactivity for these stepped platinum surfaces. The main focus of our research is to analyze the dependence of the catalytic reactivity and selectivity of the industrially relevant reactions, such as condensation of light alcohols and hydrogenation of furfural, on the surface structure of Pt nanoparticles. The different stepped and kinked Pt surfaces provide thereby a lot of active sites for these reactions, thus detailed insight in the reaction mechanisms can be obtained. The theoretical calculations will be performed using the exchange-correlation functional PBE implemented in the Vienna ab initio simulation package (VASP). [3] The analysis of the adsorption and coadsorption sites, adsorption energies, transition states and the favorable reaction pathways of the investigated reactions will be the main objective of this research. [1] K. An, G. A. Somorjai, ChemCatChem 2012, 4, 1512. [2] S. Motoo, N. Furuya, Electroanal Chem 1984, 172, 339. [3] G. Kresse, J. Hafner, Phys. Rev. B 1994, 49, 14251.

O 107.2 Fri 10:45 TRE Phy

CH_2 Stabilization at Steps on Ru(0001) by Co-Adsorbates

— Xunhua Zhao[1], Harald Kirsch[1], Zefeng Ren[2], •Sergey V. Levchenko[1], and R. Kramer Campen[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Peking University, Beijing, CN

Despite numerous studies, the stability of various one-carbon (1C) species, which determines the hydrocarbon-chain growth mechanism in industrially important processes such as the Fischer-Tropsch (FT) synthesis, is still debated. In particular, it was shown recently that H co-adsorption at Ru(0001) terraces stabilizes adsorbed CH_2, which makes it a much more likely candidate for the chain building block [1]. In this work, we use DFT with the PBE functional plus a van der Waals interaction correction vdW^{surf} [2] to study the effect of CH co-adsorption on the stability of CH_2 at stepped Ru(0001) surface. We show that both the barrier for CH_2 dissociation and that for the diffusion of CH away from the steps increase 2- to 3-fold compared to isolated 1C species. The theoretical study explains the vibrational sum-frequency generation spectroscopy measurements of this system [3]. The results of the combined theoretical/experimental study highlight the large influence of co-adsorbates on step-bound 1C moieties and provide means of reconciling previous apparently contradictory results on the FT synthesis.—[1] H. Kirsch *et al.*, J. Catal. **320**, 89 (2014); [2] V. Ruiz *et al.*, PRL **108**, 146103 (2012); [3] H. Kirsch *et al.*, JPC C **120**, 24724 (2016).—X. Zhao's current address: Chemistry Department, Princeton University, Princeton, NJ 08544, USA.—This work received funding from the UNICAT Cluster of Excellence.

O 107.3 Fri 11:00 TRE Phy

DFT modeling of formic acid decomposition over late transition metals: on the road to lower activation barriers — •Jan Kučera and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

Low temperature decomposition of formic acid (FA) to regain pure H_2 is among the processes suggested as one of the potential H_2-storage alternatives to designs employing compressed hydrogen. Heterogeneous catalysts based on late transition metals, in particular Pd or Au particles dispersed on oxide supports, selectively decompose formic acid already at low temperatures, however, so far the achieved efficiencies are below those required for commercial polymer electrolyte membrane fuel cells.

The general goal of our computational study - based mainly on periodical density functional theory (DFT) calculations - relates to the identification of the key effects operating in FA decomposition at Pd and Au-based surfaces and at complex metal/oxide interfaces. Despite the fact that in principle only two dehydrogenation steps are involved, FA decomposition represents a complex catalytic system. We will focus on the elucidation of three phenomena that might be critical for the reaction energetics: (i) modification of catalytic properties by the formation of bimetallic surfaces, (ii) the role of intermolecular forces in the formate decomposition step due to dimer configurations or the interaction with the solvent, and (iii) the effect of Au-hydride formation at the interface with CeO_2.

O 107.4 Fri 11:15 TRE Phy

Trends in catalytic activity of Ni-based electrodes for the hydrogen evolution reaction — •Hannah Schlott[1], Marc Ledendecker[2], Markus Antonietti[3], Menny Shalom[4], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Max-Planck-Institut für Eisenforschung, Düsseldorf — [3]Max-Planck-Institute of Colloids and Interfaces, Potsdam — [4]Chemistry Department, Ben Gurion University of the Negev, Israel

Metallic binary compounds have emerged in resent years as highly active and stable electrocatalysts toward the hydrogen evolution reaction. The origin of their high activity from a theoretical and experimental point of view is elucidated. Different metallic ceramics (Ni_3S_2, Ni_3N, and Ni_5P_4) are grown directly on Ni support in order to avoid any contaminations. DFT calculations were performed to obtain a deeper understanding of possible active adsorption sites and the observed catalytic stability. It is found that the heteroatoms P, S, and N actively take part in the reaction. Due to the anisotropic nature of the materials, a variety of adsorption sites with highly coverage-dependent properties exist, leading to a general shift in hydrogen adsorption free energies ΔG_H close to zero. Extending the knowledge gained about the here described materials, a new catalyst is prepared by modifying a high surface Ni foam, for which current densities up to $100\,\mathrm{mA\,cm^{-2}}$ at around $0.15\,\mathrm{V}$ are obtained.

[1] M. Ledendecker, H. Schlott, M. Antonietti, B. Meyer, M. Shalom, *Adv. Energy Mater.* **2016**, 1601735.

O 107.5 Fri 11:30 TRE Phy

What is the Most Promising Dopant for the Deacon Process at RuO_2 ? — •Zhen Yao and Karsten Reuter — Technische Universität München, Germany

The Deacon process is a sustainable way to recover high purity Cl_2 from waste HCl in chemical industry. RuO_2 is a most promising catalyst for this process, i.e. the catalytic oxidation of HCl to chlorine and water. A currently pursued route to further improve on its activity is a deliberate doping of the bulk oxide. To guide corresponding experimental endeavors we perform a density-functional theory based computational screening study for a wide range of metal dopant atoms at the RuO_2(110) facet. We use a three-dimensional descriptor matrix, evaluating the rate-controlling Cl desorption energy, the dopant surface segregation energy, as well as the dopant stability against precipitation into bulk oxide grains. Our results suggest Cu doping to represent an optimum compromise between stability and catalytic activity enhancement.

O 107.6 Fri 11:45 TRE Phy

Thermal lattice Boltzmann method for catalytic flows — •Daniel Berger[1], Ana Smith[2,3], David Smith[3], and Jens Harting[1,4] — [1]Forschungszentrum Jülich GmbH, Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy — [2]Institute for Theoretical Physics I, University of Erlangen-Nürnberg — [3]Ruđer Bošković Institute, Zagreb, Croatia — [4]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

Many catalyst devices employ porous or foam-like structures to optimize the surface to volume ratio in order to maximize the catalytic efficiency. The porous structure leads to a complex macroscopic mass and heat transport. Local heat accumulation changes the local reaction conditions, which in turn affects the catalytic turn over rate and eventually compromises the stability of the catalytic device.

We present a thermal multicomponent model based on the entropic lattice Boltzmann method (J. Kang *et al.*, Phys. Rev. B **89**, 063310 (2014)) to simulate catalytic reactions through porous media. This method reproduces the Navier-Stokes equations and allows the tracking of temperature dynamics. The viscosity, diffusivity, and heat capacities are calculated from the Lennard-Jones parameters of the gases, while the chemical surface reactions are incorporated in a very flexible fashion through the flux boundary conditions at the walls.

To show the strength and flexibility of this model and our implementation, we will report the catalytic turn-over for a wide range of porosities and reaction conditions.

O 107.7 Fri 12:00 TRE Phy

Is DFT accurate enough for modeling chemical kinetics? — •Sandra Döpking[1], Daniel Strobusch[2], Christoph Scheurer[2], Craig Plaisance[2], Karsten Reuter[2], and Sebastian Matera[1] — [1]FU Berlin, Germany — [2]TU München, Germany

Targeting at an understanding of interplay between bond making and bond breaking and observed reactivity, first-principles based kinetic methodologies for heterogenous catalysis employ energetic information derived from electronic structure calculations. These energies, usually obtained on the density functional theory (DFT) level, have typically a potential error of 0.2 eV-0.3 eV.

We present a systematic approach to address the propagtion of these errors to the kinetic model's result based on adaptive sparse grids for the sampling of the error space. We demonstrate the approach on a model for the oxygen evolution on Co_3O_4[1]. Our results indicate that the simulated reactivities carry an uncertainty of more than five orders of magnitude, questioning the trustability of the model. However, a decomposition of this uncertainty into contributions of different input errors reveals that only a small number of DFT energies have an impact. So, it is still possible to draw conclusions about the potential driving forces behind catalytic activity, although the activity itself can not be estimated accurately. Besides a qualified discussion of the effect of the modeling error, the approach can be employed for the reduction of the number of expensive first-principles simulations or for computational materials screening. [1] C. Plaisance and R. A. van Santen, J. Am. Chem. Soc. 137, 14660-14672 (2015)

O 107.8 Fri 12:15 TRE Phy

Solving the master equation without kinetic Monte Carlo: Tensor train approximations for a CO oxidation model — •Patrick Gelss[1], Sebastian Matera[1], and Christof Schütte[1,2]

— [1]Freie Universität Berlin, Germany — [2]Zuse Institut Berlin, Germany

Kinetic Monte Carlo (kMC) simulations have become an important tool for modeling chemical kinetics on catalytic surfaces. Their appealing feature is the unbiased solution of the Markovian master equation, which results from a given microkinetic mechanism, while not being affected by the *curse of dimensionality*. However, the need to perform one reaction step after the other makes kMC ineffective for stiff problems, which are characterized by a large disparity in the values of the employed rate constants. We have developed an alternative approach with tunable accuracy, which directly solves the master equation by exploiting the Tensor Train Format[1]. Using a reduced model for the CO oxidation on RuO_2(110), we benchmark the approach against highly accurate kMC simulations. We demonstrate that numerical accuracy and linear scaling in the system size can be achieved for a large range of input parameters. The advantage over the kMC approach is illustrated for a problem with increasing stiffness, where our approach is hardly affected but the computational costs for kMC explode.

[1] P. Gelß, S. Matera, C. Schütte, J. Comput. Phys., 314, pp. 489–502 (2016)

O 107.9 Fri 12:30 TRE Phy

On the effect of electromagnetic field heterogeneities on the chemical kinetics on nano-structured photocatalysts — •Sebastian Matera[1], Martin Hammersachmidt[2], Sandra Döpking[1], Sven Burger[2], and Frank Schmidt[2] — [1]FU Berlin, Germany — [2]Zuse Institute Berlin, Germany

When going from single crystal surfaces to structured catalysts, such as powders or nano-particles, the complexity of the problem dramatically increases. Besides the obvious higher structural complexity, the electromagnetic field, driving photocatalysis, might become heterogeneous on a nanoscale level. We present a simple model for the CO_2 reduction on titania anatase, which addresses the impact of these heterogeneities on the photocatalytic kinetics by coupling kinetic Monte Carlo with electromagnetic wave simulations. Our results indicate that catalytic activity might vary significantly on a single facet of a nanocrystal. Moreover, the coverage situation might change laterally on this facet and we have a concomitant change of the rate-determining steps. This heterogeneity on all levels of photocatalytic activity makes it extremely difficult to draw mechanistic conclusions from experimental studies on such structured catalysts, where only the spatially averaged activity can be addressed.

O 107.10 Fri 12:45 TRE Phy

Water-Gas Shift Reaction Catalysis in Supported Ionic Liquid Phase — •Robert Stepić[1], Nataša Vučemilović-Alagić[1,2], Daniel Berger[1,4], Christian Wick[1,2], Jens Harting[4,5], Ana-Sunčana Smith[1,2], and David M. Smith[2,3] — [1]PULS Group and Exellence Cluster: EAM, FAU, Erlangen, Germany — [2]CLS Group, RBI, Zagreb, Croatia — [3]CCC, FAU, Erlangen, Germany — [4]Forschungszentrum Jülich, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Nürnberg, Germany — [5]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, Netherlands

The water-gas shift reaction is one of the most important reactions in industry, as it is a key step in the production of hydrogen. Novel systems have been developed with highly active transition metal catalysts immobilized in a thin layer of ionic liquid on a porous support. Here we present a joint study of such a system using methods of quantum chemistry and molecular dynamics. The mechanism and energetics of the water-gas shift reaction catalysis via a ruthenium-based transition metal complex is determined with density functional theory calculations using a series of constrained optimizations and transition state searches. The ionic liquid on alumina support is studied by fully atomistic molecular dynamics simulations, where a proper force field is characterized by reproducing the experimentally observed x-ray reflectivity and diffusion coefficients. The ultimate goal of this study is to bridge the gap between multiple scales and provide a theoretical prediction of output, and optimization, of these important catalytic systems (see also modeling of gas flows by Daniel Berger et al.).

O 108: Graphene: Adsorption, Intercalation and Other Aspects

Time: Friday 10:30–13:00 Location: TRE Ma

O 108.1 Fri 10:30 TRE Ma

Radiation reduced CNM formation from halogenated biphenylthiols — •Sascha Koch[1], Christoph D. Kaiser[1], Lena Frommeyer[1], Patrick Stohmann[1], Tarek Abu-Husein[2], Andreas Terfort[2], and Armin Gölzhäuser[1] — [1]Department of Physics, Universität Bielefeld, Universitätsstrasse 25, 33615 Bielefeld, Germany — [2]Department of Chemistry, Goethe-Universität Frankfurt, Max-von-Laue-Straße 7, 60438 Frankfurt, Germany

Carbon Nano Membranes (CNM) are mechanical stable and homogeneous quasi 2D systems which are formed by the electron radiation induced cross linking of molecules in specific self-assembled monolayers (SAM) grown on substrates like e.g. gold or copper. Contrary to graphene, as the most popular 2D system, the CNM structural and functional properties can be tailored by the selection and composition of appropriate precursors for the SAM formation as for instance phenylthiols or naphthalenes [1,2]. Here, the study of SAMs from halogenated biphenylthiols on a Au(111) substrate is presented. These precursor molecules allow in contrast to hydrogenated biphenylthiols the cross linking of SAMs for the formation of a CNM at a highly reduced electron doses. Additionally, this specific doping of biphenyls provides an insight to the mechanisms of the formation of CNMs. [1] P. Angelova et al., ACS Nano, 2013, 7, 6489-6497 [2] A. Turchanin and A. Gölzhäuser, Adv. Mat. 2016, 28 6075-6103

O 108.2 Fri 10:45 TRE Ma

Graphene/Polymer Composite Membranes for Nano- and Ultrafiltration — •Lukas Madauss[1], Jens Schumacher[2], Oliver Ochedowski[1], Jens Meyer[2], Henning Lebius[3], Brigitte Band-d'Etat[3], Eugenia Toimil Molares[4], Christina Trautmann[4], Mathias Ulbricht[2], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, Duisburg, Germany — [2]Universität Duisburg-Essen, Essen, Germany — [3]CIMAP, Caen, France — [4]GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, Germany

Nanoporous graphene is currently investigated as a promising membrane material in which selective pores can be created depending on the requirements of the application [1]. Here, we report on the irradiation of nanoporous graphene/polymer composite membranes with swift heavy ions and consecutive track etching. The ions directly create atomic pores in the graphene lattice while cylindrical tracks consisting of damaged material are created in the polymer support. Chemical etching converts the ion tracks in the polymer into large open channels [2] without attacking the graphene layer. The graphene coverage is significantly improved by protecting graphene by a PMMA layer during the track etching process. Our method presents a facile route to create high-quality suspended graphene on a flexible polymeric membrane with pores of tunable size. The development of porous graphene/polymer composite membranes is promising for fast and selective ultrafiltration separation processes.

[1] S. P. Surwade, Nature Nanotechnology, 10, 459-464, 2015 [2] T.W. Cornelius, NIMB, 265, 553-557, 2007

O 108.3 Fri 11:00 TRE Ma

Optically switchable hybrid graphene/carbon nanomembrane field effect transistors — •Antony George, Zian Tang, David Kaiser, Christof Neumann, Andreas Winter, and Andrey Turchanin — Friedrich Schiller University Jena, Institute of Physical Chemistry, D-07743 Jena, Germany

Field effect transistors (FETs) based on 2D materials are of great interest for applications in ultrathin electronic devices and especially for sensing technology. Here we demonstrate the possibility to add an optical switchability to graphene devices by hybridizing the graphene channel with optically active azobenzene molecules. The azobenzene molecules have been incorporated to the graphene FET channel by building a van der Waals heterostructure with chemically functionalizable 1 nm thin carbon nanomembranes (CNM). Under exposure with 365 nm and 455 nm light azobenzene molecules undergo -cis and-trans molecular conformations resulting in switching of the molecular dipole. We show that these transformations triggered by external optical stimulation induces switching of the graphene FETs between two operation modes.

O 108.4 Fri 11:15 TRE Ma

Insight into the wetting of a graphene-mica slit pore with a monolayer of water — •Hu Lin, Andre Schilo, Rauf Kamoka, Nikolai Severin, Igor M. Sokolov, and Jürgen P. Rabe — Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Graphene-mica slit pores are prepared by mechanical exfoliation of graphite onto a freshly cleaved muscovite mica surface in dry nitrogen. We followed their wetting and dewetting with water by scanning force microscopy (SFM) and Raman spectroscopy, which allows to unravel doping and strain effects upon both wetting and dewetting. SFM reveals that the wetting water layer is one monolayer thick, slightly thinner than a single layer of graphene. Raman spectra exhibit a reduction of the graphene D' peak intensity upon wetting, and a recurrence of the peak when the water layer dewets the slit pore. We attribute the D' peak to direct contact of the graphene with the ionic mica surface in dry conditions. Analyses of the 2D and G peak positions, the corresponding peak positions and the widths, imply that graphene on dry mica is charge doped and variably strained. A monolayer of water in between graphene and mica removes doping and reduces strains. This supports that in dry conditions graphene is in direct contact with the mica surface, while a complete monolayer of water wetting the slit pore decouples the graphene from the mica substrate both mechanically and electronically.

O 108.5 Fri 11:30 TRE Ma

Substrate topography and annealing of Co/Gr/SiC(0001) investigated by means of photoemission electron microscopy — •Richard Hönig, Philipp Espeter, Peter Roese, Karim Shamout, Hermann Kromer, Ulf Berges, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4a, 44227 Dortmund, Germany

The realization of carbon electronics requires semiconducting substrates, therefore epitaxial graphene on silicon carbide is a promising candidate. Challenges with this system are the covalently bonded buffer layer impacting the electronic properties, and the limited graphene grain size depending on the preparation conditions.

Here, the so-called confinement controlled sublimation is applied to yield a high grain size. The characterization of the samples has been carried out by photoemission electron microscopy (PEEM) which combines surface sensitivity with a mesoscopic resolution and unique contrast mechanisms. Images of samples prepared under high vacuum or under inert gas conditions are presented.

In order to decouple the buffer layer as well as for tailoring the properties of this multilayer system, the intercalation of metals underneath graphene is a common method. Consequently, we will present the first attempts of cobalt intercalation.

O 108.6 Fri 11:45 TRE Ma

Oxygen intercalation at the graphene/Ni(111) interface — •Luca Bignardi[1], Paolo Lacovig[1], Matteo Dalmiglio[1], Fabrizio Orlando[1,2], Aliakbar Ghafari[1,3], Luca Petaccia[1], Alessandro Baraldi[1,4], Rosanna Larciprete[5], and Silvano Lizzit[1] — [1]Elettra - Sincrotrone Trieste, Trieste, Italy — [2]Paul Scherrer Institut - Villingen PSI, Switzerland — [3]Helmholtz-Zentrum Berlin, Berlin, Germany — [4]Università degli Studi di Trieste, Trieste, Italy — [5]CNR - Istituto dei Sistemi Complessi, Rome, Italy

Intercalation of atomic species at the graphene-substrate interface is an effective way to decouple graphene (GR) from the metal on which it is grown, restoring the Dirac cone and tuning the GR-substrate interaction. The intercalation of oxygen was found to be successful, independently of the extent of the graphene-metal interaction, upon a suitable choice of oxygen partial pressure and sample temperature. Herein we report on the intercalation and de-intercalation of oxygen at the strongly interacting Gr/Ni(111) interface. Synchrotron-radiation based high-resolution X-ray photoelectron spectroscopy was used to characterise the intercalation mechanism and the nature of the compounds at the interface. We observed that the intercalated oxygen efficiently decouples the GR layer quenching the hybridisation with the metal substrate. Angle-resolved photoelectron spectroscopy measurements showed the restoration of the Dirac cone band-structure. Moreover, X-ray photoelectron diffraction added further insight into the structure of GR in the different phases of the process.

O 108.7 Fri 12:00 TRE Ma

Graphene phonons in inelastic electron tunnelling spectroscopy — •Johannes Halle[1], Nicolas Néel[1], Mads Brandbyge[2], and Jörg Kröger[1] — [1]Technische Universität Ilmenau, Ilmenau, Germany — [2]Technical University of Denmark, Lyngby, Denmark

Graphene on Ir(111) was intercalated by Li, Cs, and Ni. Inelastic electron tunnelling spectroscopy (IETS) unraveled remarkably strong signatures of graphene phonons for Li and Cs intercalants. For Ni-intercalated graphene, in contrast, phonon signals stayed below the detection limit of the low-temperature scanning tunnelling microscope (STM). On the basis of previously determined phonon dispersion branches the IETS features were assigned to acoustic and optical graphene phonons at the M point of the surface Brillouin zone. Additional experiments unveiled that the IETS signal increased with increasing Li coverage. Moreover, decreasing the separation between STM tip and graphene from the tunnelling to contact ranges led to a significant lowering of the phonon spectroscopic signatures. Combining these results, and comparing to transport calculations based on density functional theory, we discuss possible mechanisms that appropriately describe inelastic excitations with non-zero wave vectors via electron injection from an STM tip. Financial support by the Deutsche Forschungsgemeinschaft through Grant No. KR 2912/10-1 is acknowledged.

O 108.8 Fri 12:15 TRE Ma

Electronic transport properties of novel nanosensors based on graphene and beyond — •Frank C. Maier[1], Ganesh Sivaraman[1], Fabio A.L. de Souza[2], Rodrigo G. Amorim[3], Wanderla L. Scopel[2], Ralph H. Scheicher[4], and Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Departamento de Fisica, Universidade Federal do Espirito Santo, Vitoria/ES, Brazil — [3]Universidade Federal Fluminense, Departamento de Física, Volta Redonda/RJ, Brazil — [4]Department of Physics and Astronomy, Materials Theory, Uppsala University, Sweden

In this work, we investigate the sensing abilities of graphene based-materials. Specifically, we focus of pristine graphene and on a hybrid graphene/hexagonal boron nitride monolayer. Using density functional theory based simulations together with the non-equilibrium Green's functions formalism we are able to calculate the electronic transport across these materials, which serve as a reference. At a next step we choose small molecules (such as NO2, CO2, H2S, benzene derivatives, etc.) and attach these covalently and/or non-covalently on the graphene materials. We first analyze the structural and electronic properties of these modified graphene-based monolayers and the molecule specific signatures. Our aim is to predict their electronic transport properties and evaluate the change in the properties and the charge transfer with respect to the type of the attached molecule. In the end, we discuss our results in view of using graphene-based sensors for label-free detection of molecules and binding events.

O 108.9 Fri 12:30 TRE Ma

Switching the reactivity of graphene on Ir(111) by hydrogen intercalation. — •Richard Balog[1], Andrew Cassidy[1], Line Kyhl[1], Jakob Jorgensen[1], Antonia Cabo[1], Luca Bignardi[1], Paolo Lacovig[2], Silvano Lizzit[2], Philip Hofmann[1], and Liv Hornekaer[1] — [1]Department of Physics and Astronomy and Interdisciplinary Nanoscience Center iNANO, Aarhus University, Aarhus C DK-8000, Denmark — [2]Elettra-Sincrotrone Trieste S.C.p.A., S.S. 14 Km 163.5, 34149 Trieste, Italy

In this paper I will present XPS and STM data revealing the modified reactivity of graphene towards hydrogen when intercalated. First I will show that the extent of hydrogen intercalation can be monitored by the progressive downshift of C1s spectra until fully decoupled a quasi-freestanding graphene is formed on Ir(111). Secondly, I will show that this intercalation affects the reactivity of graphene towards H atoms but also vibrationally excited H2 molecules. I will show that while graphene on Ir(111) can be functionalized upon exposure to vibrationally excited H2, the reactions is fully suppressed in a quasi-freestanding state. Controlling the reactivity of graphene towards outer environment simply by modification of its interaction with an underlying substrate paves the way for future application of (functionalized) graphene in everyday devices.

O 108.10 Fri 12:45 TRE Ma

Intercalation and Deintercalation of Lithium at the Ionic Liquid|Graphite(0001) Interface — •Florian Buchner[1], Jihyun Kim[2], Christiane Adler[2], Joachim Bansmann[2], and R. Jürgen

Behm[1,2] — [1]Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89081 Ulm, Germany — [2]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

The intercalation and deintercalation of lithium (Li) on the graphite anode in Li-ion batteries is essential for their function. This was investigated in a model study under ultrahigh vacuum conditions as a function of temperature employing X-ray and UV photoelectron spectroscopy (XPS / UPS). After vapor deposition of metallic Li, partially charged Li$^{\delta+}$ atoms were identified on graphite(0001) at 80 K, while, they diffuse into the bulk at 300 K. Interestingly, the ionic liquid (IL) 1-butyl-1-methyl-pyrrolidinium bis-(trifluoromethylsulfonyl)amide [BMP][TFSA], which is a promising solvent/electrolyte, can be used as a probe to measure Li$^{\delta+}$ deintercalation. After adsorption of a [BMP][TFSA] (sub-)monolayer on lithiated graphite at 80 K, the sample was heated to 300 K. Both the gradual shifts of all adsorbate-related XP peaks at > 230 K and the simultaneous lowering of the work function indicate the accumulation of partially charged Li$^{\delta+}$ atoms at the IL|graphite(0001) interface. This is accompanied by a partial decomposition of the IL adlayer (LiF, Li$_2$S, and LiN$_3$, etc.), which we associate with the initial stages of the chemical formation of the electrode|electrolyte interface (EEI), which in turn is crucial for the function of batteries.

O 109: Tribology and Structure of Surfaces: Misc.

Time: Friday 10:30–13:00 Location: WIL A317

Invited Talk O 109.1 Fri 10:30 WIL A317

Discovery of 1D spin-polarized states at step edges of topological crystalline insulators — •Paolo Sessi — Universität Würzburg

Topological crystalline insulators (TCIs) are topological materials where the existence of surface Dirac states is guaranteed by crystal symmetries. This protection mechanism promises a rich phenomenology in response to crystal perturbations. In my presentation, I will report on the discovery of robust 1D spin-polarized channels naturally emerging at TCI surfaces once translational invariance is broken [1]. I will illustrate how 1D channels can be easily obtained in the prototypical TCI Pb$_{1-x}$Sn$_x$Se without the need of any sophisticated preparation technique. In particular, by correlating topographic and electronic structure information, I will show that 1D states naturally emerge at step edges consisting of an odd number of atomic layers, where translational invariance is broken, while even step edges maintain translational symmetry and are featureless. By systematically acting on the crystals stoichiometry, I will demonstrate how these 1D states are directly linked to the existence of a topologically non-trivial bulk band structure. A minimal toy model and realistic tight-binding calculations allow to identify them as spin-polarized at bands connecting two Dirac points. Finally, I will show how, contrary to 1D topological states known so far, their protection mechanisms result in a striking robustness to defects, strong magnetic fields, and elevated temperature.

[1] P. Sessi *et al.*, Science *in press.*

O 109.2 Fri 11:00 WIL A317

Temperature dependent Contact Ageing effects for Diamond and Silica Interfaces — •Matthias Vorholzer, Dirk Dietzel, and André Schirmeisen — Institute of Applied Physics, Justus-Liebig-University, Giessen, Germany

Contact ageing describes the temporal evolution of interface conditions. While this topic is well known on the macroscale, recent experiments have shown, that ageing can also play an important role in nanoscale contacts [1,2,3], where ageing is supposed to influence parameters like e.g. interface matching, contact area, or the apparent stiffness of a contact. In most cases nanoscale contact ageing is assumed to be a thermally activated process. Thus, temperature dependent measurements are a viable way to survey and thoroughly explore the relevant interface processes. Here, we present experimental data with well-defined ageing times up to 10 s for Silica-Silica and Silica-Diamond interfaces, gathered with an UHV-AFM between 15 K and 300 K using the slide-hold-slide protocol [1]. Our experimental approach gives access to both static friction and contact stiffness, which can then be compared to theoretical predictions. For each temperature the anticipated logarithmic ageing is observed, yet the temperature dependence contradicts simple scenarios based solely on thermal activation [2]. Thus, more complex and realistic ageing scenarios are currently considered to describe all aspects of contact ageing.

[1] Q. Li et al., Nature 480, 233 (2011)

[2] M. Feldmann et al., PRL 112, 155503 (2014)

[3] M. Feldmann et al., PRL 117, 025502 (2016)

O 109.3 Fri 11:15 WIL A317

Antimony Nanoparticles Sliding on MoS$_2$: The Breakdown of Superlubricity — •Dirk Dietzel[1], Jan Brndiar[2], Ivan Stich[2], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, University of Giessen, Germany — [2]CCMS, Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia

Structural lubricity is an intriguingly simple concept, that predicts ultra-low friction between substrate and slider as long as a structural mismatch prevents effective interlocking of atomic potentials at the interface. In principle, this concept should be applicable to almost any material combination. However, in experiments it is found that superlubricity is rather exotic than widespread. Often, Interface contamination must be considered a limiting factor. But even under ideal conditions, structural superlubricity can be inhibited by the mechanical stability of the materials [1]. Here, we analyze this aspect by nanomanipulation experiments for Sb nanoparticles on HOPG and MoS$_2$. Despite the similarity of these layered lubrication materials, both show significantly different frictional behavior. More specifically, MoS$_2$ shows a breakdown of superlubricity, which becomes evident by checking the scaling laws of structural lubricity [2]. To explain this breakdown we have performed additional DFT simulations, which revealed significantly heightened interface interactions, that are sufficient to drive the Sb/MoS$_2$ system out of superlubricity.

[1] T .A. Sharp, L. Pastewka, M. O. Robbins. PRB 93, 121402 (2016)

[2] D. Dietzel, M. Feldmann, U. D. Schwarz, H. Fuchs, A. Schirmeisen. PRL 111, 235502 (2013)

O 109.4 Fri 11:30 WIL A317

Effect of additives and external fields on lubricating properties of nematic liquid crystals — •Pritam Kumar Jana[1], Wei Chen[2], Mikko J. Alava[1], and Lasse Laurson[1] — [1]COMP Centre of Excellence, Department of Applied physics, Aalto University, P.O. Box 11100, Aalto 00076, Finland — [2]Computer Network Information Center, Chinese Academy of Sciences, Beijing 100190, China

Several studies have been performed to understand the structural and dynamical properties of liquid crystal lubricants under external pressure and shear stress, mainly due to the observations of ultra-low friction in such systems [1]. However, to balance between efficiency and effective cost, more extensive investigations are required. In the present study, we construct a full atomistic model where a nematic liquid crystal, 4-cyano-4-hexylbiphenyl (6CB), and a short alkane chain, hexane (C6H14), are used as lubricant and additives, respectively, and mica serves as the confining surfaces. When the sliding velocity of the upper mica plate is low enough, thin films of both pure 6CB and pure C6H14 show stick-slip dynamics. However, for the same film thickness liquid crystals exhibit higher friction as compared to hexane. In addition for thick films effective viscosities of pure liquid crystals remain constant and approximately similar to bulk viscosity. When film thickness decreases effective viscosities increase. We also consider mixtures of 6CB and C6H14, by varying their proportions, as well as the effect of external electric fields, to study the resulting lubrication properties.

[1] C. Manzato, A. S. Foster, M. J. Alava, and L. Laurson. Physical Review E 91, 012504 (2015)

O 109.5 Fri 11:45 WIL A317

Temperature dependent investigation of Ni layers on Pd with Positron annihilation induced Auger electron spectroscopy, XPS and STM — •Samantha Zimnik, Marcel Dickmann, Sebastian Vohburger, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany

Positron annihilation induced Auger Electron Spectroscopy (PAES) is a powerful technique to gather information about the elemental composition of the topmost atomic layer of a specimen. The positron beam facility NEPOMUC at the research reactor of the Heinz Maier-Leibnitz Zentrum in Garching delivers the world's most intense positron beam and enables measurement times of only a few minutes per PAES spectrum. A new sample holder allows controlling of the sample temperature during the measurement up to 500°C. Thus, time and temperature-dependent PAES have become possible and hence enable the in-situ observation of the surface segregation process. The surface spectrometer at NEPOMUC uses the complementary techniques PAES, X-ray photoelectron spectroscopy (XPS) and Scanning Tunneling Microscopy (STM) to characterize both, the elemental composition of the surface and its topology. Recent studies on sub-monolayers of Ni on Pd using time- and temperature dependent PAES will be presented.

O 109.6 Fri 12:00 WIL A317

Dipole-mediated single-molecule manipulation — •Grant Simpson[1], Víctor García-López[2], James Tour[2], and Leonhard Grill[1] — [1]University of Graz, Graz, Austria — [2]Rice University, Houston, Texas, USA

It has been long known that the scanning tunneling microscope (STM) is the perfect tool not only for imaging single molecules on surfaces, but also can be used to manipulate such molecules in a variety of ways. The classical method of lateral manipulation is either pushing or pulling via van der Waals interaction with the STM tip. In the current work it is shown that the electric field of the tip plays an important role when a dipole moment exists within a molecule. The dipolar nanocar, investigated here on the Ag(111) surface, displays rotational and translational motion under the influence of the electric field of the tip. Furthermore, the spatial dependence of the tip position with respect to the molecule reveals that the dipole moment of the molecule is the deciding factor for the direction of motion. The rotation and translation of the nanocar can therefore be carefully controlled.

O 109.7 Fri 12:15 WIL A317

Tiefenaufgelöste Wasserstoffinventarbestimmung mittels Massenspektroskopie nach Laserablation — •Jannis Oelmann, Niels Gierse, Sebastijan Brezinsek, Michaele Freisinger und Christian Linsmeier — Institut für Energie und Klimaforschung - Plasmaphysik, Forschungszentrum Jülich GmbH, 52425 Jülich, Deutschland

Eine quantitative Bestimmung des Wasserstoffgehalts in Materialien wie Metallen oder funktionellen Schichten ist essentiell in Herstellungsprozessen, beispielsweise von Solarzellen oder Festkörperbatterien. Vorgestellt wird eine Methode zur tiefenaufgelösten Bestimmung des absoluten Wasserstoffgehalts von Festkörpern ohne Probenpräparation. Zur besseren Unterscheidung vom Hintergrund wird das Wasserstoffisotop Deuterium (D_2) in Titandideuteridschichten auf Wolframsubstraten, welche mittels Magnetronsputtern hergestellt wurden, detektiert. Der Partialdruck von Deuterium wird dazu in einer Vakuumkammer nach Einzelschuss-Laserablation über Quadrupolmassenspektroskopie bestimmt. Eine quantitative Bestimmung des Deuteriumgehalts der Probe wird durch Kalibration des Massenspektrometers über Kalibrationslecks ermöglicht. Es wird die dritte Harmonische ($\lambda = 355$ nm) eines Nd:YVO_4-Lasers mit einer Impulsenergie von bis zu $E = 50$ mJ bei einer Laserimpulslänge von $\tau = 35$ ps genutzt. Folglich liegt für diese Laserparmeter die thermische Eindringtiefe in der gleichen Größenordnung wie die optischen Eindringtiefe, was schussaufgelöste Tiefenprofilmessungen durch weitere Ablationsprozesse an der selben Probenposition ermöglicht.

O 109.8 Fri 12:30 WIL A317

Chemistry of artificial 2D orbitals — •Aizhan Sabitova[1,2], Jeffrey Rawson[2,3,4], Stefan Tautz[1,2], and Ruslan Temirov[1,2] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA - Fundamentals of Future Information Technology — [3]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich, Germany — [4]Institute of Inorganic Chemistry, RWTH Aachen, Germany

Two-dimensional (2D) electron systems represent a fascinating area of research. Several bottom-top approaches to engineering of such systems with defined energy spectra have been presented recently [1-4]. In our work we pattern a commensurate monolayer of 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) on Ag(111) using a low-temperature scanning tunneling microscope to produce vacancies and study their electronic structure. Produced vacancies possess electronic orbitals that appear as a bound state below the onset of dispersive 2D interface state of PTCDA/Ag(111). Orbitals of two vacancies interact to form bonding and anti-bonding pair of orbitals, shapes of which were visualized by scanning tunneling spectroscopy imaging. This hybridization can be readily understood by analogy with chemically interacting s-orbitals. We show that vacancy structures of more complex shapes demonstrate effects of multi-orbital hybridization.

[1] K.K. Gomes et al., Nature 483, 306-310 (2012) [2] K. Seufert et al., Nano Lett. 13, 6130-6135 (2013) [3] W-X. Qiu et al., arXiv:1609.01876v1 [4] R. Drost et al., arXiv:1611.01049v2

O 109.9 Fri 12:45 WIL A317

Monitoring corrosion in nano confinement in real time using white light interferometry — •Claudia Merola[1], Hsiu-Wei Cheng[1], Ying-Ju Chen[1], and Markus Valtiner[2] — [1]Max Planck Institute, Düsseldorf, Germany — [2]Technische Universität Bergakademie, Freiberg, Germany

Crevice corrosion (CC) still remains one of the most difficult types of corrosion to detect and to prevent. Most often CC occurs in narrow fissures where oxygen access is poor and a stagnant electrolyte solution is present. Experimentally it is a challenge to obtain in-situ information of processes in confined geometries and to establish well defined confined situations in the first place. Here, white light interferometry has been used, for the first time, to study and monitor in situ the initial stages of the crevice corrosion process of thin layers of Nickel in different concentrations of NaCl solutions. Using Mica as a crevice former in an electrochemical surface apparatus allowed us to provide a deeper understanding of the initiation of the corrosion process. Electrochemical potential ramps were applied at different rates and different concentrations of NaCl led to different corrosion mechanism, based on a variation of the material transport mechanism into and out of the confined zones. Our results reveal that CC proceeds as a self-catalyzed pitting inside the confined zone and provides a surprising real-time view of the initial corrosion of confined surfaces, and hence may contribute to a deeper general understanding, and ultimately prevention, of localized corrosion.

O 110: Molecular Films: Morphology, Electronics, Photovoltaics

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

Invited Talk O 110.1 Fri 10:30 GER 38

Ceramics for Metal-Organic Frameworks (MOFs) based devices — •Paolo Falcaro — Graz University of Technology — The University of Adelaide — International Institute for Nano/Meso Materials Science

Metal organic frameworks (MOFs) are a class of ultra-porous materials with exceptionally high accessible surface area due to the framework produced by the inorganic nodes coordinated by organic ligands.1,2 An increasing number of studies are investigating MOFs for a variety of functional applications including sensing, microelectronics, energy production, drug delivery and microfluidics.3 However, MOF-based device fabrication requires synthetic protocols for the controlled functionalization of the porous crystals and the integration in suitable platforms.4 Ceramics have been recently employed for the synthesis,5,6 crystal engineering,6 functionalization,7,8 and patterning9,10 of MOFs. This presentation will summarize the recent progress in this emerging field.

References (1) Furukawa et al. Science 2013, 341(6149), 1230444. (2) Kitagawa et al. Angew. Chem. Int. Ed. 2004, 43(18), 2334. (3) Chem. Soc. Rev. 2014, 43 - special issue on MOFs. (4) Falcaro, et al. Chem. Soc. Rev. 2014, 43(16), 5513. (5) Buso et al. Chem. Mater. 2011, 23(4), 929. (6) Reboul et al. Nat. Mater. 2012, 11(8), 717. (7) Doherty et al. Acc. Chem. Res. 2014, 47(2), 396. (8) Ricco et al. J. Mater. Chem. A 2013, 1(42), 13033. (9) Zanchetta et al. Chem. Mater. 2015, 27(3), 690. (10) Okada et al. Adv. Funct. Mater. 2014, 24(14), 1969.

O 110.2 Fri 11:00 GER 38

Heterochiral to Homochiral Transition in Pentahelicene 2D Crystallization Induced by Second-Layer Nucleation — •Anaïs Mairena[1], Laura Zoppi[2], Johannes Seibel[1], Alix Tröster[3], Konstantin Grenader[3], Manfred Parschau[1], Andreas Terfort[3], and Karl-Heinz Ernst[1,2] — [1]Empa , Dübendorf, Switzerland — [2]University Zürich, Zürich, Switzerland — [3]Goethe-Universität, Frankfurt, Germany

Chirality is ubiquitous in the molecular world, but the principles of intermolecular recognition are still poorly understood. A promising approach towards a better understanding of chiral interactions is the study of self-assembly of chiral molecules on surfaces with submolecular-resolution scanning tunneling microscopy.

The self-assembly of helical racemic pentahelicene ([5]H, C22H14) on Cu(111) leads,at very low coverages to formation of non-covalently-bonded homochiral dimers. At coverages close to the monolayer (ML), two distinct long-range ordered structures have been observed. They both have homochiral dimers as building blocks. One structure consists of a conglomerate of homochiral domains, while the second structure is a racemate composed of homochiral pairs with opposite handedness. At full ML coverage only the racemic structure prevails. Above ML coverage, a transition from the denser racemate phase into the less dense homochiral conglomerate phase occurs. The observation of such transition in the 1st layer, induced by 2nd layer nucleation is unprecedented in surface science. It indicates a long-range chiral communication between 2nd layer islands and other areas on the surface.

O 110.3 Fri 11:15 GER 38

Electronic Properties of Tailored Co-Salophene Based Building Blocks on Ag(111) — •Micha Elsebach[1], Emil Sierda[1], Bernhard Bugenhagen[2], Marc Prosenc[2], Roland Wiesendanger[1], and Maciej Bazarnic[1] — [1]Institute for Nanostructures and Solid State Physics, University of Hamburg, D-20355 Hamburg, Germany — [2]Institute of Inorganic Chemistry, University of Hamburg, D-20146 University of Hamburg, Germany

Spintronic devices based on molecules are a promising approach for the future of information technology. Recently we showed that Co-salophenes can be used for the fabrication of such a device on Au(111) [1]. The basic building blocks for this device are 2Br-Co-salophenes and 3Br-3Co-salophenes. These molecules can be covalently linked by the use of an on-surface Ullmann reaction. On the Au(111)-surface the Kondo effect inhibits the control of the molecules' magnetic centers by an external magnetic field. Therefore we are searching for a different substrate material, on which all properties of the molecules are preserved, excluding the Kondo screening.

In this talk I will present STM studies on the electronic properties of single molecules as well as molecular chains formed by Ullmann reaction on Ag(111). The results show that the electronic structure of the molecules is promising for a working spintronic device, and that there is no Kondo effect on the Ag(111)-substrate.

[1] Bazarnik et al. Nano Letters 2016 16 (1), 577-582

O 110.4 Fri 11:30 GER 38

Single molecule manipulation via inelastic electron tunneling — •Gitika Srivastava[1], Tibor Kudernac[2], Manfred Parschau[1], Peter Stacko[3], Natsuki Ito[4], Takashi Hirose[4], Kenji Matsuda[4], Bernard Lucas Feringa[3], and Karl-Heinz Ernst[1,5] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — [2]University of Twente, The Netherlands — [3]Univeristy of Groningen, The Netherlands — [4]Kyoto University, Japan — [5]University of Zürich, Switzerland

Manoeuvring individual molecules over a clean and unmodified surface is challenging, yet possible using surface sensitive techniques like Scanning Tunneling Microscopy (STM). Electronic and vibrational excitation by means of inelastic electron tunnelling from the tip of STM has been observed to have brought out subsequent dynamical processes on surfaces. We investigate the influence of inelastic electron tunnelling on helical molecules and have observed molecular motions like hopping and rotation. First results of single molecular dynamics of these molecules at low temperatures (7K) on Cu(111) and Au(111) surfaces are presented and discussed. In addition, we present latest results on molecular machines, a topic that has been awarded the Chemistry Nobel Prize in 2016.

O 110.5 Fri 11:45 GER 38

Determination of large converse piezoelectric effect on a single molecule — Oleksander Stetsovych[1], •Martin Svec[1], Pingo Mutombo[1], Ondrej Krejci[1], Irena Stara[2], Ivo Stary[2], and Pavel Jelinek[1] — [1]Institute of Physics, CAS, Praha, Czech republic — [2]Institute of Chemistry and Biochemistry, CAS, Praha, Czech republic

The converse piezoelectric effect is a phenomenon, in which a mechanical strain is generated in a material due to an applied electrical field. Demonstration of the piezoelectric effect on nanoscale remains a challenge. In this work, we investigate the piezoelectric effect in single 2,17-Bis(acetylsulfanyl) heptahelicene (BA7H) molecules on Ag(111), using the non-contact atomic force microscopy (AFM). The BA7H on the substrate forms various islands, which can be effectively disassembled to individual molecules by the AFM tip, to exclude collective influence on the piezoelectric measurements. The acetylsulfanyl group at the terminal of the molecule exposed to the tip can be reversibly rotated between two metastable configurations via tip interactions. We characterized the bias-induced deformations of the BA7H and found that the piezoelectric constant is independent of the acetylsulfanyl group conformation, thereby demonstrating the piezoelectric effect is intrinsic to the helicene core. The total energy DFT calculations reveal strong charge transfer between BA7H molecule and the metallic substrate, which gives rise to a vertical electric dipole, which causes together with a soft vibrational mode of the molecule the strong piezoelectric effect.

O 110.6 Fri 12:00 GER 38

Lazarevicite-type short-range ordering in ternary III-V nanowires — •Michael Schnedler[1], Isabelle Lefebvre[2], Tao Xu[2,3], Verena Portz[1], Gilles Patriarche[4], Jean-Philippe Nys[2], Sébastien Plissard[2,5], Philippe Caroff[2,6], Maxime Berthe[2], Holger Eisele[7], Rafal Dunin-Borkowski[1], Philipp Ebert[1], and Bruno Grandidier[2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Germany — [2]Dép. ISEN, Institut d'Electronique, de Microélectronique et de Nanotechnologie, CNRS, UMR 8520, Lille Cedex, France — [3]Key Laboratory of Advanced Display and System Application, Shanghai University, PRC — [4]Laboratoire de Photonique et de Nanostructures (LPN), CNRS, Université Paris-Saclay, Marcoussis, France — [5]Laboratoire d'Analyse et d'Architecture des Systémes (LAAS), CNRS, Université de Toulouse, France — [6]Dep. of Electronic Materials Engineering, Research School of Physics and Engineering, ANU, Canberra, Australia — [7]Institut für Festkörperphysik, Technische Universität Berlin, Germany

Stabilizing ordering instead of randomness in alloy semiconductor materials is a powerful means to change their physical properties. We used STM and TEM to reveal an unrecognized ordering in ternary III-V materials. The lazarevicite short-range order, found in the shell of $InAs_{1-x}Sb_x$ nanowires, is driven by the strong Sb-Sb repulsion along $\langle 110 \rangle$ atomic chains during their incorporation on unreconstructed $\{110\}$ sidewalls. Its spontaneous formation under group-III rich conditions of growth offers the prospect to broaden the limited classes of ordered structures occurring in III-V semiconductor alloys.

O 110.7 Fri 12:15 GER 38

All-Carbon Nanocapacitors from Graphene–Carbon Nanomembrane–Graphene Heterostructures — •Emanuel Marschewski[1], Xianghui Zhang[1], Thomas Weimann[2], Paul Penner[1], Daniel Emmrich[1], Peter Hinze[2], and Armin Gölzhäuser[1] — [1]Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig

We demonstrated the fabrication and characterization of all-carbon capacitors (ACCs) composed of multilayer stacks of dielectric carbon nanomembranes (CNMs) that are sandwiched between two CVD graphene sheets that act as conducting electrodes. CNMs were formed from a series of phenylthiol homologues, i.e. biphenylthiol (BPT), p-terphenylthiol (TPT), and p-quaterphenylthiol (QPT). Two-layer and six-layer CNMs were used as the dielectric layer between the top and bottom trilayer graphene electrodes.The junction areas of the nanocapacitors range from 1 to 2500 μm^2. The frequency response of nanocapacitors has been measured with an LCR meter and the impedance spectra could be analyzed with a simple equivalent circuit. The dielectric constant of oligophenyl-based multilayer CNMs could be determined from the junction capacitance. These results suggest that the combination of graphene and CNMs as well as other 2D materials in nanoscale functional devices may provide a promising approach toward further development of molecular electronics devices.

O 110.8 Fri 12:30 GER 38

Diffusion Properties of Molecular Dopants in Organic

Semiconducting Polymers — Patrick Reiser[1,3], Vipilan Sivanesan[2,3], •Sebastian Beck[2,3], Wolfram Jaegermann[1,3], and Eric Mankel[1,3] — [1]Institute for Materials Science, Technische Universität Darmstadt — [2]Kirchhoff-Institut für Physik, Universität Heidelberg — [3]InnovationLab GmbH, Heidelberg

In this study we investigate the diffusion of a solution-processable metal-organic molybdenum complex (Mo(tfd-$CO_2Me)_3$) acting as p-dopant in Poly(3-hexylthiophen) (P3HT) thin films. In general, doping of organic semiconductors significantly increases the charge carrier concentration and improves transport and injection at contacts. However, in photo-active layers and at donor-acceptor interfaces a molecular dopant can act as exciton quencher. Therefore the diffusivity of molecular dopants is of interest for device stability and lifetime. Here, the dopant diffusion is measured at room temperature in 50nm polymer films using long-term Photoemission Electron Spectroscopy (PES) measurements. Molar surface fractions are derived from characteristic core-level emission lines. A simple analytical model can be employed to determine diffusion coefficients from time-dependent changes in surface doping ratios. We observe an exponential concentration dependency of the diffusion constant, which gives insight into the specific diffusion mechanism.

O 110.9 Fri 12:45 GER 38

Polling Ferroelectric BiFeO3 Photoelectrodes for Switchable Charge-Transfer in the Photoelectrochemical Energy-Conversion Process — •Nasori Nasori, Dawei Cao, Zhijie Wang, Yang Xu, and Yong Lei — Prof-Schmidt-Straße 26, 98693 Ilmenau, Institute for Physics & IMN MacroNano Ilmenau University of Technology

We report BiFeO3 ferroelectric photoelectrodes with switchable charge transfer property to break the limits imposed by conventional semiconductor. Because of the prominent ferroelectric properties, the photoelectrodes are able to tune the transfer of photo-excited charges generated either in BiFeO3 or the surface modifiers by manipulating the poling conditions of the ferroelectric domains. At 0 V vs Ag/AgCl, the photocurrent canbe switched from 0 mAcm-2 to 10 mAcm-2 and the open-circuit potential changes from 33 mV to 440 mV, when the poling bias of pretreatment is manipulated from -8 V to +8 V. Additionally, the pronounced photocurrent from charge injection of the excited surface modifiers can be quenched by switching the polling bias from +8 V to -8 V.

O 111: Nanostructures at Surfaces: Molecular Systems III

Time: Friday 10:30–13:00 Location: REC/PHY C213

O 111.1 Fri 10:30 REC/PHY C213

Resolving molecular products of astro-photochemistry: light-induced hydrogenation of 1,2-bis(2-phenylethynyl)benzene — •Martin Svec[1], Jack Hellerstedt[1], Ales Cahlik[1], Oleksandr Stetsovych[1], Maria Moro Lagares[1], Irena Stara[2], Ivo Stary[2], and Pavel Jelinek[1] — [1]Institute of Physics, CAS, Praha, CR — [2]Institute of Chemistry and Biochemistry, CAS, Praha, CR

The interaction between photons and molecules is as enticing as it is elusive. Typically, light-induced reactions have complicated reaction pathways and a diverse range of products that are difficult to characterize with (liquid) solution based measurements. The advent of on-surface preparation and scanned probe measurement techniques has greatly advanced the ability to resolve complicated reactions by direct observation of structural and conformational changes. We extend this a step further by considering the possibility of reactions occurring in the dilute limit, e.g. high and ultrahigh vacuum (UHV) conditions, the nearest local approximation of the interstellar medium of our universe.

In this paradigmatic astro-photochemistry experiment, a dilute gas (in UHV) of phenyl-based molecules (1,2-bis(2-phenylethynyl)benzene) is exposed to high intensity UV light during deposition onto a single crystal metal substrate. The products are subsequently studied via low temperature (5K) scanning probe techniques capable of resolving molecular structure at the atomic level. We observe chemically altered products, assembled in geometrically distinct superstructures. Linear assemblies can exceed 250nm in length. These are identified using theoretical simulations and comparison with the AFM/STM data.

O 111.2 Fri 10:45 REC/PHY C213

Pyridyl-functionalized triarylamines self-assembled on Au(111) — •Leonid Solianyk[1], Juan Carlos Moreno-López[1], Jun Li[1], Stefano Gottardi[1], Mihaela Enache[1], Ute Meinhardt[2], Milan Kivala[2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — [2]Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Germany

Engineering of molecular nanostructures on well-defined inorganic surfaces is essential for the development of nanoelectronic devices. In order to build up the nanostructures with atomic precision, ultimate control over the underlying interactions is needed. In our work, we investigated the self-assembly of pyridyl-functionalized triarylamines on Au(111) by scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED). For deposition of submonolayer coverage onto Au(111) held at room temperature, a close-packed phase as well as a hexagonal nanoporous network were observed to co-exist. The close-packed phase is stabilized by hydrogen bonding while the nanoporous network is held together by metal-ligand interactions with native gold atoms. Thermal annealing at 180°C results in the exclusive formation of a second Au-coordinated hexagonal nanoporous network with a larger pore size. Based on STM and LEED data the structural models and the intermolecular as well as molecule-substrate interactions will be discussed. Moreover, XPS data add information about the chemical state of the structures and corroborate the findings.

O 111.3 Fri 11:00 REC/PHY C213

Controlled On-Surface Synthesis of Organic and Organometallic Macrocycles — •Qitang Fan[1], Tao Wang[2], Cici Wang[2], Junfa Zhu[2], Min Chen[1], Malte Zugermeier[1], Claudio K. Krug[1], Julian Kuttner[1], Gerhard Hilt[1], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]National Synchrotron Radiation Laboratory, University of Science and Technology of China

Macrocycles and cyclic polymers have properties distinctly different from those of their linear counterparts. While effective approaches for their synthesis in solution remain scarce, on-surface synthesis has proven to be a viable alternative due to the inherent template effects. The controlled formation of hyperbenzene and organometallic macrocycles has been achieved on (modified) metal surfaces from 4,4"-dibromo-m-terphenyl (DBMTP) precursor molecules. Hyperbenzene, a hexagon consisting of 18 phenyl rings, forms on Cu(111), Ag(111) and Au(111) with different yields, which are maximized under pseudo-high dilution conditions. On clean Cu(110), DBMTP reacts to form zigzag organometallic chains linked with C-Cu-C bonds. However, with a template based on a Cu(110)-(2 x 1)O supergrating, cyclic organometallic tetragons and hexagons are obtained on the Cu stripes (with width from 2.6 nm to 3.6 nm).These methods may pave the way for the synthesis of other macrocycles.

O 111.4 Fri 11:15 REC/PHY C213

On-surface synthesis and characterization of nonsymmetrical single-molecule nodes — •Christophe Nacci[1], Andreas Viertel[2], Stefan Hecht[2], and Leonhard Grill[1] — [1]University of Graz, Graz, Austria — [2]Humboldt-University, Berlin, Germany

On-surface reactions are a promising strategy for synthetizing complex molecular architectures that are potentially relevant in the field of novel nanostructures and molecular electronics. Suitable design of molecular building blocks is required to construct molecular nanostructures with a well-defined size, geometry and composition [1]. A molecular node, i.e. a junction where several molecular wires merge, represents a key component in monomolecular electronic circuits, but its growth requires a precise and well-defined arrangement of different building blocks. Here, we report the first construction of a chemically and geometrically well-defined covalent architecture made of one central node and three molecular wires arranged in a non-symmetrical fashion in order to ensure different conjugation pathways [2]. Slight modifications of the molecular building blocks results in significant change of the outcome of the chemical reactions involved in the on-surface synthesis process on the Au(111) surface. The electrical characterization of individual non-symmetric molecular nodes by pulling them off a supporting surface with the tip of a scanning tunneling microscope will be discussed [2]. [1] L. Grill et al., Nature Nanotechnology 2, 687 (2007) [2] C. Nacci et al., Angew. Chem. Int. Ed. 55, 13724 (2016)

O 111.5 Fri 11:30 REC/PHY C213

Structural analysis of small carbon cage molecules with low temperature scanning probe microscopy — •Jalmar Tschakert[1], Daniel Ebeling[1], Marvin Stiefermann[1], Marina Sekutor[2], Peter Schreiner[2], and André Schirmeisen[1] — [1]Institute of Applied Physics - Justus Liebig University, Gießen, Germany — [2]Institute of Organic Chemistry - Justus Liebig University, Gießen, Germany

Diamondoids are small hydrogen terminated carbon cage molecules that are composed of one or more unit cages of the diamond lattice. Self-assembled monolayers of such molecules are known for their outstanding electronic properties [1,2]. Here we study the self-assembly process of tetramantane molecules (i.e., a diamondiod that consists of four diamond unit cages) on Cu(111) and Au(111) surfaces by low temperature atomic force microscopy with CO-functionalized tips. This allows us to determine the precise orientation and arrangement of the adsorbed molecules within 2D islands, which gives new insight into the underlying mechanism of the self-assembly process of these molecules.

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[1] *Science* **316**, 1460-1462 (2007)
[2] *Nature Nanotechnology* **11**, 267-272 (2016)

O 111.6 Fri 11:45 REC/PHY C213

Photophysical properties of semiconducting armchair-edge graphene nanoribbons — •Seyed Khalil Alavi[1,2], Markus Pfeiffer[1], Boris Senkovskiy[3], Andrea Bliesener[3], Jingyi Zhu[3], Samuel Michel[3], Alexei V. Fedorov[4], Raphael German[3], Dirk Hertel[1], Danny Haberer[4], Luca Petaccia[5], Felix R. Fischer[4], Klaus Meerholz[1], Paul van Loosdrecht[3], Alexander Grüneis[3], and Klas Lindfors[1] — [1]Department of Chemistry, University of Cologne, Luxemburger Str. 116, 50939 Köln, Germany — [2]Institut für Angewandte Physik der Universität Bonn, Wegelerstr. 8, 53115, Bonn, Germany — [3]II. Physikalisches Institut, Universität zu Köln, Zülpicher Strasse 77, 50937 Köln, Germany — [4]Department of Chemistry, University of California at Berkeley, Tan Hall 680, Berkeley, CA 94720, USA — [5]Elettra Sincrotrone Trieste, Strada Statale 14 km 163.5, 34149 Trieste, Italy

Armchair graphene nanoribbons are novel one-dimensional semiconductors with well defined structure and promising optoelectronic properties. We present here for the first time observation of fluorescence from graphene nanoribbons and photophysical characterization for aligned nanoribbons on insulating substrates. We further determine the excitonic resonances in the material by wavelength dependent Raman spectroscopy. From photoluminescence measurements we obtain polarized non-bleaching emission that is excited by light polarized along the ribbon. We observe a clear spectral shift from the position of the lowest exciton. The emission is attributed to bright defects in the material, which is demonstrated by controlled photochemical induction.

O 111.7 Fri 12:00 REC/PHY C213

Substrate mediated electronic interactions of organic charge-transfer complexes on Ag(111) — •Kathrin Müller[1], Nico Schmidt[2], Stefan Link[1], Michael Grunst[3], Rene Riedel[3], Walter Malone[4], Abdelkader Kara[4], Ulrich Starke[1], Milan Kivala[3], and Meike Stöhr[2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [3]Department of Chemistry and Pharmacy University Erlangen-Nürnberg, Germany — [4]Department of Physics University of Central Florida Orlando, USA

The use of organic molecules in electronic devices is gaining increasing interest due to their low cost, flexibility and easy processability. However, organic molecules often show weak intermolecular interactions limiting the charge carrier mobility. The use of electronically complementary molecules, which exhibit strong intermolecular interaction, might overcome this problem. Here we report on the self-assembly and the electronic properties of two complementary molecules containing electron-withdrawing and -donating cyano- and methoxy-groups, respectively, on Ag(111). The investigations of the structural and electronic properties of homogeneous layers containing only one species as well as heterogeneous layers containing both were carried out by STM, STS, XPS, ARPES, UPS, LEED and DFT calculations. The molecules are strongly interacting with each other leading to an alignment of the lowest unoccupied molecular orbitals (LUMOs). However, we also observe strong molecule/substrate interactions and thus we speculate that the LUMO alignment is mediated by the metallic substrate.

O 111.8 Fri 12:15 REC/PHY C213

Imaging on-surface hierarchical assembly of chiral organometallic polymers — •Laerte L. Patera[1,2,3], Zhiyu Zou[2,4], Carlo Dri[2,3,5], Cristina Africh[2], Jascha Repp[1], and Giovanni Comelli[2,3] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]IOM-CNR Laboratorio TASC, Area Science Park, 34149 Trieste, Italy — [3]Department of Physics, University of Trieste, 34127 Trieste, Italy — [4]Abdus Salam International Centre for Theoretical Physics, 34151 Trieste, Italy — [5]Elettra - Sincrotrone Trieste S.C.p.A., 34149 Trieste, Italy

We report the first real-time observation of the self-assembly mechanisms driving the hierarchical expression of supramolecular chirality, for 10,10'-dibromo-9,9'-bianthryl on Cu(111). Molecular recognition steers a multi-level chirality transfer, leading first to the growth of chiral organometallic chains and then to the formation of enantiopure islands. The structure of the polymeric networks has been determined by means of non-contact atomic force microscopy (nc-AFM), while high-speed scanning tunnelling microscopy (STM) revealed details of the surface kinetics. The direct observation of the assembly mechanisms allowed us to evaluate the enantioselectivity of the interchain coupling, shedding light on the driving forces of the hierarchical chirality expression. Our results provide an extended characterization of processes involved in the sequential self-assembly of enantiopure structures, paving the way for the design of functional supramolecular architectures.

O 111.9 Fri 12:30 REC/PHY C213

Imaging the electronic structure of on-surface generated acenes — •Justus Krüger[1], Frank Eisenhut[1], Thomas Lehmann[1], José M. Alonso[2], Dmitry Skidin[1], Dolores Pérez[2], Enrique Guitián[2], Dmitry A. Ryndyk[1], Christian Joachim[3], Diego Peña[2], Francesca Moresco[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, Max Bergmann Center of Biomaterials, and Center for Advancing Electronics Dresden, TU Dresden, 01069 Dresden — [2]CIQUS and Departamento de Química Orgánica, Universidade de Santiago de Compostela. Santiago de Compostela 15782 — [3]GNS & MANA Satellite, CEMES, CNRS, 29 rue J. Marvig, 31055 Toulouse Cedex

We present the fabrication of acenes (polycyclic hydrocarbons formed by the linear fusion of several benzene rings) on metallic surfaces. In particular, scanning tunneling microscopy and spectroscopy of single hexacene molecules is performed to directly visualize the frontier orbital resonances and to capture their narrow energy gap. Due to the high reactivity of hexacene under ambient conditions, scanning probe investigations at the single molecule level could not be obtained so far. In this work, we proof the scalability of a recently introduced on-surface reaction [1] to generate and stabilize hexacene directly on Au(111) by making use of oxygen-containing precursors. In the last part of this talk, we analyze the electronic resonances of long acenes on Au(111) as function of their length. [1] ACS Nano, 2016, 10 (4), pp 4538-4542

O 111.10 Fri 12:45 REC/PHY C213

Thermal Fluctuations of Structured Adhered Bio-Membranes Probed with Nanometer/Microsecond Resolution — •Cornelia Monzel[1,2,3], Daniel Schmidt[4,5], Ana-Suncana Smith[4], Udo Seifert[5], Kheya Sengupta[2], and Rudolf Merkel[1] — [1]Forschungszentrum Jülich, Germany — [2]Centre Interdisciplinaire de Nanoscience de Marseille, France — [3]present address: Institut Curie, France — [4]Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [5]Universität Stuttgart, Germany

Bio-membrane adhesion is essential for life and understanding its physical basis is key for further insight into many vital processes. Here, we explore bio-membrane adhesion to heterogeneously distributed linkers, as mimicked by micropatterns of adhesive and nonadhesive regions. As bio-membrane, we use closed lipid shells, so-called giant unilammellar vesicles (GUV) which bind to the patterned linkers, but, intriguingly, exhibit a fluctuating membrane within nonadhesive regions. The thermally excited fluctuations result in an entropic repulsion spatially separating the membrane from the substrate. Additional attractive and repulsive interactions near the substrate determine the final shape of the membrane, which we explore using different adhesion pattern and applying osmotic pressure changes. We further advance Reflection Interference Contrast Microscopy and develop Dynamic Optical Displacement Spectroscopy to monitor membrane undulations with up to 4nm and 10^(-6)s resolution. From the analysis of this data and by expanding the theoretical framework a coherent view of this structured adhered membrane and its surface interaction is obtained.

O 112: Overview Talk STM and Molecular Machines: Karl-Heinz Ernst

Time: Friday 13:15–14:00 Location: HSZ 01

Invited Talk O 112.1 Fri 13:15 HSZ 01
Helical Molecules and Surfaces: Self-Assembly, Spin Filtering and Unidirectional Motors — •Karl-Heinz Ernst — Empa, Swiss Federal Laboratories for Materials Research and Technology — Department of Chemistry, University of Zurich

The Nobel Prize for Chemistry 2016 is shared by Jean-Pierre Sauvage, J. Fraser Stoddard and Ben Feringa for the development of molecular machines. The three researchers designed molecules with subunits that moved relative to each other in a controlled manner, and therefore founded a new field in chemistry. Some of their molecules can, for example under influence of light, even fulfill work, and laid the foundation for nanoscopic motors, like molecular escalators, molecular muscles and nanocars. These functional molecules are believed to have a large potential and it is expected that they become useful some days in nanomedicine or as intelligent materials.

After brief introduction into artificial devices based on natural motor proteins I will present our involvement in the realization of the first successful electrical current-driven, unidirectional motion of a synthetic molecule designed and synthesized by the Feringa group. Moreover, we very briefly report spin-dependent filtering of electrons by monolayers of helical molecules.

O 113: Thin Films, Nanostructures and Nanoparticles II

Time: Friday 10:15–13:00 Location: ZEU 114

O 113.1 Fri 10:15 ZEU 114
Shear Exfoliation of layered silica in organic solvents — •Michael Huth and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

There is a large interest in the delamination of layered silica for the production of nanocomposites. Those nanocomposites can be used for several applications, like reinforcement, flame retardant agent, or barrier applications. For all those applications, a uniform dispersion of monolayers in the nanocomposites is essential for the improvement of overall performance. In this work, layered silicaes with different intercalated molecules, so-called intercalated agents are used. Those agents change the interlayer distance between the layers forming the silica flake. The influence of those changes on the dispersion process, as well as on the morphology of the dispersed plates is investigated. The dispersions of clay are processed using a shear exfoliation in chloroform. The dispersions consist of layered silica flakes of ~ 1.5 μm length and with a thickness down to 3 nm, equivalent less than four monolayers. The obtained high aspect ratio flakes, were characterized by microscopy (TEM and AFM), UV-Vis and gravimetric measurement. The results show that high interlayer distances favor a stable dispersion of layered silicaes with a thickness of just a few monolayers.

O 113.2 Fri 10:30 ZEU 114
Gas permeation through free-standing carbon nanomembranes — •Petr Dementyev[1], Polina Angelova[2], Henning Vieker[2], Daniel Emmrich[1], and Armin Gölzhäuser[1] — [1]Universität Bielefeld, Fakultät für Physik, Universitätsstr. 25, Bielefeld — [2]CNM Technologies GmbH, Herforder Str. 155a, Bielefeld

Despite membranes-based gas separation can provide lower operation costs compared to distillation and sorption methods, membranes of superior permeance and selectivity are still under development. 2D materials seem to be promising in this context, as nanoporous membranes with the least thickness and no tortuosity would provide the ultimate permeation rate and could potentially work as molecular sieves.

Herein we employ a newly developed high vacuum permeation setup to study mass transport through free-standing carbon nanomembranes (CNMs). CNMs are formed out of self-assembled monolayers of molecules and are mechanically stable. Furthermore, CNMs can be fabricated on a large scale, and their properties are widely tunable depending on the preparation conditions.

Various CNMs were probed towards permeation of helium, neon, nitrogen, oxygen, argon and carbon dioxide. Mass-spectrometry detection enabled to determine the permeation rate and the membrane selectivity. Some of the samples were found to have defects with a characteristic size of 100 nm which was confirmed by helium ion microscopy. In turn, the intact samples were proved to be dense but highly selective to helium. We discuss the mechanism of gas separation as well as the origin of defects.

O 113.3 Fri 10:45 ZEU 114
Transfer and characterization of covalently modified large area graphene — •Felix Rösicke[1,2], Marc A. Gluba[1], Christoph Kratz[3], Timur Shaykhutdinov[3], Norbert H. Nickel[1], Jörg Rappich[1], and Karsten Hinrichs[3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]SALSA - School of Analytical Sciences Adlershof, Berlin, Germany — [3]Leibniz - Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Berlin, Germany

We have investigated the electrochemical grafting of CVD grown large area graphene, as grown on copper, by p-(N-maleimido)phenyl residues from the respective diazonium salt (p (N maleimido)phenylbenzenediazonium tetrafluoroborate). The samples were characterized using Raman backscattering and infrared spectroscopic ellipsometry measurements, both prior and after transfer to a thin gold film on silicon. Optical simulations of the C=O vibrations were performed, determining the thickness of the functional layer to approximately 4 nm, showing the possibility of a lossless transfer. Furthermore, AFM-IR experiments were performed to confirm both the thickness and homogeneity of the maleimido layer. To prove the reactivity of the p-(N-maleimido)phenyl layer, the Michael addition of a thiol was monitored via IR-microscopy. Considering the variety of possible diazonium cations, this opens the possibility to the use of modified graphene as tailored modular building block for facile and specific surface functionalization.

O 113.4 Fri 11:00 ZEU 114
Pyrolysis of carbon nanomembranes studied by gas permeation measurements — •André Beyer, Nils Klement, Riko Korzetz, Xianghui Zhang, Berthold Völkel, and Armin Gölzhäuser — Physics of Supramolecular Systems and Surfaces, Bielefeld University, 33615 Bielefeld, Germany

Carbon nanomembranes (CNMs) from aromatic self-assembled monolayers are made by electron exposure of the molecular monolayers, resulting in cross-linked membranes which are 1 nm thick and exhibit molecular sieving characteristics in gas permeation experiments [1]. Annealing at 1200 K in vacuum transforms CNMs into nanocrystalline graphene [2, 3]. Here, this transformation process is studied by gas permeation measurements of CNMs after annealing at different intermediate temperatures in the range between 600 K and 900 K. To this end, CNMs were placed onto polydimethylsiloxane (PDMS) membranes after completion of the annealing process to determine their gas permeation characteristics with different gases (He, Ne, CO_2, Ar, Kr, N_2). A resistance model is employed to discriminate the permeation characteristics of the annealed CNMs from the PDMS support membranes [1]. It is found that a major part of the transformation process occurs at temperatures between 670 K and 770 K.

[1] M. Ai et al., Adv. Mater. 26 (2014) 3421.

[2] A. Turchanin et al., Adv. Mater. 21 (2009) 1233.

[3] A.Turchanin, et al., ACS Nano 5 (2011) 3896.

O 113.5 Fri 11:15 ZEU 114

Transparent Graphene Electrodes for Biomedical Applications — •Pranoti Kshirsagar[1], Thomas Chassé[3], Monika Fleischer[2], and Claus J. Burkhardt[1] — [1]NMI Natural and Medical Sciences Institute at the University of Tübingen, 72770 Reutlingen (Germany) — [2]Institute for Applied Physics and Center LISA+, Eberhard Karls University Tübingen, 72076 Tübingen (Germany) — [3]Institute of Physical and Theoretical Chemistry and Center LISA+, Eberhard Karls University Tübingen, 72076 Tübingen (Germany)

Since its isolated preparation in 2004, graphene is one of the most extensively researched materials. However, the entry of graphene into the field of biomedicine is relatively recent. Microelectrode arrays (MEAs) are often used to record the cellular activity from cells like neurons or cardiomyocytes. Au, TiN, Pt and PEDOT-CNTs are some of the electrode materials which are excellently suited for the cellular recordings. However, all these materials are opaque posing limitation for applications such as optogenetics and calcium imaging.

Here we present the development of MEAs with transparent graphene electrode and their application. 2.5 cm x 2.5 cm largely monolayer graphene is CVD grown and subsequently transferred onto the conduction lines of a MEA substrate. Detailed correlative scanning electron microscopy (SEM) and Raman spectroscopy is performed confirming the presence of graphene after each processing step. SEM is used for visualization of graphene and Raman confirms the number of layers. Graphene micro electrodes of 30 micron diameter are fabricated with this reliable process and successfully tested with cell cultures.

15 min break

O 113.6 Fri 11:45 ZEU 114

Patterned 2-D materials by laser ablation and self-assembly — •Daniel Rhinow[1], Natalie Freese[2], Julian Scherr[3], Andreas Terfort[3], André Beyer[2], Armin Gölzhäuser[2], and Norbert Hampp[4] — [1]Max-Planck-Institut für Biophysik, Abteilung Strukturbiologie, 60438 Frankfurt, Deutschland — [2]Universität Bielefeld, Fakultät für Physik, 33501 Bielefeld, Deutschland — [3]Goethe-Universität Frankfurt, Fachbereich Chemie, 60438 Frankfurt, Deutschland — [4]Philipps-Universität Marburg, Fachbereich Chemie, 35032 Marburg, Deutschland

Self-assembled monolayers (SAMs) of thiols on gold can be patterned using a variety of physical and chemical methods. Irradiation of SAMs on gold with a pulsed 532 nm laser beam leads to thermal desorption of thiol molecules. The gaps are filled with a second thiol SAM and a patterned SAM is obtained. Photothermal patterning of SAMs enables the fabrication of arbitrary structured monolayers with lateral dimensions in the centimetre range. We demonstrate that phothothermal desorption of aromatic thiols can be used to produce patterned two-dimensional materials. Patterned carbon nanomembranes have been analyzed by helium ion microscopy, scanning electron microscopy and photoelectron spectroscopy.

O 113.7 Fri 12:00 ZEU 114

Surface-Enhanced Characterization of Nanoparticle Surfaces — •Christian Kuttner[1,2], Roland P.M. Höller[1], Martin Mayer[1,2], Max J. Schnepf[1], and Andreas Fery[1,2,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [2]Cluster of Excellence Centre for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden, Germany — [3]Physical Chemistry of Polymeric Materials, Technische Universität Dresden, 01069 Dresden, Germany

We present the retrieval of molecular information at nanoparticle surfaces using surface-enhanced Raman scattering (SERS). The electric-field enhancement of the localized surface plasmon resonances (LSPRs) of noble metal nanoparticles can be exploited for the local characterization of their molecular surface near field. [1]

Consequently, we studied the nanoparticles' ligand corona in dispersion and its exchange based on the example of low-molecular-weight surfactants against high-molecular-weight proteins. [2]

[1] Höller, R.P.M. *et al.*, *ACS Nano* **2016**, *10*, 5740–5750.

[2] Tebbe, M. *et al.*, *ACS Appl. Mater. Interfaces* **2015**, *7*, 5984–5991.

O 113.8 Fri 12:15 ZEU 114

***In-situ* Small-angle X-ray Scattering and UV-vis spectroscopy Investigations of the Formation and Growth of Inorganic Nanoparticles by Microwave-Assisted Solvothermal Synthesis** — •Robert Wendt[1], Eike Gericke[1], Dragomir Tatchev[2], Armin Hoell[3], Markus Wollgarten[3], Simone Raoux[3], and Klaus Rademann[1] — [1]Humboldt-Universität zu Berlin, Berlin, Germany — [2]Bulgarian Academy of Sciences, Sofia, Bulgaria — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Microwave-assisted solvothermal syntheses (MWASS) have become subject of renewed fundamental interests in the preparation of crystalline and monodisperse inorganic nanoparticles (NPs). Main features of MWASS are distinguished control and exact on-line determination of pressure and temperature inside the autoclave-type reactors. The advantage is the efficient internal volumetric "in-core" heating by direct coupling of MW energy to the reaction molecules. It allows high heating rates with small thermal gradients and strongly decreased reaction times based on the Arrhenius law. This work includes innovative *in-situ* investigations of the formation and growth mechanisms of inorganic NPs by this new developed MWASS-system. It allows exact additions of precursor solution into the sealed reactor and withdrawals of colloid solution at any time. Thereby, we are able to investigate and characterize the NPs in a time-range of seconds by *in-situ* UV-Vis spectroscopy and SAXS and *ex-situ* by TEM, EELS and EXAFS. These results provide new insights in the formation and growth mechanisms.

O 113.9 Fri 12:30 ZEU 114

Metrology on Nascent Soot Particles from Flames by Helium Ion Microscopy — •Daniel Emmrich[1], Maurin Salamanca[2], Lena Ruwe[2], Henning Vieker[1], André Beyer[1], Katharina Kohse-Höinghaus[2], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems, Bielefeld University, 33615 Bielefeld, Germany — [2]Department of Chemistry, Bielefeld University, 33615 Bielefeld, Germany

Soot emissions from combustion processes are a problem for environment and health. A detailed understanding on the formation process of soot is a prerequisite for the development of strategies to reduce the emission of soot. While mature soot particles are spherical aggregates with dimensions of 20-50 nm, nascent soot particles are smaller and structurally inhomogeneous. Thus, especially the latter poses challenges in their characterization. In this study, we extracted soot particles from flames of different fuels and use helium ion microscopy (HIM) to determine size and shape of the particle down to a size of 2 nm. HIM is a scanning technique similar to scanning electron microscopy (SEM) but taking advantage from the higher mass of the helium ions. The use of helium ions in comparison to electrons in SEM enables higher contrast accompanied with high resolution, high surface sensitivity and low beam currents resulting in low sample damage. This microscope enables high throughput and high resolution to follow the growth of nascent soot particles taken at different distances from the burner surface [1, 2]. [1] M. Schenk et al., ChemPhysChem, 14, 3248 (2013) [2] M. Schenk et al., Proc Combust Inst, 35, 1879 (2015)

O 113.10 Fri 12:45 ZEU 114

Mean free path of slow electrons retrieved from velocity map imaging of aerosol particles — •Maximilian Goldmann[1], Bruce L. Yoder[1], Stavros Amanatidis[1], Egor Chasovskikh[1], Lukas Lang[1], Andras Bodi[2], David Luckhaus[1], and Ruth Signorell[1] — [1]Laboratorium für physikalische Chemie, ETH Zürich, 8093 Zürich — [2]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen

Electron mean free paths are important quantities for a number of physico-chemical phenomena ranging from aerosol physics and chemistry to radiation damage of biological tissues. We introduce and apply a novel method to determine the electron mean free path of low energy electrons in solid and liquid materials by velocity map imaging photoelectron spectroscopy of neutral aerosol particles using vacuum ultraviolet light. We extract the electron mean free path by comparing experimental with simulated photoelectron velocity map images of aerosol particles. For the simulation, we use a detailed scattering model [1].

Experimental photoelectron spectra of potassium chloride nanoparticles [2], liquid water droplets [1], and liquid-coated nanoparticles are presented. These photoelectron images were recorded at the VUV beamline at Paul Scherrer Institute and by means of a home-built table-top laser system.

[1] R. Signorell et al., Chem. Phys. Lett. 658, 1 (2016).

[2] M. Goldmann et al., J. Chem. Phys. 142, 224304 (2015).