Surface Science Division
Fachverband Oberflächenphysik (O)

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Overview of Invited Talks and Sessions

(Lecture halls HSZ 01, 02, GER 37, 38, REC C 213, TRE Ma, Phy, WIL A317, B321, and C107;
Poster P1A, P1C, P2/EG, P2/1OG, P2/2OG)

Prize Talks Prepending Surface Science Sessions

PRV II	Mon	15:00–15:30	WIL B321	**Hartree-Fock simulation of hematite surfaces with *a posteriori* calculation of correlation energy** — •David Scholz, Thomas Stirner
PRV V	Wed	15:00–15:30	WIL A317	**Toward Atomic-Scale Optical Spectroscopy in Plasmonic STM Junctions** — •Takashi Kumagai

Invited Talks

O 5.1	Mon	10:30–11:00	GER 38	**Predominance of non-adiabatic effects in zero-point renormalization of electronic energies.** — •Xavier Gonze, Anna Miglio, Véronique Brousseau-Couture, Gabriel Antonius, Yang-Hao Chan, Steven Louie, Giantomassi Matteo, Michel Côté
O 6.2	Mon	10:45–11:15	REC C 213	**Excited State Dynamics at Interfaces with Organic Semiconductors** — •Petra Tegeder
O 7.4	Mon	11:15–11:45	TRE Ma	**Surface templating in on-surface synthesis: Directing the reaction pathway** — Antje Kutz, Md Taibur Rahman, Ville Haapasilta, Chiara Venturini, Ralf Bechstein, André Gourdon, Adam S. Foster, •Angelika Kühnle
O 11.1	Mon	10:30–11:00	WIL C107	**A microscopic view of graphene quantum Hall edge states with STM and AFM measurements** — •Joseph A. Stroscio
O 15.1	Mon	15:00–15:30	REC C 213	**Molecular nanostructures on metals vs. graphene: towards preserving functional properties** — •Meike Stöhr
O 16.3	Mon	15:30–16:00	TRE Ma	**Nanotuning via local work function control: Ethylene hydrogenation on supported Pt nanoclusters** — •Ueli Heiz, Marian D. Rötzer, Maximilian Krause, Andrew S. Crampton, Bokwon Yoon, Uzi Landman
O 17.4	Mon	15:45–16:15	TRE Phy	**Tales of 1000 and 1.2 electrons: Grand Canonical Simulations of Electrified Interfaces using Implicit Solvation Models** — •Nicolas G. Hörmann
O 17.7	Mon	16:45–17:15	TRE Phy	**Electrochemical microcalorimetry - measuring the entropy of electrochemical reactions** — •Rolf Schuster
O 18.1	Mon	15:00–15:30	WIL A317	**Probing Nanophotonic Modes and Optical Phase Shaping of Electron Beams in Ultrafast Transmission Electron Microscopy** — •Armin Feist
O 19.6	Mon	16:15–16:45	WIL C107	**Atomic scale neural circuitry capable of self-adaptation** — •Brian Kiraly
O 20.3	Mon	16:00–16:30	WIL B321	**Polarons in oxide surfaces** — •Cesare Franchini
O 41.2	Tue	10:45–11:15	TRE Ma	**Molecular switches at surfaces** — •Petra Rudolf
O 41.5	Tue	11:45–12:15	TRE Ma	**Molecular Nanoprobe - utilizing a single molecule as detector** — •Markus Leisegang
O 42.1	Tue	10:30–11:00	TRE Phy	**Exploring the Design Space of Organic Semiconductors with Machine Learning** — •Harald Oberhofer

O 42.2	Tue	11:00–11:30	TRE Phy	**Machine learning for molecular nanorobotics** — •Christian Wagner
O 42.8	Tue	12:45–13:15	TRE Phy	**Theory-informed Machine Learning for Interface Structure Reconstruction from Experimental Data** — Eric Schwenker, Chaitanya Kolluru, Spencer Hills, Arun Mannodi Kanakkithodi, Fatih Sen, Michael Sternberg, •Maria Chan
O 44.1	Tue	10:30–11:00	WIL B321	**Attosecond coherent manipulation of electrons in tunneling microscopy** — •Manish Garg, Klaus Kern
O 44.7	Tue	12:15–12:45	WIL B321	**Ultrafast dynamics of charge transfer and Frenkel excitons in molecular thin films** — •Benjamin Stadtmüller
O 45.3	Tue	11:00–11:30	WIL C107	**In-situ identification of catalytically active surface sites using electrochemical STM** — •Aliaksandr Bandarenka
O 61.1	Wed	10:30–11:00	GER 38	**Hybrid Perovskites: polarons, excitons and phase diagrams** — •Georg Kresse, Menno Bokdam, Ryosuke Jinnouchi
O 62.1	Wed	10:30–11:00	REC C 213	**Towards FAIR experimental data** — •Claudia Draxl
O 62.7	Wed	12:15–12:45	REC C 213	**Reproducible data analysis with Snakemake** — •Johannes Köster
O 63.2	Wed	10:45–11:15	TRE Ma	**The art of molecular manipulation with the scanning tunneling microscope: controlled rotations** — •Nicolas Lorente
O 64.9	Wed	12:30–13:00	TRE Phy	**On-surface Chemical Reactions of Heterocycles for Functional Nanomaterials** — •Shi-Xia Liu
O 67.1	Wed	10:30–11:00	WIL C107	**The shiniest gold (111) surface** — Weronica Linpe, Jonas Evertsson, Giuseppe Abbondanza, Alfred Larsson, Gary Harlow, Johan Zetterberg, Lisa Rämisch, Sebastian Pfaff, •Edvin Lundgren
O 70.1	Wed	15:00–15:30	GER 38	**Electron-phonon interactions in realistic materials** — •Fabio Caruso
O 71.1	Wed	15:00–15:30	REC C 213	**Detection of strong interaction between electrons and antiferromagnetic magnons in $\mathbf{Ba_{1-x}K_xMn_2As_2}$** — Tianlun Yu, Rui Peng, Guanghan Cao, •Haichao Xu, Donglai Feng
O 73.3	Wed	15:30–16:00	TRE Phy	**1.*Real-space investigation of the influence of polar species on ice structure** — •Karina Morgenstern
O 99.3	Thu	11:00–11:30	GER 38	**Exploration of complex interfacial networks and 2D tesselations** — •Johannes V Barth
O 102.1	Thu	10:30–11:00	TRE Phy	**Video STM of particle diffusion on crowded surfaces** — •Joost Wintterlin
O 106.1	Thu	15:00–15:30	GER 38	**Huge quantum effects on the 250 K superconducting lanthanum hydride** — •Ion Errea
O 107.5	Thu	16:00–16:30	REC C 213	**Coupling of electronic and atomic degrees of freedom in surface-stabilized quasi-1D systems** — •Wolf Gero Schmidt
O 112.1	Thu	15:00–15:30	WIL C107	**Positron Beams for Elemental and Structure Analysis of Surfaces** — •Christoph Hugenschmidt
O 119.1	Fri	10:30–11:00	REC C 213	**theoretical studies on the state and fate of single atom catalysts: from hydroformylation to CO oxidation** — •Felix Studt
O 120.1	Fri	10:30–11:00	TRE Ma	**Ultrafast charge transfer dynamics in 2D heterostructures** — •Giulio Cerullo, Stefano Dal Conte, Zilong Wang, Chiara Trovatello
O 120.3	Fri	11:15–11:45	TRE Ma	**Dynamic non-linear multi-frequency analysis: investigating the electron-transfer theory** — •Fabio La Mantia
O 120.7	Fri	12:30–13:00	TRE Ma	**Resolving Chemical Bond Dynamics at an Electrode Surface** — •Tanja Cuk
O 121.3	Fri	11:00–11:30	TRE Phy	**Photoelectron spectroscopy at liquid/solid interfaces** — •Hendrik Bluhm

Invited talks of the joint symposium SYSD

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:55	HSZ 02	**Disentangling transport in topological insulator thin films down to the nanoscale** — •Felix Lüpke
SYSD 1.2	Mon	9:55–10:20	HSZ 02	**Spintronics with Terahertz Radiation: Probing and driving spins at highest frequencies** — •Tom Sebastian Seifert, Tobias Kampfrath

SYSD 1.3	Mon	10:20–10:45	HSZ 02	**Non-radiative voltage losses in organic solar cells** — •Johannes Benduhn
SYSD 1.4	Mon	10:45–11:10	HSZ 02	**Multivalent ions for tuning the phase behaviour of protein solutions** — •Olga Matsarskaia
SYSD 1.5	Mon	11:10–11:35	HSZ 02	**Network Dynamics under Constraints** — •Malte Schröder
SYSD 1.6	Mon	11:35–12:00	HSZ 02	**Exciton spectroscopy of van der Waals heterostructures** — •Philipp Nagler

Invited talks of the joint symposium SYAS

See SYAS for the full program of the symposium.

SYAS 1.1	Mon	15:00–15:30	HSZ 02	**Ultrafast Coherent Spin-Lattice Interactions in Ferromagnets** — •Steven L. Johnson
SYAS 1.2	Mon	15:30–16:00	HSZ 02	**Ab-initio treatment of ultrafast spin-dynamics** — •Sangeeta Sharma, J. K. Dewhurst
SYAS 1.3	Mon	16:00–16:30	HSZ 02	**Light-wave driven Spin Dynamics** — •Martin Schultze, Sangeeta Sharma, Markus Münzenberg
SYAS 1.4	Mon	16:45–17:15	HSZ 02	**All-coherent subcycle switching of spins by THz near fields** — •Christoph Lange
SYAS 1.5	Mon	17:15–17:45	HSZ 02	**Ultrafast optically-induced spin transfer in ferromagnetic alloys** — •Stefan Mathias

Invited talks of the joint symposium SYBD

See SYBD for the full program of the symposium.

SYBD 1.1	Tue	9:30–10:00	HSZ 02	**Materials innovation driven by data and knowledge systems** — •Surya Kalidindi
SYBD 1.2	Tue	10:00–10:30	HSZ 02	**Network Theory Meets Materials Science** — •Chris Wolverton, Murat Aykol, Vinay Hegde
SYBD 1.3	Tue	10:30–11:00	HSZ 02	**Verification and error estimates for ab initio data** — •Claudia Draxl
SYBD 1.4	Tue	11:15–11:45	HSZ 02	**Identifying Domains of Applicability of Machine Learning Models for Materials Science** — •Mario Boley, Christopher Sutton, Luca M. Ghiringhelli, Matthias Rupp, Jilles Vreeken, Matthias Scheffler
SYBD 1.5	Tue	11:45–12:15	HSZ 02	**Deep learning of low-dimensional latent space molecular simulators** — •Andrew Ferguson

Invited talks of the joint symposium SYWH

See SYWH for the full program of the symposium.

SYWH 1.1	Wed	15:00–15:30	HSZ 02	**Engineering 2D materials with a twist** — •Cory Dean
SYWH 1.2	Wed	15:30–16:00	HSZ 02	**Flat Bands and Correlated Electronic States in Two Dimensional Atomic Crystals** — •Eva Y. Andrei
SYWH 1.3	Wed	16:00–16:30	HSZ 02	**Lightwave electronics and valleytronics in van der Waals layered materials** — •Rupert Huber
SYWH 1.4	Wed	16:30–17:00	HSZ 02	**Interaction and Topological Effects in Atomically Thin Two-dimensional Materials** — •Steven G. Louie
SYWH 1.5	Wed	17:00–17:30	HSZ 02	**Excitons in 2D Semiconductors and Heterostructures** — •Alexander Högele

Invited talks of the joint symposium SYED

See SYED for the full program of the symposium.

SYED 1.1	Thu	9:30–10:00	HSZ 01	**Ultrafast electron dynamics at laser-irradiated surfaces** — •Baerbel Rethfeld

SYED 1.2	Thu	10:00–10:30	HSZ 01	**Unraveling Momentum-Dependent Electron-Phonon Coupling and its Role in the Origin of Charge Density Wave Phases** — •Bradley Siwick, Martin Otto, Jan-Hendrik Pohls, Laurent Rene de Cotret, Mark Sutton
SYED 1.3	Thu	10:30–11:00	HSZ 01	**Light MATTERs!!!** — •Hrvoje Petek, Andi Li, Zehua Wang, Marcel Reutzel
SYED 1.4	Thu	11:15–11:45	HSZ 01	**Quantum localization and delocalization of charge carriers in molecular organic crystals** — •Jochen Blumberger
SYED 1.5	Thu	11:45–12:15	HSZ 01	**Single-Atom Catalysis (SAC): How Structure Influences Reactivity** — •Gareth Parkinson

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Thu	9:30–10:00	HSZ 02	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs
SYES 1.2	Thu	10:00–10:30	HSZ 02	**Mechanics of life: Cellular forces and mechanics far from thermodynamic equilibrium** — •Timo Betz
SYES 1.3	Thu	10:30–11:00	HSZ 02	**A hydrodynamic approach to collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.4	Thu	11:15–11:45	HSZ 02	**The spindle is a composite of two permeating polar gels** — David Oriola, Benjamin Dalton, Franziska Decker, Frank Julicher, •Jan Brugues
SYES 1.5	Thu	11:45–12:15	HSZ 02	**Adding magnetic properties to epitaxial graphene** — •Rodolfo Miranda
SYES 2.1	Thu	15:00–15:30	HSZ 01	**Interactions in assemblies of surface-mounted magnetic molecules** — •Wolfgang Kuch
SYES 2.2	Thu	15:30–16:00	HSZ 01	**Towards phononic circuits based o optomechanics** — •Clivia M. Sotomayor-Torres
SYES 2.3	Thu	16:00–16:30	HSZ 01	**Optical properties of 2D materials and heterostructures** — •Janina Maultzsch
SYES 2.4	Thu	16:45–17:15	HSZ 01	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 2.5	Thu	17:15–17:45	HSZ 01	**Infrared signatures of the coupling between vibrational and plasmonic excitations** — •Annemarie Pucci

Invited talks of the joint symposium SYDW

See SYDW for the full program of the symposium.

SYDW 1.1	Thu	15:00–15:30	HSZ 02	**Statics and Dynamics of Soft Wetting** — •Bruno Andreotti
SYDW 1.2	Thu	15:30–16:00	HSZ 02	**Modelling imbibition, dynamic wetting and evaporation on structured surfaces and porous coatings** — •Tatiana Gambaryan-Roisman, Noemi Ghillani
SYDW 1.3	Thu	16:00–16:30	HSZ 02	**Droplets on shaped liquid and electrically switchable surfaces** — •Glen McHale
SYDW 1.4	Thu	16:45–17:15	HSZ 02	**Liquid-liquid Dewetting: From Spinodal Breakup to Dewetting Morphologies and Rates** — •Ralf Seemann, Stefan Bommer, Roghayeh Shiri, Sebastian Jachalski, Dirk Peschka, Barbara Wagner
SYDW 1.5	Thu	17:15–17:45	HSZ 02	**Droplet durotaxis and engulfment on yielding viscoelastic gels** — •Anne Juel

Sessions

O 1.1–1.3	Mon	9:30–11:00	CHE 89	**Focus Session: Topological Phenomena in Synthetic Matter I (joint session DS/O)**
O 2.1–2.11	Mon	9:30–13:00	POT 151	**Heterostructures, interfaces and surfaces (joint session HL/O)**
O 3.1–3.12	Mon	9:30–13:00	POT 81	**2D semiconductors and van der Waals heterostructures I (joint session HL/DS/O)**

O 4.1–4.1	Mon	9:30–10:15	TRE Phy	**Overview Talk: Martin Aeschlimann**
O 5.1–5.8	Mon	10:30–12:45	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions I (joint session O/HL/CPP/DS)**
O 6.1–6.11	Mon	10:30–13:30	REC C 213	**Organic Molecules on Inorganic Substrates I: Electronic, Optical and other Properties**
O 7.1–7.12	Mon	10:30–13:45	TRE Ma	**Focus Session: Functional Molecules at Surfaces I**
O 8.1–8.11	Mon	10:30–13:15	TRE Phy	**Ultrafast Electron Dynamics I: Surfaces and Interfaces (joint session O/MA)**
O 9.1–9.13	Mon	10:30–13:45	WIL A317	**Plasmonics and Nanooptics I: Local Probes and Raman (joint session O/CPP)**
O 10.1–10.13	Mon	10:30–13:45	WIL B321	**Oxides I: Growth and Characterization**
O 11.1–11.12	Mon	10:30–13:45	WIL C107	**2D Materials I: Electronic Structure, Excitations, etc. (joint session O/CPP/HL)**
O 12.1–12.2	Mon	11:15–12:15	CHE 89	**Focus Session: Topological Phenomena in Synthetic Matter II (joint session DS/O)**
O 13.1–13.3	Mon	11:30–12:15	ZEU 255	**2D Materials (joint session CPP/O)**
O 14.1–14.10	Mon	15:00–17:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions II (joint session O/HL/CPP/DS)**
O 15.1–15.11	Mon	15:00–18:00	REC C 213	**Organic Molecules on Inorganic Substrates II: Mainly Porphyrins**
O 16.1–16.12	Mon	15:00–18:15	TRE Ma	**Nanoscale Heterogeneous Catalysis**
O 17.1–17.9	Mon	15:00–17:45	TRE Phy	**Solid-Liquid Interfaces I: Reactions and Electrochemistry**
O 18.1–18.11	Mon	15:00–18:00	WIL A317	**Plasmonics and Nanooptics II: Ultrafast and Nonlinear Phenomena (joint session O/CPP)**
O 19.1–19.12	Mon	15:00–18:15	WIL C107	**2D Materials II: Electronic Structure, Excitations, etc. (joint session O/CPP/HL)**
O 20.1–20.11	Mon	15:30–18:30	WIL B321	**Oxides II: Structures, Interactions and Reducibility**
O 21.1–21.3	Mon	16:30–17:15	ZEU 260	**Interfaces and Thin Films I (joint session CPP/O/DY)**
O 22.1–22.8	Mon	18:15–20:00	P1A	**Poster Session - 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction**
O 23.1–23.2	Mon	18:15–20:00	P1A	**Poster Session - Electron-Driven Processes at Surfaces and Interfaces**
O 24.1–24.3	Mon	18:15–20:00	P1A	**Poster Session - Electronic-Structure Theory: General**
O 25.1–25.3	Mon	18:15–20:00	P1A	**Poster Session - Focus Sessions: Innovation in Machine learning PRocEsses for Surface Science (IMPRESS)**
O 26.1–26.4	Mon	18:15–20:00	P1A	**Poster Session - Graphene: Growth, Structure and Substrate Interaction**
O 27.1–27.2	Mon	18:15–20:00	P1A	**Poster Session - Graphene: Electronic Structure, Excitations, etc.**
O 28.1–28.11	Mon	18:15–20:00	P1A	**Poster Session - Scanning Probe techniques: Method Development**
O 29.1–29.3	Mon	18:15–20:00	P1A	**Poster Session - Solid-liquid Interfaces: Structure, Spectroscopy**
O 30.1–30.11	Mon	18:15–20:00	P1A	**Poster Session - Surface Magnetism**
O 31.1–31.7	Mon	18:15–20:00	P1C	**Poster Session - Metal substrates: Structure, Epitaxy and Growth**
O 32.1–32.13	Mon	18:15–20:00	P1C	**Poster Session - Organic Molecules on Inorganic Substrates: Adsorption and Growth**
O 33.1–33.11	Mon	18:15–20:00	P1C	**Poster Session - Plasmonics and Nanooptics: Applications and other Aspects**
O 34.1–34.8	Mon	18:15–20:00	P1C	**Poster Session - Topological Insulators**
O 35.1–35.5	Mon	18:15–20:00	P1C	**Poster Session - Tribology: Surfaces and Nanostructures**
O 36.1–36.8	Tue	9:30–11:30	CHE 89	**2D Materials and their Heterostructures I (joint session DS/O/HL)**
O 37.1–37.1	Tue	9:30–10:15	TRE Phy	**Overview Talk: Bjørk Hammer**
O 38.1–38.12	Tue	9:30–13:00	ZEU 260	**Interfaces and Thin Films II (joint session CPP/O/DY)**
O 39.1–39.13	Tue	10:30–13:45	GER 38	**2D Materials III: Growth and Heterostructures (joint session O/HL)**

O 40.1–40.10	Tue	10:30–13:00	REC C 213	**Organic Molecules on Inorganic Substrates III: Electronic, Optical and other Properties**
O 41.1–41.8	Tue	10:30–13:00	TRE Ma	**Focus Session: Functional Molecules at Surfaces II**
O 42.1–42.8	Tue	10:30–13:15	TRE Phy	**Focus Session: Innovation in Machine learning PRocEsses for Surface Science (IMPRESS)**
O 43.1–43.13	Tue	10:30–13:45	WIL A317	**Plasmonics and Nanooptics III: Periodic Structures and Theory**
O 44.1–44.10	Tue	10:30–13:30	WIL B321	**Ultrafast Electron Dynamics II (joint session O/MA)**
O 45.1–45.11	Tue	10:30–13:30	WIL C107	**Solid-Liquid Interfaces II: Reactions and Electrochemistry**
O 46.1–46.8	Tue	14:00–16:00	POT 81	**2D semiconductors and van der Waals heterostructures IV (joint session HL/DS/O)**
O 47.1–47.15	Tue	18:15–20:00	P2/EG	**Poster Session - 2D Materials: Electronic Structure, Excitations, etc.**
O 48.1–48.12	Tue	18:15–20:00	P2/EG	**Poster Session - Electronic Structure of Surfaces: Spectroscopy, Surface States**
O 49.1–49.10	Tue	18:15–20:00	P2/EG	**Poster Session - Organic Molecules on Inorganic Substrates: Electronic, Optical and Other**
O 50.1–50.12	Tue	18:15–20:00	P2/EG	**Poster Session - Plasmonics and Nanooptics: Fabrication and Characterization**
O 51.1–51.3	Tue	18:15–20:00	P2/1OG	**Poster Session - Metal Substrates: Adsorption and Reaction of Small Molecules**
O 52.1–52.12	Tue	18:15–20:00	P2/1OG	**Poster Session - New Methods: Experiments**
O 53.1–53.5	Tue	18:15–20:00	P2/1OG	**Poster Session - Oxides and Insulators: Adsorption and Reaction of Small Molecules**
O 54.1–54.2	Tue	18:15–20:00	P2/1OG	**Poster Session - Semiconductor substrates: Adsorption and Reaction of Small Molecules**
O 55.1–55.5	Tue	18:15–20:00	P2/2OG	**Poster Session - Nanostructured Surfaces and Thin Films**
O 56.1–56.5	Tue	18:15–20:00	P2/2OG	**Poster Session - Nanostructures at Surfaces: Dots, Particles, Clusters**
O 57.1–57.3	Tue	18:15–20:00	P2/2OG	**Poster Session - Surface Dynamics: Phase Transitions and Elementary Processes**
O 58.1–58.8	Tue	18:15–20:00	P2/2OG	**Poster Session - Ultrafast Electron Dynamics at Surface and Interfaces**
O 59.1–59.12	Wed	9:30–13:00	POT 81	**2D semiconductors and van der Waals heterostructures V (joint session HL/DS/O)**
O 60.1–60.1	Wed	9:30–10:15	TRE Phy	**Overview Talk: Leo Gross**
O 61.1–61.11	Wed	10:30–13:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions III (joint session O/HL/CPP/DS)**
O 62.1–62.9	Wed	10:30–13:15	REC C 213	**Focus Session: Big Data in Aquisition in ARPES (joint session O/CPP)**
O 63.1–63.12	Wed	10:30–13:45	TRE Ma	**Focus Session: Functional Molecules at Surfaces III**
O 64.1–64.12	Wed	10:30–13:45	TRE Phy	**Organic Molecules on Inorganic Substrates IV: Adsorption, Growth and Networks**
O 65.1–65.12	Wed	10:30–13:30	WIL A317	**Plasmonics and Nanooptics IV: Waveguides and Antennas**
O 66.1–66.13	Wed	10:30–13:45	WIL B321	**2D Materials IV: Interfacial Interactions (joint session O/HL/CPP)**
O 67.1–67.11	Wed	10:30–13:30	WIL C107	**Solid-Liquid Interfaces III: OER, ORR, CO2RR, etc.**
O 68.1–68.4	Wed	15:00–17:15	HSZ 04	**PhD Focus Session: Symposium on "Magnetism – A Potential Platform for Big Data?" (joint session MA/AKjDPG/O)**
O 69.1–69.4	Wed	15:00–16:00	GER 37	**Tribology: Surfaces and Nanostructures (joint session O/CPP)**
O 70.1–70.9	Wed	15:00–17:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions IV (joint session O/CPP/DS/HL)**
O 71.1–71.9	Wed	15:00–17:30	REC C 213	**Electronic Structure of Surfaces I**
O 72.1–72.10	Wed	15:00–17:30	TRE Ma	**Scanning Probe Techniques I: STM-ESR and Method Development (joint session O/CPP)**
O 73.1–73.12	Wed	15:00–18:15	TRE Phy	**Organic Molecules on Inorganic Substrates V: Adsorption, Growth and Networks**

O 74.1–74.10	Wed	15:00–17:30	WIL B321	**Nanostructured Surfaces and Thin Films I: Synthesis and Properties (joint session O/CPP)**
O 75.1–75.8	Wed	15:00–17:00	WIL C107	**Metal Substrates: Growth Studies**
O 76.1–76.11	Wed	15:30–18:15	WIL A317	**Plasmonics and Nanooptics V: Tunable Structures and Nanoparticles (joint session O/CPP)**
O 77.1–77.8	Wed	18:15–20:00	P2/EG	**Poster Session - 2D Materials: Stacking and Heterostructures**
O 78.1–78.3	Wed	18:15–20:00	P2/EG	**Poster Session - Focus Session: Functional Molecules at Surfaces - Motion and Intramolecular Processes**
O 79.1–79.5	Wed	18:15–20:00	P2/EG	**Poster Session - Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interaction**
O 80.1–80.6	Wed	18:15–20:00	P2/EG	**Poster Session - Graphene: Adsorption, Intercalation and Doping**
O 81.1–81.3	Wed	18:15–20:00	P2/EG	**Poster Session - New Methods: Theory**
O 82.1–82.2	Wed	18:15–20:00	P2/EG	**Poster Session - Organic Molecules on Inorganic Substrates: Networks and Overlayers**
O 83.1–83.14	Wed	18:15–20:00	P2/EG	**Poster Session - Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy**
O 84.1–84.14	Wed	18:15–20:00	P2/EG	**Poster Session - Solid-Liquid Interfaces: Reactions and Electrochemisty**
O 85.1–85.3	Wed	18:15–20:00	P2/EG	**Poster Session - Supported Nanoclusters: Structure, Reactions, Catalysis**
O 86.1–86.9	Wed	18:15–20:00	P2/EG	**Poster Session - Organic Molecules on Inorganic Substrates: Electronic, Optical and other Properties II**
O 87.1–87.8	Wed	18:15–20:00	P2/1OG	**Poster Session - Nanostructures at Surfaces: 1D and 2D Structures and Networks**
O 88.1–88.1	Wed	18:15–20:00	P2/1OG	**Poster Session - Nanostructures at Surfaces: Other Aspects**
O 89.1–89.5	Wed	18:15–20:00	P2/1OG	**Poster Session - Oxide and Insulator Surfaces: Structure, Epitaxy and Growth**
O 90.1–90.2	Wed	18:15–20:00	P2/1OG	**Poster Session - Semiconductor Substrates: Metallic Nanowires, Overlayers, etc.**
O 91.1–91.3	Wed	18:15–20:00	P2/1OG	**Poster Session - Semiconductor Substrates: Structure, Epitaxy and Growth**
O 92.1–92.8	Wed	18:15–20:00	P2/1OG	**Poster Session - Ultrafast Electron Dynamics at Surface and Interfaces II**
O 93.1–93.8	Thu	9:30–12:00	HSZ 101	**Surface Magnetism (joint session MA/O)**
O 94.1–94.5	Thu	9:30–10:45	CHE 89	**2D Materials and their Heterostructures II (joint session DS/O/HL)**
O 95.1–95.5	Thu	9:30–10:45	CHE 91	**Thin Oxides and Oxide Layers I (joint session DS/HL/O)**
O 96.1–96.1	Thu	9:30–10:15	TRE Phy	**Overview Talk: Charlie Sykes**
O 97.1–97.13	Thu	9:30–13:00	ZEU 255	**Wetting and Liquids at Interfaces and Surfaces I (joint session CPP/O/DY)**
O 98.1–98.6	Thu	10:30–12:00	GER 37	**Graphene I: Growth, Structure and Substrate Interaction (joint session O/TT)**
O 99.1–99.11	Thu	10:30–13:30	GER 38	**Organic Molecules on Inorganic Substrates VI: Adsorption, Growth and Networks**
O 100.1–100.10	Thu	10:30–13:00	REC C 213	**Electronic Structure of Surfaces II**
O 101.1–101.5	Thu	10:30–13:00	TRE Ma	**Ertl Young Investigator Award Competition**
O 102.1–102.11	Thu	10:30–13:30	TRE Phy	**Heterogeneous Catalysis on Metals**
O 103.1–103.11	Thu	10:30–13:15	WIL A317	**Topology and Symmetry Protected Materials I**
O 104.1–104.9	Thu	10:30–12:45	WIL B321	**Ultrafast Electron Dynamics III (joint session O/MA)**
O 105.1–105.9	Thu	10:30–12:45	WIL C107	**Scanning Probe Techniques II: Method Development (joint session O/CPP)**
O 106.1–106.9	Thu	15:00–17:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions V (joint session O/HL/DS/CPP)**
O 107.1–107.9	Thu	15:00–17:30	REC C 213	**Semiconductor Surfaces (joint session O/HL)**
O 108.1–108.11	Thu	15:00–17:45	TRE Ma	**Electron-Driven Processes at Surfaces and Interfaces**
O 109.1–109.10	Thu	15:00–17:30	TRE Phy	**Heterogeneous Catalysis on Metal Oxides**
O 110.1–110.12	Thu	15:00–18:00	WIL A317	**Surface Magnetism I (joint session O/MA)**

O 111.1–111.9	Thu	15:00–17:15	WIL B321	**Nanostructured Surfaces and Thin Films II: 1D and 2D Systems (joint session O/CPP)**
O 112.1–112.9	Thu	15:00–17:30	WIL C107	**Development of Novel Methods I**
O 113	Thu	19:00–19:30	HSZ 01	**Annual General Meeting of the Surface Science Division**
O 114	Thu	19:30–20:30	HSZ 01	**Post-Deadline Talks**
O 115.1–115.1	Fri	9:30–10:15	TRE Phy	**Overview Talk: Susan Stipp**
O 116.1–116.9	Fri	9:30–12:15	ZEU 260	**Wetting and Liquids at Interfaces and Surfaces II (joint session CPP/DY/O)**
O 117.1–117.8	Fri	10:30–12:30	GER 37	**Graphene II: Adsorption, Intercalation and Doping (joint session O/TT)**
O 118.1–118.13	Fri	10:30–13:45	GER 38	**Surface Magnetism II (joint session O/MA)**
O 119.1–119.8	Fri	10:30–12:45	REC C 213	**Oxides III: Single-Atom Catalysis, Iron Oxides**
O 120.1–120.7	Fri	10:30–13:00	TRE Ma	**Focus Session: Nonequilibrium Electron Transfer Across Interfaces in Real Time**
O 121.1–121.11	Fri	10:30–13:30	TRE Phy	**Solid-Liquid Interface IV: Structure and Spectroscopy**
O 122.1–122.10	Fri	10:30–13:00	WIL A317	**Topology and Symmetry Protected Materials II**
O 123.1–123.10	Fri	10:30–13:00	WIL B321	**Nanostructured Surfaces and Thin Films III: Dots, Particles, Clusters (joint session O/CPP)**
O 124.1–124.12	Fri	10:30–13:30	WIL C107	**Development of Novel Methods II**
O 125.1–125.1	Fri	14:00–14:45	HSZ 02	**Overview Talk: Roland Wiesendanger (joint session O/CPP/DS)**

Annual General Meeting of the Surface Science Division

Thursday 19:00–19:30 HSZ 01

- Bericht
- Wahl
- Verschiedenes

O 1: Focus Session: Topological Phenomena in Synthetic Matter I (joint session DS/O)

Topological insulators are a striking example of materials in which topological invariants are manifested in robustness against perturbations. Topology has emerged as an abstract, yet surprisingly powerful, new paradigm for controlling the flow of an excitation, e.g. the flow of electrons or light. This interdisciplinary Focus Session aims at discussing the latest experimental and theoretical results in the fast developing field of topological phenomena in synthetic matter. The recent merging of topology and cold atoms, photonics, mechanics and many more fields promises a considerable impact on these disciplines. We bring together leading theoretical and experimental experts from the fields of topological phenomena in synthetic matter to discuss recent progress and interdisciplinary synergy emerging at the interface of these fields. Furthermore, we give an overview to young scientists of exciting possibilities of interdisciplinary research in these fields with the special focus on the practical applications of fundamental science.

Organizers: S. Klembt, R. Thomale, S. Höfling (Uni Würzburg) and A. Szameit (Uni Rostock)

Time: Monday 9:30–11:00 Location: CHE 89

Invited Talk O 1.1 Mon 9:30 CHE 89

In situ fabrication of (Bi,Sb)-based topological insulator - superconductor hybrid devices — •Peter Schüffelgen — Forschungszentrum Jülich, Peter Grünberg Institute 9, Jülich, Germany

With their experimental verification in 2007, topological insulators render a new and fascinating material class. A band inversion in the bulk of a 3D topological insulator creates a 2D metallic Dirac system at the physical surface of those 3D crystals. The surface Dirac states are topologically protected and have their spin locked to their momentum. This intrinsic quantum spin texture enables the realization of novel technologies, such as elusive Majorana quantum bits. In this talk, I will introduce the material class of (Bi,Sb)-based topological insulators and discuss experimental challenges. I will present an in situ process that makes it possible to construct hybrid devices comprised of topological and superconductive nanostructures fully under ultra-high vacuum conditions via molecular beam epitaxy. A combination of stencil lithography and selective area growth allows for the realization of a variety of superconductor-topological insulator hybrid devices and solves the associated fabrication challenges.

Invited Talk O 1.2 Mon 10:00 CHE 89

Atomic monolayers as two-dimensional topological insulators — •Ralph Claessen — Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany

Two-dimensional topological insulators (2D-TIs) are characterized by hosting spin-polarized conducting band states at their one-dimensional (1D) edges, giving rise to the quantum spin Hall (QSH) effect. As pointed out in the seminal work of Kane and Mele, graphene would constitute the most simple realization of a QSH insulator if it were not for its almost negligible spin-orbit interaction. It has been suggested that going to heavier group IV monolayers (such as Sn-derived "stanene") could remedy this problem, but a convincing demonstration of such 2D TIs is still lacking. Recently it has been found that going to the neighboring groups III and V in the Periodic Table provides a promising alternative approach. Here I will discuss our recent photoemission (ARPES) and scanning tunneling microscopy (STM) studies of such monolayer systems. Particular focus will be on the case of bismuthene deposited on a SiC(0001) substrate, which is identified as a large band-gap QSH insulator with almost atomically confined 1D edge states. Time permitting I will also address our recent discovery of possible topological behavior in triangular In monolayers on SiC.

Invited Talk O 1.3 Mon 10:30 CHE 89

Exceptional Topology of Non-Hermitian Systems — •Jan Carl Budich — Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

In a broad variety of physical situations ranging from classical settings to open quantum systems, non-Hermitian (NH) Hamiltonians have proven to be a powerful and conceptually simple tool for effectively describing dissipation. Motivated by recent experimental discoveries in synthetic materials, a major focus of research has developed on investigating the topological properties of such NH systems. In this talk, we present our latest results in this rapidly growing field. Specifically, we discuss the occurrence of novel gapless topological phases unique to NH systems. There, the role of spectral degeneracies familiar from Hermitian systems such as Weyl semimetals is played by exceptional points at which the effective NH Hamiltonian becomes non-diagonalizable. Furthermore, we show how guiding principles of topological matter such as the bulk boundary correspondence are qualitatively changed in the NH realm.

O 2: Heterostructures, interfaces and surfaces (joint session HL/O)

Time: Monday 9:30–13:00 Location: POT 151

O 2.1 Mon 9:30 POT 151

Determining the band alignment of copper oxide-gallium oxide heterostructures — •Sebastian Leonard Benz, Martin Becker, Angelika Polity, Sangam Chatterjee, and Peter Jens Klar — Institute for Experimental Physics I and Center for Materials Research (LaMa), Justus Liebig University Giessen, Germany

The copper oxides cuprite (Cu_2O) and tenorite (CuO) are ideal candidates for solar cells as they promise high conversion efficiencies according to the Shockley-Queisser limit[1]. However, both cannot readily be doped n-type, hampering charge-carrier extraction of the photoexcited electron-hole pairs. The combination of the copper oxides with gallium sesquioxide is considered an excellent heterojunction system for overcoming this challenge. In such a pn junction, the p-type copper oxide layer will act as absorber and the transparent n-type gallium sesquioxide as window layer. In these devices, the band alignment at the internal interface is crucial for the device performance. Here, we study the band alignments of different copper oxide-gallium sesquioxide heterostructures by X-ray photoelectron spectroscopy. Within the experimental margin of error, Cu_2O-α-Ga_2O_3 appears to offer the most favourable band alignment for photovoltaic applications.

[1] William Shockley and Hans J. Queisser (March 1961). Journal of Applied Physics. 32 (3): 510*519.

O 2.2 Mon 9:45 POT 151

Nanometer Scale Characterization of Al/TiOx/SiOx Electron Selective Passivating Contacts Utilizing Advanced TEM Methods — •Christoph Flathmann[1], Tobias Meyer[1], Valeriya Titova[2,3], Jan Schmidt[2,3], and Michael Seibt[1] — [1]University of Goettingen, IV. Physical Institute, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute for Solar Energy Research Hamelin (ISFH), Emmerthal, Am Ohrberg 1, 31860, Germany — [3]Institute of Solid-State Physics, Leibniz University Hannover, Hannover, Appelstraße 2, 30167, Germany

One promising possibility to further increase photovoltaic efficiency and to enable new solar cell designs is the development of carrier selective passivating contacts. A particularly interesting electron selective passivating contact consists of an n-type crystalline Si base with tunnel silicon oxide ($\mathrm{SiO_x}$), atomic layer deposited sub-stoichiometric titanium oxide ($\mathrm{TiO_x}$) and aluminum as a rear contact. It is commonly assumed that $\mathrm{SiO_x}$ ensures high chemical interface passivation, whilst oxygen vacancies in the $\mathrm{TiO_x}$ result in an increased open circuit voltage. However, the detailed interplay of structure, composition and electrical properties is not entirely understood yet. We, therefore, apply various STEM techniques, such as EDX, EELS and 4D-STEM, to characterize such contacts for differently treated samples. The analytical methods show strong interdiffusion at the interfaces; in particular, intermixing of Al and $\mathrm{TiO_x}$ appears to be important for contact quality. Furthermore, the capabilities of medium resolution 4D-STEM to elucidate properties of such interfaces are explored.

O 2.3 Mon 10:00 POT 151

direct insight into the structure-property relation of interfaces from first-principles crystal structure prediction — •lin sun[1], miguel a. l. marques[2,3], and silvana botti[1,3] — [1]Institut für Festkörpertheorie und Optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut für Physik - Martin-Luther-Universität Halle, D-06099 Halle, Germany — [3]European Theoretical Spectroscopy Facility

In this work we develop an efficient and accurate computational scheme aimed at a full understanding of heterogeneous materials. Our approach is a variant of the minima-hopping method for global crystal structure prediction. Specifically, we implement a constraint library and we enable variations of the atomic density in proximity to the interface. DFT and DFTB calculations supply necessary energy and forces to the minima-hopping algorithm. With this method, we find a rich polymorphism in the reconstructions of tilt boundaries in polycrystalline silicon, with recurring bonding patterns that we classify in increasing energetic order. In several cases, we succeed in identifying atomic arrangements that are significantly more stable than previously predicted structures, while in other cases we show that the algorithm can recover, without experimental input, geometries that had been built by hand to match experimental data. We extend then the calculations to other group IV elements, and compare lowest energy reconstructions of C, Si, Ge and Sn grain boundaries. Finally, a clear relation between bonding patterns and electrically active interface states is unveiled and discussed.

O 2.4 Mon 10:15 POT 151

Effect of KF and RbF post-deposition treatments on the electronic structure of the CdS/Cu(In,Ga)Se2 interface in thin-film solar cells investigated by Kelvin Probe and Photoelectron Yield Spectroscopy — •Marin Rusu[1], Tim Kodalle[2], Leo Choubrac[1], Sergiu Levcenco[1], Nicolas Barreau[3], Christian Kaufmann[2], Rutger Schlatmann[2], and Thomas Unold[1] — [1]Struktur und Dynamik von Energiematerialien, Helmholtz-Zentrum Berlin für Materialien und Energie, Lise-Meitner Campus, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]PVcomB, Helmholtz-Zentrum Berlin für Materialien und Energie, Schwarzschildstr. 3, 12489 Berlin, Germany — [3]Institut des Matériaux Jean Rouxel (IMN)-UMR6502, Université de Nantes, 2 rue de la Haussinière, 44322 Nantes Cedex 3, France

We investigate the impact of potassium fluoride (KF) and rubidium fluoride (RbF) post-deposition treatments on electronic features of the Cu(In,Ga)Se2 (CIGSe) layer and CdS/CIGSe interface in a sequential time-dependent CdS thickness evolvement over the chemical bath deposition (CBD) process. Kelvin Probe and Photoelectron Yield Spectroscopy methods have been employed. Although we observe similarities with the reported data, we observe additional distinct features. We find that after an initial CBD stage the valence band maximum of the CIGSe surface is significantly shifted (by 180-620 mV) towards the Fermi level. In addition, K and Rb act as compensating dopants in CdS. Energy level diagrams are proposed and discussed.

O 2.5 Mon 10:30 POT 151

Template-Guided Programmable Janus Heteronanostructure Arrays for Efficient Plasmonic Photocatalysis — •Zhiqiang Zeng, Rui Xu, Huaping Zhao, and Yong Lei — Technische Universität Ilmenau, 98693, Ilmenau, Germany.

Janus heteronanostructures (HNs), as an important class of anisotropic nanomaterials, could facilitate synergistic coupling of diverse functions inherited by their comprised nanocomponents. Nowadays, synthesizing deterministically targeted Janus HNs remains a challenge. Here, a general yet scalable technique is utilized to fabricate an array of programmable Janus HNs based on anodic aluminum oxide binary-pore templates. By designing and employing an overetching process to partially expose four-edges of one set of nanocomponents in a binary-pore template, selective deposition and interfacing of the other set of nanocomponents is successfully achieved along the exposed four-edges to form a densely packed array of Janus HNs on a large scale. In combination with an upgraded two-step anodization, the synthesis provides high degrees of freedom for both nanocomponents of the Janus HNs, including morphologies, compositions, dimensions, and interfacial junctions. Arrays of TiO2-Au and TiO2/Pt NPs-Au Janus HNs are designed, fabricated, and demonstrated about 2.2 times photocurrent density and 4.6 times H2 evolution rate of that obtained from their TiO2 counterparts.

30 min. break.

Invited Talk O 2.6 Mon 11:15 POT 151

Exciton-Polariton Topological Insulator — •Sebastian Klembt — Technische Physik, Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Topological insulators (TIs) constitute a striking example of materials in which topological invariants are manifested in robustness against perturbations. The most striking characteristic is the emergence of topological edge states at the interface between areas with distinct topological invariants. The observable physical effect is unidirectional, robust edge transport, immune to disorder or defects. TIs have at first been observed in the integer quantum Hall effect in fermionic systems of correlated electrons. However, during the past decade the concepts of topological physics have been introduced into numerous fields beyond condensed matter, including photonic systems. Recently, TIs were proposed in exciton-polariton systems organized as honeycomb lattices, under the influence of a magnetic field. Exciton-polaritons are the new eigenstate quasiparticles resulting from the strong coupling of quantum well excitons to light in an optical microcavity mode. Here, we demonstrate experimentally the first exciton-polariton TI and as such the first symbiotic light-matter TI. In polaritonic honeycomb lattices, we show the existence of a $C = 2$ Chern TI, manifesting in a chiral, topologically protected edge mode. Notably, due to the driven-dissipative nature of polaritons this is an open system, with a strong non-linearity still preserving the topological mode.

O 2.7 Mon 11:45 POT 151

Quantum spin Hall quantum point contacts — •niccolo traverso ziani[1], bjoern trauzettel[2], christoph fleckenstein[2], lorenzo privitera[2], and maura sassetti[1] — [1]Università degli Studi di Genova, Genova, Italy — [2]Universitaet Wuerzburg, Wuerzburg, Deutschland

The edges of two-dimensional topological insulators are fashinating systems. In order to fully exploit their potential, gaps need to be induced. While superconducting gaps can be implemented, magnetic and interaction-related ones seem to be experimentally challenging. We propose a wide range of possibilities enabled by the gaps that can open when constrictions between helical edges[1] are created. Jackiw-Rebbi charges[2], Majorana bound states[3], parafermions[4] and Floquet bound states[5] are addressed.

[1] J. Strunz, J. Wiedenmann, C. Fleckenstein, L. Lunczer, W. Beugeling, V. L. Mueller, P. Shekhar, N. Traverso Ziani, S. Shamim, J. Kleinlein, H. Buhmann, B. Trauzettel, and L. W. Molenkamp, Nat. Phys. (2019).

[2] C. Fleckenstein, N. Traverso Ziani, and B. Trauzettel EPL (Europhysics Letters) 121, 57003 (2018).

[3] C. Fleckenstein, N. Traverso Ziani, and B. Trauzettel, in preparation

[4] C. Fleckenstein, N. Traverso Ziani, and B. Trauzettel, Phys. Rev. Lett. 122, 066801 (2019)

[5] C. Fleckenstein, N. Traverso Ziani, L. Privitera, M. Sassetti, and B. Trauzettel, arXiv:1908.11719

O 2.8 Mon 12:00 POT 151

Correlation of optical properties and interface morphology in type-II semiconductor heterostructures — •Luise Rost, Jannick Lehr, Milan Maradiya, Wolfgang Stolz, and Wolfram Heimbrodt — Department of Physics and Materials Sciences Center, Philipps-Universität Marburg, Germany

The (Ga,In)As/GaAs/Ga(As,Sb) material system is used for lasers operating over a wide spectral range in the infrared. To further optimize the design of such heterostructures, it is important to have deep understanding of the influence of the interface morphology and the charge carrier dynamic through the interface. Here (Ga,In)As/GaAs/Ga(As,Sb) type-II double quantum well heterostructures has been grown by metall-organic vapor phase epitaxy. A growth interruption procedure was used to intentionally modify the morphology of the internal interfaces. The heterostructures were investigated using continuous wave and time-resolved photoluminescence spectroscopy. A correlation was revealed between the interface morphology and optical and kinetic properties. AFM images of the as grown interface surfaces show substantially smoother interfaces both on vertical as well as lateral length scales. We will illustrate that for every used material there is a matching growth interruption time to further enhance the optical response of such a type-II heterostructure.

O 2.9 Mon 12:15 POT 151

First-principles study of the structural and electronic properties of the GaAsxP1-x surface — •Marsel Karmo and Erich Runge — TU ILmenau, Weimarer Str.32, 98693 ILmenau

GaAsP is a III-V semiconductor alloy, which forms crystals in zincblende structure. Due to its high electron mobility, it is an important material in optoelectronics, mainly for solar cells. For the latter, it is important to understand the surface relaxation and reconstruction in the P-rich MOVPE process. We use the Vienna Ab initio Simulation Package (VASP) to perform first-principles calculations to identify the composition-dependent surface reconstructions and bonding-sites for adsorbates.

O 2.10 Mon 12:30 POT 151

Copper iodide thin films: Dynamic AFM studies of local electrical properties — •Tillmann Stralka, Chang Yang, Holger von Wenckstern, and Marius Grundmann — Solid State Physics, Leipzig, Germany

The search for high-performance p-type transparent conductive materials has been a major challenge in decades [1]. Copper iodide (CuI) or alloys based on CuI [2] could offer a solution, since CuI does outperform all other known p-type TCMs, concerning transmittance in the visible spectrum as well as electrical conductivity at room temperature [3]. In this contribution polycrystalline CuI thin films grown by sputtering, are investigated. Hereby we try to understand the impact of grains and grain boundaries (GBs) on transport mechanisms. Topographic features as GBs lead to a depletion of majority charge carriers and even a localized inversion (two dimensional electron gas) within GBs [4]. To acquire morphological and electrical properties with a high spatial resolution we employ atomic force microscopy, which additionally offers different modes to characterize electrical properties (such as: capacitance, conductivity and work function). These measurements will be conducted and evaluated with a novel approach that offers voltage spectroscopy and localization of sub-nm sized objects at the same time and furthermore correlate topographic features with electrical properties.

[1] M. Grundmann et al., J.Phys.D.Apps.Phys., 49(213001), 2016 [2] T. Jun et al., Adv. Mater. 30(1706573), 2018 [3] C. Yang et al., PNAS 113(412929) [4] M. Kneiß et al., Adv. Mater. Interfaces, 5(6), 2018

O 2.11 Mon 12:45 POT 151

Stability and Tunneling Transport Properties of $NiSi_2$-Si Interfaces — •Florian Fuchs[1,2,3,4], Sibylle Gemming[2,3], and Jörg Schuster[1,2,3,4] — [1]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [2]Chemnitz University of Technology, Chemnitz, Germany — [3]Center for Advancing Electronics Dresden (cfaed), Dresden, Germany — [4]Forschungsfabrik Mikroelektronik, Berlin, Germany

Metal-semiconductor interfaces are of huge importance for applications and are considered for various modern device architectures. We study the interface between $NiSi_2$ and silicon on the basis of density functional theory. Different crystal orientations and strain states are investigated systematically. The energetically most favorable interface orientation is worked out, which can explain recent experimental observations [1]. Using atomistic quantum transport simulation, the tunneling transport through the interface is calculated [2]. The transport is related to underlying properties including the Schottky barrier height and the effective mass. This is done on the basis of the Wentzel-Kramers-Brillouin approximation, which can describe the tunneling transport reasonably well. Finally, the Schottky barrier height and its strain dependence is discussed in the context of the metal-induced gap states model.

[1] Khan et al., *Appl. Sci.* **9**, 3462 (2019)
[2] Fuchs et al., *J. Phys.: Condens. Matter* **31**, 355002 (2019)

O 3: 2D semiconductors and van der Waals heterostructures I (joint session HL/DS/O)

Time: Monday 9:30–13:00 Location: POT 81

O 3.1 Mon 9:30 POT 81

Demonstration of a broadband Photodetector Based on a Two-Dimensional Metal-Organic Framework — •Himani Arora[1,2], Renhao Dong[3], Tommaso Venanzi[1,2], Jens Zscharschuch[1], Harald Schneider[1], Manfred Helm[1,2], Xinliang Feng[3], Enrique Cánovas[4], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Faculty of Physics & Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany — [3]Faculty of Chemistry and Food Chemistry & Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany — [4]Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA Nanociencia), 28049 Madrid, Spain

Electrically-conducting metal-organic frameworks (MOFs) have gained considerable attention in last years. In this regard, we report a novel semiconducting Fe3(THT)2(NH4)3 (THT, 2,3,6,7,10,11-triphenylenehexathiol) two-dimensional MOF. The developed MOF films reveal a free-charge band-like transport with a record-high Hall mobility of 230 cm2 V-1 s-1 at room temperature. We further demonstrate a proof-of-concept photodetector based on Fe3(THT)2(NH4)3 MOF films, operative in UV-to-NIR range. Due to IR bandgap of the MOF samples (0.45 eV), the photodetectors are best operated at cryogenic temperatures by suppressing the noise from thermally-activated charge carriers to obtain a clear signal from optically generated carries. Our work reports the first proof-of-concept MOF photodetector, revealing MOFs as promising candidates for optoelectronics.

O 3.2 Mon 9:45 POT 81

Theory of synchrotron-based spectroscopic techniques on two-dimensional materials — •Dominik Christiansen, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

High energy radiation enables the spectroscopic analysis of core level electronic excitations.

First, we develop a theoretical framework for X-ray absorption spectroscopy (XAS) including electronic and structural information obtained from near-edge XAS and extended XAS [1]. Analysing graphene as exemplary material, we show that the characteristic behaviour of the XAS spectra can be derived from the semi-empirical tight-binding approach by considering the spatially non local light-matter interaction.

Second, we develop a theory of exciton dynamics in time and angle resolved photoemission spectroscopy investigating the exciton formation and thermalization in ultrathin transition-metal dichalcogenides [2,3].

[1] B. Buades *et al.*, Optica **5**, 000502 (2018)
[2] D. Christiansen *et al.*, Phys. Rev. B **100**, 205401 (2019)
[3] M. Selig *et al.*, 2D Mater. **5**, 035017 (2018)

O 3.3 Mon 10:00 POT 81

The Ultimate Radiative Emission Rate of van der Waals materials — •Mark Kamper Svendsen[1], Yaniv Kurman[2], Ido Kaminer[2], and Kristian Sommer Thygesen[1] — [1]Techincal University of Denmark, Kgs. Lyngby, Denmark — [2]Technion University, Haifa, Israel

We consider the coupling between intersubband transitions in few layer transition metal dichalcogenide(TMD) stacks and graphene plasmons. Specifically, we consider few layer TMD quantum wells[1] of different thicknesses, squeezed in between a metallic substrate and a graphene sheet. Using a new, non-perturbative combined MQE-DFT time domain methodology to calculate the state evolution, we find radiative rates exceeding 1 THz and extreme Purcell factors of more than 1E6. Interestingly, we find that for certain combinations of the TMD stack width and graphene Fermi level, graphene plasmon launching becomes the dominant method of emission. This could potentially point to interesting new possibilities in graphene plasmonics.

[1] Schmidt, P., Vialla, F., Latini, S. et al. Nano-imaging of intersubband transitions in van der Waals quantum wells. Nature Nanotech 13, 1035*1041 (2018) doi:10.1038/s41565-018-0233-9

O 3.4 Mon 10:15 POT 81

Excitation-induced optical nonlinearities and charge carrier localization in atomically thin TMD semiconductors — •Daniel Erben[1], Alexander Steinhoff[1], Michael Lorke[1,2], Christian Carmesin[1], Matthias Florian[1], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen — [2]BCCMS, University of Bremen

To interpret the nonlinear optical properties of atomically thin transition metal dichalcogenides (TMD), the density of photoexcited carriers is of central importance. However, in experiments the excited carrier density is practically not accessible. For the case of above band-gap optical pumping of TMD monolayers, we utilize the semiconductor Bloch equations to determine the excitation density as function of the optical pump fluence. Our theory includes Pauli-blocking, band-gap renormalization, dephasing and screening of the Coulomb interaction due to excited carriers. The excitation density strongly depends on the wavelength of the exciting laser pulse. For pumping at the band gap, Pauli blocking of available phase space and renormalizations of the single particle energies are the dominant sources of a nonlinear density dependence, even at small pump fluence. In another study, we investigate the charge-carrier confinement in TMD nanobubbles. The latter are formed during stacking processes and exhibit quantum light emission upon optical excitation. We demonstrate that the emission originates from strong carrier localization, which is caused by the interplay of surface wrinkling, strain-induced confinement, and local changes of the dielectric environment. These effects combine to a specific localization signature that is found in recent spatially resolved photoluminescence experiments.

O 3.5 Mon 10:30 POT 81

Near-field photoluminescence of two-dimensional semiconductors — •Vlastimil Křápek, Petr Dvořák, Martin Konečný, Lukáš Kejík, Michal Horák, and Tomáš Šikola — CEITEC, Brno University of Technology, Purkyňova 123, 61200 Brno, Czech Republic

Layered two-dimensional semiconductors are ideal light sources for onchip integration. They exhibit strong luminescence even at elevated temperature, are very compact, highly tunable, and capable of single-photon emission. Since the wavelength of the light is considerably larger than the physical dimensions of the emitter, near-field handling of the emission with a deeply subwavelength spatial resolution would be of great importance. Here we present fully near-field photoluminescence experiment of two-dimensional semiconductors, with a surface plasmon interference device (SPID) used for the excitation and scanning near-field optical microscopy (SNOM) for the collection.

A SPID is formed by an opaque gold layer with the thickness of about 200 nm with the subwavelength grooves serving as sources of surface plasmon polaritons (SPP) [1]. We characterize the electric near field of SPP by SNOM, demonstrating the ability of SPP to excite the semiconductor placed on the SPID. We also demonstrate the polarization sensitivity of the experiment [1,2]. Next, we put various layered two-dimensional semiconductors on top of the SPID and characterize their SPP-excited luminescence by SNOM, demonstrating subwavelength spatial resolution.

[1] P. Dvořák et al., Opt. Express **25**, 16560 (2017).

[2] P. Dvořák et al., Nanoscale **10**, 21363 (2018).

O 3.6 Mon 10:45 POT 81

2D Semiconductors in moving and standing phonon fields — •Tobias M. Petzak, Emeline D. S. Nysten, and Hubert J. Krenner — Lehrstuhl für Experimentalphysik 1, Institut für Physik, Universität Augsburg, Universitätstr. 1, 86159 Augsburg, Germany

In this work, we prepare two-dimensional layers of transition metal dichalcogenides (TMDCs) such as MoS_2, $MoSe_2$, WS_2 or WSe_2 via micromechanical exfoliation and transfer them into the propagation path of a Surface Acoustic Wave (SAW) directly on a $LiNbO_3$ substrate via viscoelastic stamping. The electric field of the SAW couples to the electron system of the monolayer semiconductors and, thus, we gain insight into the dynamics of photogenerated charges in the sample in a non-invasive, completely contact-free, way.

Additionally, we coupled WSe_2 monolayers to the phononic modes of a high quality factor SAW resonator. This resonator-based spectroscopy increases the sensitivity of our technique. In spectrally resolved experiments using the resonator we are able to resolve the absorption edge of the 2D semiconductor which is in agreement with photoluminescence data. The latter results mark the first major step toward highly sensitive SAW spectroscopy employing SAW resonators.

30 min. break

O 3.7 Mon 11:30 POT 81

Interlayer excitons in $MoSe_2/WSe_2$ heterobilayers — •Johannes Michl[1], Oliver Iff[1], Maximilian Waldherr[1], Sefaattin Tongay[2], Martin Kamp[1], Sven Höfling[1], and Christian Schneider[1] — [1]Technische Physik, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Arizona State University

Two dimensional materials such as monolayers of transition metal dichalcogenides (TMDs) offer a wide range of possibilities for investigation due to their unique optical properties, resulting from the exotic valley physics and the strong Coulomb interaction. By stacking two different TMDs, a van der Waals heterostructure is formed. This heterobilayer can exhibit a type-II band alignment, enabling formation of interlayer excitons, with the electron and the hole residing in separate layers. As the heterobilayer is formed, spatially periodical moiré potentials occur due to the lattice mismatch and twist of the different monolayer materials. The moiré potential is predicted to have a great impact on the interaction of light with the interlayer excitons. We discuss the observation of interlayer excitons in $MoSe_2/WSe_2$ heterobilayers performing μ-PL measurements. Due to the weaker coupling strength between the electron and hole in the spatially separated arrangement, the luminscence from the interlayer excitons is shifted around 200 nanometers. The interlayer excitonic resonance is further characterized by a distinct, non-trivial peak structure, which indicates the involvement of a moiré superpotential.

O 3.8 Mon 11:45 POT 81

Interlayer excitons and band alignment in MoS_2/GaSe heterostructures. — •Christian Wagner[1,2], Mahfujur Rahaman[2], Dietrich R.T. Zahn[2], and Sibylle Gemming[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany

We study the influence of the $(\mathrm{GaSe})_n/(\mathrm{MoS}_2)_m$ heterostack composition on the band alignment and the interlayer exciton energy using *ab initio* calculations.

The electronic interaction between individual layers in a 2D heterostack is often reasonably described by a perturbation of the physical effects of the isolated layers by additional electrostatic doping and screening. In terms of optical properties, however, the formation of bound interlayer excitons composed of electrons from one layer and holes from the neighboring layer is possible. These states are measured experimentally by photoluminescence and photocurrents, e.g. in the case of MoS_2 on GaSe due to its type-II band alignment [1].

The interlayer excitons can be approximately located in k-space and energy from density functional theory by relating the band structures of the heterostack to the band structure of the individual layers. This is allowed due to the weak hybridization of electronic states between the two materials. Furthermore, the many-body description allows extracting the exciton binding energies and oscillator strengths in order to obtain the respective spectral signatures.

[1] M. Rahaman *et al.*, J. Phys.: Condens. Matter **31**, 114001 (2019)

O 3.9 Mon 12:00 POT 81

Biexcitons in 2D transition metal dichalcogenide from first principle: binding energies and fine structure — •Abderrezak Torche and Gabriel Bester — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, D-20146 Hamburg, Germany

Reducing the dimensionality of a system enhances quasiparticles interaction and leads to the formation of Coulomb bound complexes which govern most of the optical properties of semiconductors. Among these complexes, biexcitons are of special interest. Theoretically, first principle treatment of biexcitons, on the same theoretical footing as excitons and trions, is now possible thanks the the newly developed methodology of Ref. [1] which uses a hybrid approach combining configuration interaction and green function methods for the description of many-electrons many-holes excitations. This methodology is applied here to study the binding and fine structure of biexcitons in different transition metal dichalcogenides. The resulting binding energies agree better with experimental values a compared to previous effective mass treatment. The fine structure of biexcitons is shown to be highly dependent on temperature and become very dense (e.g. have many sub-peaks that are separated by hundreds of micro-eV to few meV) at room temperature.

[1] Torche, A., and Bester, G. (2019).PRB,100(20), 201403.

O 3.10 Mon 12:15 POT 81

In-plane anisotropy of the photon-helicity induced linear Hall effect in few-layer WTe$_2$ — •Simon Steinhauser[1,2], Paul Seifert[1,2], Florian Sigger[1,2], Jonas Kiemle[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], Christoph Kastl[1,2,4], Ursula Wurstbauer[1,2,5], and Alexander Holleitner[1,2] — [1]Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, D-85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstrasse 4, D-80799 München, Germany — [3]Advanced Materials Laboratory, Tsukuba, Ibaraki 305-0044, Japan — [4]Molecular Foundry, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley, California 94720, USA — [5]Institute of Physics, University of Münster, Wilhelm-Klemm-Strasse 10, D-48149 Münster, Germany

Using Hall photovoltage measurements, we demonstrate that a linear transverse Hall voltage can be induced in few-layer WTe$_2$ under circularly polarized illumination. We find that the photon-helicity induced Hall effect is strongly anisotropic with respect to the crystal axis. Our results are consistent with the Berry curvature and its dipolar distribution due to the breaking of inversion symmetry. We also studied how the Hall voltage changes with varying layer numbers. Time resolved optoelectronic autocorrelation spectroscopy shows the comparatively long spin lifetime of carriers caused by the momentum-indirect electron and hole pockets in WTe$_2$.

O 3.11 Mon 12:30 POT 81

Characterization of interlayer excitons in MoSe$_2$-WSe$_2$ heterostructures in high magnetic fields — •Johannes Holler[1], Michael Kempf[3], Jonas Zipfel[1], Mariana Ballottin[2], Anatolie Mitioglu[2], Philipp Nagler[1], Michael Högen[1], Alexey Chernikov[1], Peter Christianen[2], Christian Schüller[1], and Tobias Korn[3] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]High Field Magnet Laboratory (HFML EMFL), Radboud University Nijmegen, Netherlands — [3]Institut für Physik, Universität Rostock, Germany

In the recent years, the research on transition-metal dichalchogenides (TMDCs) and especially their heterostructures has increased a lot. These heterostructures are fabricated by stacking two different TMDCs on top of each other. With the right material combination, a type-II band alignment can be achieved and electrons and holes are spatially separated forming so-called interlayer excitons (IEXs).

Here, we study these IEXs in MoSe$_2$-WSe$_2$ heterostructures. In low-temperature PL measurements in magnetic fields of up to 30T, we observe a giant valley-selective splitting and a resulting near-unity valley polarization. In time-resolved measurements, we track the buildup of IEX valley polarization in the magnetic field. We also find a clear dependence of the magnetic-field behavior of the IEX on the stacking angles.

O 3.12 Mon 12:45 POT 81

Defect-related photoluminescence of WS$_2$ monolayers — •Marcel Ney, Aswin Asaithambi, Lukas Madauss, Marika Schleberger, Axel Lorke, and Günther Prinz — Faculty of Physics and CENIDE, University Duisburg-Essen, Germany

Two-dimensional transition metal dichalcogenide (TMD) monolayers interact efficiently with visible light due to the direct band gap nature at the K-point in momentum space. The result of the quantum confinement effects in two dimensions is a strong electron-hole Coulomb interaction, leading to a large exciton binding energy, which makes this material very promising for optoelectronic devices.

We will present low-temperature photoluminescence-spectroscopy (PL) measurements, which show the influence of laser-irradiation with different excitation powers on WS$_2$ monolayers grown on a standard Si/SiO$_2$ substrate via a chemical vapor deposition (CVD) process.

In the PL investigations, we observed a defect-related emission D$_1$, which can be assigned to adsorbate-decorated defect complexes [1]. The nature of this defect-related state investigated by laser-power-dependent measurements, will be presented in this contribution. During a laser excitation cycle, a laser-activated emission with a higher energy than the defect-related emission D$_1$, occurs. Furthermore, another defect-related emission D$_2$ was observed. Due to the annealing properties after laser-irradiation we identify this emission as a monosulfur vacancy decorated with physisorbed adsorbates [2].

[1] Z. He et al., ACS Nano 10, 5847 (2016)

[2] V. Carozo et al., Science Advances 3, e1602813 (2017)

O 4: Overview Talk: Martin Aeschlimann

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

Topical Talk O 4.1 Mon 9:30 TRE Phy

Chasing excited electrons in energy, momentum space, and time — •Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Kaiserslautern, Germany

Optically excited (hot) electrons play a crucial role for many fundamental chemical and physical phenomena occurring at surfaces, interfaces, and in bulk materials. For the investigation of such processes, time-resolved photoelectron spectroscopy turned out to be a very powerful tool through its direct access to single electron as well as transient band-structure dynamics. Recent technological breakthroughs in the development of ultrashort pulsed light sources and electron spectrometers have paved the way for a completely new generation of real-time photoemission experiments. In this presentation, I will demonstrate the potential of time-resolved momentum microscopy to study the electronic fingerprints of the elastic and inelastic scattering processes occurring at surfaces and (metal-organic) hybrid interfaces. The results reveal the unique opportunity of momentum microscopy to directly trace relaxation pathways of excited electrons in momentum space.

O 5: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions I (joint session O/HL/CPP/DS)

Electronic-structure calculations from first principles have become an indispensable and ubiquitous tool in materials modeling, design, and discovery. One of the outstanding challenges in this area is to study materials at finite temperature, in order to achieve a more realistic description of materials properties and to enable direct comparison with experimental data. To address this challenge it will be necessary to move beyond the static-ions approximation, and to devise systematic approaches for incorporating the effects of electron-phonon coupling, phonon-phonon interactions, and phonon-assisted quantum processes in state-of-the-art electronic-structure methods. The invited lectures will cover recent progress in the broad area of electron-phonon physics from the point of view of first-principles calculations. More generally, the symposium will also cover other areas of first-principles computational materials science (basic methods and applications).

Claudia Draxl (Humboldt-Universität zu Berlin, Germany), Feliciano Giustino (University of Texas at Austin, USA), Matthias Scheffler (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany)

Time: Monday 10:30–12:45 Location: GER 38

Invited Talk O 5.1 Mon 10:30 GER 38

Predominance of non-adiabatic effects in zero-point renormalization of electronic energies. — •Xavier Gonze[1,2], Anna Miglio[1], Véronique Brousseau-Couture[3], Gabriel Antonius[4,5], Yang-Hao Chan[4], Steven Louie[4], Giantomassi Matteo[1], and Michel Côté[3] — [1]UCLouvain, Belgium. — [2]Skoltech, Moscow, Russia. — [3]Dept. Physique, U. Montréal, Canada. — [4]Dept. Physics, U. California Berkeley & Materials Sci. Div. NBNL Berkeley, CA, USA. — [5]Dept. Chim., Bio. & Physique, U. Québec Trois-Rivières, Canada.

Electron-phonon interaction induces variation of bandgaps with temperature, and zero-point motion renormalization (ZPR) even at 0K. Ignored in most calculations, ZPR has been evaluated recently for several materials, often relying on the adiabatic approximation, reasonably valid for materials without infrared (IR) activity, but eagerly applied to other materials. We present the first large-scale (29 materials) first-principles evaluation of ZPR beyond the adiabatic approximation [1]. For materials with light elements the ZPR is often larger than 0.3 and up to 1.1 eV: it is useless to go beyond G0W0 without including ZPR in such materials. For IR-active materials, global agreement with experimental data is obtained only with nonadiabatic effects. They even dominate ZPR for many materials. A generalized Fröhlich model that represents accurately nonadiabatic effects accounts for more than half the ZPR for a large set of materials.

[1] A. Miglio, V. Brousseau-Couture, G. Antonius, Y.-H. Chan, S.G. Louie, M. Giantomassi, M. Côté, and X. Gonze. Submitted.

O 5.2 Mon 11:00 GER 38

A generalized first-principles formalism for the electron-phonon renormalization of electronic energy eigenvalues — •Jae-Mo Lihm[1,2,3] and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

The interaction between electrons and phonons induce a temperature-dependent renormalization of electronic energy eigenvalues [1]. The perturbative theory of Allen, Heine, and Cardona (AHC) [2] enables an efficient first-principles calculation of the renormalized electronic eigenenergies. The temperature dependence of the electronic bandgap, optical responses, and topological properties of real materials have been investigated within the AHC formalism. In this study, we generalize the AHC formalism [3] so that it could be applied to a broader class of materials. We demonstrate our formalism by calculating the temperature-dependent electronic energy eigenvalues of representative materials.

[1] F. Giustino, Rev. Mod. Phys. 89, 015003 (2017)

[2] P. B. Allen and V. Heine, J. Phys. C 9, 2305 (1976); P. B. Allen and M. Cardona, Phys. Rev. B 24, 7479 (1981); 27, 4760 (1983).

[3] J.-M. Lihm and C.-H. Park, unpublished.

O 5.3 Mon 11:15 GER 38

Electron-phonon interactions beyond the Born-Oppenheimer approximation in Kohn Sham theory — •Nikitas Gidopoulos — Department of Physics, Durham University, South Road, Durham, DH1 3LE, U.K.

I shall present our work on non-adiabatic corrections to the electron-phonon matrix elements, in density functional theory beyond the Born Oppenheimer approximation, where the Kohn-Sham single-particle potential contains a non-adiabatic correction term [1]. This term depends self-consistently on the nuclear vibrational wave function. The standard expansion of the non-adiabatic KS potential around the nuclear equilibrium positions yields electron-phonon matrix elements beyond the BO approximation.

[1] NI Gidopoulos, EKU Gross, Phil. Trans. R. Soc. A 372, 20130059 (2014). http://dx.doi.org/10.1098/rsta.2013.0059

O 5.4 Mon 11:30 GER 38

Renormalized second-order perturbation theory for the band gap and single-particle excitations of solids — •Maria Dragoumi[1], Sergey V. Levchenko[2,1], Igor Ying Zhang[3,1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Skolkovo Institute of Science and Technology, Moscow, RU — [3]Fudan University, Shanghai, CN

We report an efficient implementation of renormalized second-order single-particle energies for periodic systems in an all-electron numeric atomic orbital framework. Starting from second-order perturbation theory, which is single-electron self-interaction free as a virtue of the first-order and second-order exchange diagrams, we use the Dyson equation to sum up infinite number of diagrams [1,2]. In our implementation we use Ewald summation for the long-range part of the Coulomb interaction. This results in an integrable singularity in k-space, which has to be carefully evaluated in order to ensure proper convergence with k-point mesh density. For this purpose we develop an approach based on a generalization of the Gygi-Baldereschi method. The dependence on the starting point of the perturbation theory is examined. The new approach shows a competitive or even superior performance for the description of band-energies compared to the current state-of-the-art methods such as hybrid functionals and G^0W^0 approximation. Thus, with a good starting point this method becomes a powerful tool for the prediction of band energies for a variety of materials.

[1] J. Sun and R. J. Bartlett, J. Chem. Phys. 104, 8553 (1996).

[2] A. Grüneis *et al.*, J. Chem. Phys. 133, 074107 (2010).

O 5.5 Mon 11:45 GER 38

Band structure of semiconductors and insulators from Koopmans-compliant functionals — •Riccardo De Gennaro[1], Nicola Colonna[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Laboratory for Neutron Scattering and Imaging (LNS), Paul Scherrer Institute, 5232 Villigen, Switzerland

Koopmans-compliant functionals provide a novel orbital-density-dependent framework for an accurate evaluation of spectral properties, obtained imposing a generalized piecewise-linearity condition on the total energy of the system with respect to the occupation of each orbital. In crystalline materials, due to the orbital-density-dependent nature of the functionals, minimization of the total energy leads to a ground-state set of variational orbitals that are localized and break the periodicity of the underlying lattice. Despite that, thanks to the Wannier-like character of the variational orbitals, we show that the Bloch symmetry is still preserved and it is possible to describe the electronic energies through a band structure picture. In this talk I will present results for some benchmark semiconductors and insulators, obtained by unfolding the electronic bands obtained with Gamma-point-only calculations.

O 5.6 Mon 12:00 GER 38

Dynamical vertex corrections beyond GW from time-dependent density-functional theory — •Georg S. Michelitsch[1,2], Lucia Reining[1,2], and Matteo Gatti[1,2] — [1]Laboratoire des Solides Irradiés, École Polytechnique, F-91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF)

Strong many-body effects in solid state materials are the reason for features such as satellites in electronic excitation spectra. Many-body perturbation theory approaches based on the Green's function formalism are the state-of-the-art in their understanding, commonly applied in terms of the GW approximation to the self-energy, which neglects the so-called vertex correction in Hedin's equations. Although successful for some observables such as band gaps, this approximation cannot sufficiently well describe satellite peaks observed in experiment.

Vertex corrections beyond GW can be taken into account thanks to time-dependent density-functional theory[1]. However, only adiabatic approximations have been considered so far. Here we make use of a non-adiabatic approximation[2] to investigate dynamical vertex corrections within a model self-energy. We compare our results to calculations where a static vertex is included and report first successes in terms of a correction to the satellites in the spectral function of sodium.

[1] R. Del Sole et al. *Phys. Rev. B*, 49, 8024 (1994)
[2] M. Panholzer et al. *Phys. Rev. Lett.*, 120, 166402 (2018)

O 5.7 Mon 12:15 GER 38

Large-scale benchmark of exchange-correlation functionals for the determination of electronic band gaps of solids — •Pedro Borlido[1], Thorsten Aull[2], Ahmad Huran[2], Fabien Tran[3], Miguel Marques[2], and Silvana Botti[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [3]Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria

We compile a large dataset designed for the efficient benchmarking of exchange-correlation functionals for the calculation of electronic band gaps.The dataset comprises information on the experimental structures and band gaps of 472 non-magnetic materials, and includes a diverse group of covalent-, ionic-, and van der Waals-bonded solids.

We used it to benchmark a set of 30 functionals sampling the entirety of Jacob's Ladder. This includes well established functionals such as PBE, mBJ and HSE06, as well as several other less known functionals.

The comparison of experimental and theoretical band gaps shows that mBJ is at the moment the best available density functional, closely followed by HSE06. Other functionals such as HLE16, HLE17, AK13 and TASK also show overall good performance.

O 5.8 Mon 12:30 GER 38

Assessment of Approximate Methods for Anharmonic Free Energies — •Venkat Kapil[1], Edgar Engel[2], Mariana Rossi[3], and Michele Ceriotti[1] — [1]Swiss Federal Institute of Technology, Switzerland — [2]Department of Physics, University of Cambridge, UK — [3]MPI for Structure and Dynamics of Matter, Hamburg, Germany

Quantitative estimations of thermodynamic stabilities, measured by free energies, must take into account thermal and quantum zero-point nuclear motion. While these effects are easily estimated within a harmonic approximation, corrections arising from the anharmonic nature of the interatomic potential are often crucial and their accurate computations require expensive path integral simulations. Consequently, different approximate methods for computing affordable estimates of anharmonic free energies have been developed. Understanding which of the approximations involved are justified for a given system is complicated by the lack of comparative benchmarks. We here assess the accuracy of some of the commonly used approximate methods: vibrational self-consistent field and self-consistent phonons by comparing anharmonic corrections to Helmholtz free energies against reference path integral calculations. We study a diverse set of systems, ranging from simple weakly anharmonic solids to flexible molecular crystals with freely-rotating units and conclude that efforts towards obtaining computationally-feasible anharmonic free-energies of molecular systems must focus at reducing the expense of path integral methods. *Kapil, Venkat, et al. Assessment of Approximate Methods for Anharmonic Free Energies. JCTC, 2019, doi:10.1021/acs.jctc.9b00596.*

O 6: Organic Molecules on Inorganic Substrates I: Electronic, Optical and other Properties

Time: Monday 10:30–13:30 Location: REC C 213

O 6.1 Mon 10:30 REC C 213

Molecular orientation and phase transitions of DHTAP on Cu(110) — •Claudia López-Posadas[1], Michael Györök[1], Antony Thomas[2], Thomas Leoni[2], Olivier Siri[2], Conrad Becker[2], and Peter Zeppenfeld[1] — [1]Institute of Experimental Physics, Johannes Kepler University Linz, Altenberger Str. 69, A-4040 Linz, Austria — [2]Aix-Marseille University, CNRS, CINaM, UMR 7325, F-13288 Marseille, France

The structure and orientation of 5,14-dihydro-5,7,12,14-tetraazapentacene (DHTAP) layers deposited on Cu(110) was studied using reflectance difference spectroscopy (RDS), Scanning Tunneling Microscopy (STM) and Low Energy Electron Diffraction (LEED). The evolution of the RDS signal allows to identify the sequential formation of up to three monolayers as well as a phase transition upon completion of the first one. DHTAP molecules in the first monolayer are always lying flat with their long molecular axis aligned parallel to the [-110]-direction of the Cu(110) surface. However, for subsequent layers the orientation critically depends on the deposition temperature T. At T=240K the DHTAP molecules are mostly aligned parallel to the ones in the first layer, whereas at room temperature and above their preferential orientation is along the [001]-direction, i.e., orthogonal to the molecules in the first layer. Finally, the main optical transitions and the orientation of the transition dipole moments of the DHTAP layers were extracted from the RDS spectra and compared with recent theoretical investigations on individual DHTAP molecules.

Invited Talk O 6.2 Mon 10:45 REC C 213

Excited State Dynamics at Interfaces with Organic Semiconductors — •Petra Tegeder — Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Germany

Understanding the dynamics of electronically excited molecular states after optical excitation in organic semiconductors is necessary for improvement and optimization of potential molecule-based devices such as organic photovoltaic cells or organic light emitting diodes. Using femtosecond time-resolved spectroscopies, namely two-photon photoemission (2PPE) and second harmonic generation (SHG) we studied the excited state dynamics at interfaces and within thin films of several organic semiconducting molecules. This includes the singlet fission dynamics in triisopropyl-silylethynyl-pentacene (TIPS-Pn) adsorbed on Au(111). Based on 2PPE measurements we proposed a coherent excitation of the singlet and multiexciton state, both decaying with the same time constant of 160 fs. The triplet state stabilizes on a time scale of 1.6 ps and decays to the ground state. The latter occurs within 620 ps. However, SHG measurements on TIPS-Pn films point towards a non-coherent formation of the singlet and multiexciton state. In well-ordered diindenoperylene (DIP) and perylene alkyldiimide (PDIR) films, respectively, and at differently structured DIP/PDIR interfaces we elucidated the exciton and charge transfer dynamics in the femtosecond regime using SHG.

O 6.3 Mon 11:15 REC C 213

Dynamic Momentum Mapping of Excited Molecular Wave Packets — •Kiana Baumgärtner[1], Markus Scholz[2], Christian Metzger[1], Chul-Hee Min[1], Thiago R. F. Peixoto[1], Dmytro Kutnyakhov[3], Michael Heber[3], Federico Pressacco[4], Wilfried Wurth[3,4], Anders Madsen[2], and Friedrich Reinert[1] — [1]Experimentelle Physik 7, Julius-Maximilians-Universität Würzburg, Germany — [2]European XFEL, Germany — [3]DESY Hamburg, Germany — [4]Universität Hamburg, Germany

In the last decade [1], the interpretation of the momentum distribution from static angle-resolved photoemission experiments has improved our understanding of charge transfer processes at the molecule-metal-interface [2], vibronic progression [3] as well as the geometric alignment in these systems [4]. In this contribution I will present our experimental findings on time-resolved orbital mapping of excited molecular states. We conducted pump-probe experiments on pentacene bilayers atop Ag(110) at a free-electron-laser facility with a momentum microscope. Pentacene presents an ideal material system to study not only because of its broad applicability in devices such as OFETs and OLEDs but it is also well characterized by static experiments [4,5] and it has the potential to showcase ultrafast photoinduced processes such as singlet fission.

[1] P. Puschnig et al., Science 326, 702 (2009). [2] G. Zamborlini et al., Nat. Comm. 8, 335 (2017). [3] M. Graus et al., Phys. Rev. Lett. 116, 147601 (2016). [4] M. Grimm et al., Phys. Rev. B 98, 195412 (2018). [5] M. Scholz et al., arXiv:1907.10434.

O 6.4 Mon 11:30 REC C 213

Dodecacene generated on Surface: Re-opening of the Energy

Gap — Tim Kühne[1], Frank Eisenhut[1], Fátima Garcia[3], Saleta Fernández[3], Enrique Guitián[3], Dolores Pérez[3], Georges Trinquier[5], Gianaurelio Cuniberti[2], Christian Joachim[4], Diego Peña[3], and •Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, Germany — [2]Institute for Materials Science, TU Dresden, Germany — [3]Leibniz Institute of Polymer Research, Dresden, Germany — [4]GNS & MANA Satellite, CEMES, CNRS, Toulouse Cedex, France — [5]Laboratoire de Chimie et Physique Quanties, Université Paul-Sabatier, Toulouse Cedex, France

The acene series represents a unique model system to investigate the intriguing electronic properties of extended π electron structures in the one-dimensional limit, which are important for applications in electronics and spintronics and for the fundamental understanding of electronic transport. Here we present the on-surface generation of the longest acene obtained so far: Dodecacene. Scanning tunneling spectroscopy gives access to the energy position and spatial distribution of its electronic states on the Au(111) surface. We observe that, after a progressive closing of the gap and a stabilization to about 1 eV at the length of decacene and undecacene, the energy gap of dodecacene unexpectedly increases to 1.4 eV. Considering the acene series as an exemplary general case, we discuss the evolution with length of the single tunneling resonances in comparison with ionization energy, electronic affinity, and optical gap.

O 6.5 Mon 11:45 REC C 213

Exciton Fission, Fusion, Annihilation and Quantum Beating in Deposited Tetracene Films — Kevin Oldenburg, •Ingo Barke, Chris Rehhagen, Stefan Lochbrunner, and Sylvia Speller — Institute of Physics, University of Rostock

One technique to overcome the Shockley-Queisser limit in dye-sensitized solar cells is to exploit singlet fission processes, effectively doubling the number of charge carriers per photon. Here we present photoemission electron microscopy (PEEM) data of the excited state dynamics and spatial distribution of tetracene thin films. In order to locally enhance the excitation density, plasmon excitations in mass-selected silver nanoparticles (diameter $\approx$ 10 nm) are used [1]. Signatures of a singlet fission process are visible leading to an efficient population of a triplet state with annihilation governed decay dynamics on the order of ns to μs, while we observe an intrinsic lifetime exceeding 10 μs. Complementary fluorescence lifetime microscopy (FLIM) reveals quantum beats in the signal of delayed fluorescence on the time scale of several ns which are attributed to a coherent excitation of a triplet manifold [2]. The coherence time appears to be dependent on the exciton density which is analyzed by changing the excitation power. The characteristic lifetimes obtained by PEEM are consistent with fluorescence data (see also [3]).
[1]K. Oldenburg *et al.*, J. Phys. Chem. C **123**, 1379 (2019).
[2] J. Burdett, C.J. Bardeen, JACS **134**, 8597 (2012).
[3] G.M. Akselrod *et al.*, Nat. Commun. **5**, 3646 (2014).

O 6.6 Mon 12:00 REC C 213

Good Vibrations - Mode Coupling in Fatty Acids — Michael Lackner, •Marvin Hille, and Eckart Hasselbrink — University of Duisburg-Essen, Essen, Germany

Internal vibrational energy distribution (IVR) in molecules is fundamental for understanding their chemical reactivity and research in this field has gained a lot of popularity in the past. It is, however, still fair to say that predictive power over the energy flow in vibrationally excited molecules has yet to be obtained. We will present newest findings regarding the energy flow dynamic of a fatty acid Langmuir-Blodgett film on a picosecond scale. Vibrational sum frequency generation (vSFG) spectroscopy allows precise monitoring of resonant vibrations of an adsorbate monolayer. In our setup we use a resonant ps narrowband IR laser pulse for pumping and a fs broadband IR-visible pulse pair for vSFG probing of the monolayer. Using this pump-probe setup we observed a very fast ($<$ 2ps) energy transfer to the other modes when pumping the anti-symmetric methyl or methylene stretch, followed by a longer decay (˜85 ps) into presumably bending and internal rotational modes.

O 6.7 Mon 12:15 REC C 213

excited states dynamics of unsubstituted terrylene, a text book molecule — •Boubacar Tanda Bonkano[1], Kobin Björn[2], Sergey Kovalenko[2], Stefan Hecht[2], and Julia Stähler[1] — [1]Fritz-Haber Institute of the MPG, Berlin — [2]Institut für Chemie, Humboldt Universität zu Berlin

In hybrid solar cells, the separation of the electron-hole pairs after photogeneration is a key aspect of their functionality. This requires, in hybrid inorganic/organic systems, the use of molecules that have excited states with sufficiently long lifetime to allow charge separation. In order to investigate terrylene molecules, we performed two types of time-resolved spectroscopy, time-correlated single photon counting (TCSPC) and broadband transient absorption (TA) using a white light continuum probe. The steady state absorption and emission of terrylene molecules in solution show mirrored lineshapes displaying a clear vibronic progression. Terrylene molecules have their maximum absorption and emission lines at 560 nm (2.21 eV) and 570 nm (2.17 eV) respectively. Both TCSPC and TA consistently show a decay of 3.7 ns for the excited state S_1. Our results demonstrate that terrylene molecules have long-lived excited states, and, therefore could facilitate charge separation process. First measurements of thin terrylene films indicate a significant change of absorption properties, possibly resulting from H-aggregate formation.

O 6.8 Mon 12:30 REC C 213

Unbaking a cake: Computational strategies to disentangle core-level spectroscopy signals of chemical interaction at metal-organic interfaces — •Samuel J. Hall and Reinhard J. Maurer — Department of Chemistry, University of Warwick, Coventry, CV4 7AL, United Kingdom

X-ray photo-emission spectroscopy (XPS) and x-ray absorption, so-called near-edge absorption fine structure spectroscopy (NEXAFS) provide insight into the structure, chemical interaction, and electronic properties of metal-organic interfaces. The interpretation of NEXAFS spectra is challenged by peak broadening, overlapping features and electronic hybridisation between organic and metallic states at the interface. These effects diminish the usefulness of reference spectra and literature values when it comes to peak assignment for complex metal-adsorbed molecules. In this talk, we will present a systematic computational study of the effect of molecule-metal interaction strength and overlayer structure on spectral features in NEXAFS spectroscopy. Using dispersion-inclusive Density Functional Theory and the Transition-Potential method, we have simulated NEXAFS spectra for a benchmark set of various aromatic organic compounds adsorbed on a series of (111) facets of single crystal transition metal surfaces. By decomposing the spectra into initial core state and final valence state contributions, we analyse how weak and strong molecule-metal interaction, charge transfer, and electronic hybridisation and dispersion effects manifest in spectra. On the basis of these findings, we provide suggestions for future interpretation strategies.

O 6.9 Mon 12:45 REC C 213

Manipulation of the noble metal rare earth surface alloy DyAg$_2$ by adsorption of organic molecules — •Eva Sophia Walther[1], Johannes Seidel[1], Dominik Jungkenn[1], Markus Franke[2,3], Ahmed Alhassanat[4], Hans-Joachim Elmers[4], Christian Kumpf[2,3], Martin Aeschlimann[1], and Benjamin Stadtmüller[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [3]Jülich-Aachen Research Alliance (JARA) — [4]Institute of Physics, JGU Mainz

The vast requirement for novel nano-sized information technology devices has triggered the search for functional low dimensional materials with distinct spin order. A particularly interesting case is the contact of molecular complexes and surface alloys, which combines the unique functionality of molecular complexes with the spin order of surface alloys. Here, we focus on Perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) on the DyAg$_2$ surface alloy. Alloying the topmost layer of an Ag(111) surface with Dy results in a long range ordered magnetic phase at low sample temperature. Using synchrotron-based photoemission and magnetic circular dichroism experiments we can reveal the manipulation of the electronic and magnetic properties of this surface alloy by adsorption of PTCDA. These changes of the DyAg$_2$ surface alloy are attributed to the formation of σ-like local bonds between the molecules oxygen end groups and the Dy-alloy atoms.

O 6.10 Mon 13:00 REC C 213

Direct observation of conductive polymer induced inversion layer in n-Si and correlation to solar cell performance — •rongbin wang[1,2], yusheng wang[2], chen wu[2], tianshu zhai[2], jiacheng yang[2], baoquan sun[2], steffen duhm[2], and norbert koch[1,2] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Germany — [2]Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, China

Heterojunctions formed by PEDOT:PSS films and n-type silicon were investigated by photoelectron spectroscopy. By diluting the original PEDOT:PSS solution and increasing the spin-coating speed, a series of PEDOT:PSS thin films with nominal thicknesses down to 5 nm were achieved on n-Si substrates. Large shifts of Si 2p core levels upon PEDOT:PSS deposition provide direct evidence that a dopant-free p-n junction, i.e., an inversion layer, is formed within Si. Among the investigated PEDOT:PSS formulations, the largest induced band bending within Si (0.71 eV) is found for PH1000 combined with a wetting agent and the solvent additive dimethyl sulfoxide (DMSO). Without DMSO, the induced band bending is reduced, as is also the case with a PEDOT:PSS (AI4083) formulation with higher PSS content. By comparing PEDOT:PSS/n-Si solar cells with MoOx/n-Si cells, it becomes apparent that a large contact-induced band bending does not necessarily lead to a high Voc. Adequate passivation of the silicon surface to decrease recombination and high conductivity of the covering layer are also needed to achieve high PCE devices. Reference: Wang et al., Adv. Funct. Mater. 2019, 1903440 (doi.org/10.1002/adfm.201903440)

O 6.11 Mon 13:15 REC C 213

Investigation of a Novel Tetrapodal Self-Assembled Monolayer for Orthogonal Orientation — •Valentina Rohnacher[1,2], Frank S. Benneckendorf[2,3], Sebastian Beck[1,2], Jan Freudenberg[2,3], Wolfram Jaegermann[2,4], Paolo Samorì[5], Michael Zharnikov[6], Uwe H.F. Bunz[2,3], Annemarie Pucci[1,2], and Klaus Müllen[2,7] — [1]KIP, Uni Heidelberg — [2]InnovationLab, Heidelberg — [3]TU Darmstadt — [4]OCI, Uni Heidelberg — [5]CNRS, Uni Strasbourg — [6]PCI, Uni Heidelberg — [7]MPIP, Mainz

Conformationally rigid multipodal molecules should control the orientation and packing density of functional head groups upon self-assembly on solid supports. Common tripods frequently fail in this regard, because of inhomogeneous bonding configuration and stochastic orientation. These issues are circumvented by a suitable tetrapodal diazatriptycene (DAT) moiety, bearing four thiol-anchoring group.

We performed infrared reflection-absorption spectroscopy (IRRAS) on DAT molecules assembled on gold substrates to probe the orientation. Together with the results of contact angle measurements, STM, NEXAFS and PES, a better understanding about the formation of self-assembled monolayers (SAMs) was achieved. We found out that DAT molecules form well-ordered SAMs on Au(111) substrates, whereby the tetrapodal scaffold enforces a nearly upright orientation of the terminal head group with respect to the substrate. Functionalization by condensation chemistry allows a large variety of functional head groups to be introduced to the tetrapod, paving the path towards advanced surface engineering and sensor fabrication.

O 7: Focus Session: Functional Molecules at Surfaces I

This focus session aims at discussing motion and intramolecular changes taking place in functional molecules adsorbed at surfaces. Fundamental physical and chemical processes as for instance lateral displacement, molecular dynamics, conformational changes, or chemical reactions will be considered from the experimental and theoretical point of view. Various stimuli can be employed to induce such processes: from heat and light, which address many molecules at the same time, to the tip of a scanning probe microscope that acts locally on a single molecule.

Organizers: Francesca Moresco (TU Dresden) and Leonhard Grill (University of Graz)

Time: Monday 10:30–13:45 Location: TRE Ma

O 7.1 Mon 10:30 TRE Ma

Tuning the Halogen Bond between Adsorbed Organic Molecules — Jalmar Tschakert[1], Qigang Zhong[1], Sebastian Ahles[2], Pascal Henkel[3], Tobias Schlöder[3], Carlos Romero Muniz[4], Pablo Puo[4], Ruben Perez[4], Doreen Mollenhauer[3], Hermann A. Wegner[2], Andre Schirmeisen[1], and •Daniel Ebeling[1] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Germany — [2]Institute of Organic Chemistry, Justus Liebig University Giessen, Germany — [3]Institute of Physical Chemistry, Justus Liebig University Giessen, Germany — [4]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain

Halogen bonds are ideally suited for designing molecular assemblies because of their strong directionality and the possibility of tuning the interactions by using different types of halogens or molecular rests. This is interesting for applications in supramolecular chemistry, crystal engineering, or drug design. Here, we present a new approach for tuning the 2D self-assembly process of organic molecules by adsorption to different metal surfaces. The so-called σ-hole, the positive region at the cap of a halogen, which acts as the halogen bond donor can be actively tuned by molecule-substrate interactions. Since this effect depends strongly on the polarizability of the halogen and the reactiveness of the metal substrate it can be employed for controlling intermolecular connections including their bonding angles and the selectivity of bonding sites. Our results provide new insights into the nature of halogen bonds and their complex interplay with metal surfaces.

O 7.2 Mon 10:45 TRE Ma

Giant thermal expansion triggered by alkyl chain functionalization — •Sebastian Scherb[1], Antoine Hinaut[1], Rémy Pawlak[1], Guilherme Vilhena[1], Sara Freund[1], Zhao Liu[1], Klaus Müllen[2], Thilo Glatzel[1], Akimitsu Narita[2], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Basel, Switzerland — [2]Max Planck Institute for Polymer Research, Mainz, Germany

Thermal expansion, the response in shape or size of a solid to heat, is a fundamental property governing their mechanical applicability. Due to various mechanisms involving intrinsic flexibility, conformational changes and weak intermolecular interactions, molecular architecture allows negative and large positive expansions [1]. However, understanding of the underlying mechanisms down to the molecular scale remains elusive.

Here, we investigate the influence of alkyl chain functionalization on the thermal response of molecular assemblies by non-contact AFM, STM and molecular dynamic simulations (MD) at different temperatures [2,3]. Upon heating from 5 K to 300 K the alkyl chains undergo large thermal fluctuations compared to the cores because of entropic effects and large anharmonic vibrations [3]. This results in temperature-dependent intermolecular interactions that promote a giant expansion of the networks with temperature.

[1] Liu, Z. et al. Chem. Commun. 54, 5164-5176 (2018).

[2] Hinaut et al., Nanoscale, 10, 1337-1344 (2018).

[3] Scherb, S. et al., in preparation (2019).

O 7.3 Mon 11:00 TRE Ma

On-surface assembly of supramolecular graphyne-like networks: from hydrogen- and halogen-bonded to organometallic structures — Zechao Yang[1], Lukas Fromm[2], Tim Sander[1], Julian Gebhardt[2], Tobias A. Schaub[3], Andreas Görling[2], Milan Kivala[3], and •Sabine Maier[1] — [1]Department of Physics, FAU Erlangen-Nürnberg — [2]Chair of Theoretical Chemistry, FAU Erlangen-Nürnberg — [3]Organisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg

The on-surface assembly of graphyne-like 2D networks is directive for the long-awaited synthesis of the elusive carbon allotrope graphyne. On-surface synthesis facilitates the formation of single-layered materials, however, one of the key issues in the graphyne synthesis is the control of the alkyne coupling reaction. Here, we demonstrate a supramolecular approach to assemble highly-ordered, monolayered hydrogen-/halogen-bonded and organometallic graphyne-like 2D networks from H-/Br-functionalized triethynyltriazine derivatives on Ag(111) and Au(111). The structural and electronic properties of the supramolecular graphynes have been investigated by STM in combination with DFT. We found that intermolecular N$\cdots$Br-C(sp) halogen-bonds − hitherto unexplored in surface-supported self-assemblies − lead to significantly stronger bonded networks compared to N$\cdots$H-C(sp) hydrogen-bonds. After debromination, organometallic networks with Ag/Au-bis-acetylide bonds are formed. The highly-ordered monolayers feature unoccupied electronic states that are delocalized along the networks, which is indicative for a strong reversible bonding.

Invited Talk O 7.4 Mon 11:15 TRE Ma

Surface templating in on-surface synthesis: Directing the reaction pathway — Antje Kutz[1], Md Taibur Rahman[2], Ville Haapasilta[3], Chiara Venturini[4], Ralf Bechstein[2], André Gourdon[4], Adam S. Foster[3], and •Angelika Kühnle[2] — [1]Johannes Gutenberg University Mainz — [2]Bielefeld University — [3]Aalto University — [4]CNRS, CEMES, Toulouse

On-surface synthesis constitutes a very promising strategy for creating stable functional structures on surfaces. In the past, classical reactions known from solution synthesis have been transferred onto surfaces. Due to the presence of the surface, on-surface synthesis provides the potential of directing the reaction pathway in a manner that might not be accessible in classical solution synthesis. In particular, on-surface polymerization has been discussed for creating electrical contacts in future molecular electronic devices, for which electrically insulating substrates are desired. In this talk, we present evidence for an acetylene polymerization from a terminal alkyne monomer deposited onto the (10.4) surface of the bulk insulator calcite. Moreover, the terminal alkyne forms homo-coupled dimers on the surface. Although the dimer is present, we find no indication for diacetylene polymerization. This is in sharp contrast to what is observed when directly depositing the dimers. Our work thus constitutes a demonstration for controlling the specific reaction pathway in on-surface synthesis by the presence of the surface.

O 7.5 Mon 11:45 TRE Ma

Selective on-surface synthesis of oxygen heterocycles on metals — •Andreas Doerr[1], Nemanja Kocić[1], Konstantin Amsharov[2], and Sabine Maier[1] — [1]Department of Physics, Erwin-Rommel Straße 1, 91052 Erlangen — [2]Institute for Chemistry, Kurt-Mothes-Straße 2, 06099 Halle (Saale)

Heterocycles with nitrogen, oxygen, or sulfur atoms are the basic units to incorporate chemical functionalization into carbon scaffolds. For oxygen-doped nanographenes, furan[1] and pyran - having five- and six-membered rings, respectively - are the most common ones. However, their on-surface synthesis via cyclomerization reactions remains elusive so far. Here we present a low-temperature scanning tunneling microscopy study to understand the on-surface synthesis of furan and pyran derivatives from ketone-functionalized precursors on metal surfaces. We use thermally induced CH-activation reactions to fuse two ketone-derivatives in either cis- and trans-configuration selectively. Finally, cyclomerization reactions towards furan and pyran moieties are observed after further annealing. These results are highly unexpected because ketone derivatives are mostly known to convert to cyclic trimers or tetramers in solution-based chemistry. On the surface, however, the strong interaction of the ketones with the metal surface opens up new reaction pathways.

References

[1] L. Liu, H. Klaasen, A. Timmer, H.Y. Gao, D. Barton. H. Mönig, J. Neugebauer, H. Fuchs, A. Studer: J. Am. Chem. Soc. 2018, 140, 18, 6000-6005

O 7.6 Mon 12:00 TRE Ma

UV-light assisted on-surface synthesis of polyphenyl chains — •Kathrin Schneider, Jacques Bonvoisin, and Veronique Langlais — Center of Materials Elaboration and Structural Studies (CEMES) -CNRS, 29 rue Jeanne Marvig, 31055 Toulouse, France

On surface synthesis is a powerful tool to create extended molecular structures directly on a surface such as molecular chains or networks, not synthesizable in solution. In order to get a detailed understanding of the reaction steps and to optimize the reaction parameters, we studied commercial diiodo-p-ter-phenyl as model molecules.

These iodine functionalized molecules should react between them by losing their halogen and by creating C-C bonds upon Ullmann coupling. Scanning Tunneling Microscopy and Spectroscopy (STM and STS) were used to study them on Ag(001) surface, acting as substrate and catalyst. Carbon-iodine bond dissociation energy was determined by bond cleavage with the STM tip. Unreacted molecules forming a self-assembly monolayer convert, depending on annealing temperature, into organometallic and finally to fully polymerized molecular chains. The reaction temperature could clearly be reduced by using UV-light in addition to thermal treatment. These results open the route for on-surface synthesis dealing with larger or more fragile molecules.

O 7.7 Mon 12:15 TRE Ma

Free energy QM/MM simulations of on-surface reaction pathways. — •Aurelio Gallardo[1,2], Adam Matěj[1], Jesús Mendieta-Moreno[1], and Pavel Jelínek[1,2] — [1]IOP of the Czech Academy of Sciences, Prague, Czech Republic — [2]RCPTM, Olomouc, Czech Republic

On-surface chemistry represents a fast-growing field allowing to synthetize molecular structures not available by traditional wet chemistry. In combination with high-resolution scanning probe technique providing the unprecedented spatial resolution, individual products of reactions can be precisely identified. Nevertheless, a deep understanding of the reaction mechanism under the conditions imposed by the substrate remains unknown.

Widely adopted energy reaction path techniques will only describe the potential energy landscape at zero Kelvin, while the free energy landscape at given temperature enables a more appropriated description of the reaction. Such simulations including temperature effect include the effect of entropy, vibrations modes, concerted motion, etc. Consequently, such simulations avoid local minima and allows to explore different states, revealing lower energy pathways.

We will present QM/MM simulations of strain-induced isomerization in one-dimensional metal-organic chains on Cu(111) surface [1] and pp π-conjugated polymers on Au(111) surface. The simulation demonstrates the importance of the temperature effect on proper description of the reaction mechanism.

[1] M. Telychko et al., Angew. Chem 2019, 58

O 7.8 Mon 12:30 TRE Ma

Dynamic adaptation of linear bis-hydroxamic acid modules in complex nanostructures — •Anthoula C. Papageorgiou[1], Chao Jing[1], Bodong Zhang[1], Sabine Synkule[1], Maryam Ebrahimi[1], Alexander Riss[1], Willi Auwärter[1], Li Jiang[1], Guillaume Médard[2], Joachim Reichert[1], and Johannes V. Barth[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]Chair of Proteomics and Bioanalytics, Technical University of Munich, Germany

Recently, we functionalised linear building blocks with two terminal hydroxamic acid groups and applied them to two-dimensional (2D) architectonics on the close-packed single crystal surfaces of silver and gold.[1] A combination of scanning tunnelling microscopy, atomic force microscopy, X-ray photoelectron spectroscopy and density functional theory investigations found that the molecular building block would ever so slightly adapt its shape in the environment provided by the supporting surface and its neighbouring molecules. This affords an unusual manifold of surface supramolecular motifs: two to six molecules held together by intermolecular interactions. Only a handful of these motifs organised in 2D crystals, ranging from close-packed structures to polyporous networks. Dynamic, chiral supramolecules formed enantioselectively within some of the larger network pores, demonstrating chirality transfer from host to guest. Molecular coverage, as well as the chemical state of the hydroxamic acid functional group are correlated to the complex self-assembly scenario.

1) *Angew. Chem., Int. Ed.* **2019** DOI: 10.1002/anie.201912247.

O 7.9 Mon 12:45 TRE Ma

Tailoring topological order and π-conjugation to engineer quasi-metallic polymers — •Shayan Edalatmanesh[1], Borja Cirera[2], Ana Sánchez-Grande[2], Bruno de la Torre[1,3], José Santos[2,5], Eider Rodríguez-Sánchez[2,5], Koen Lauwaet[2], Benjamin Mallada[1], Radek Zbořil[1], Rodolfo Miranda[2,6], Oliver Gröning[4], Pavel Jelínek[1,3], Nazario Martín[2,5], and David Écija[2] — [1]Regional Centre of Advanced Technologies and Materials, Czechia — [2]IMDEA Nanociencia, Spain — [3]Institute of Physics, The Czech Academy of Sciences — [4]EMPA, Swiss Federal Laboratories for Materials Science and Technology — [5]Universidad Complutense, Spain — [6]Universidad Autónoma de Madrid, Spain

Topological band theory provides a conceptual framework to predict or even engineer robust metallic states at the boundaries of topologically distinct phases. The bulk-boundary correspondence requires that a topological electronic phase transition between two insulators must proceed via closing of the electronic gap. Therefore, it can provide a conceptual solution to the instability of metallic phases in π-conjugated

1D polymers.

In this work, we demonstrated that on-surface chemical reactions of molecular precursors on pristine Au(111) surfaces result in the formation of long, defect-free, π-conjugated polymers featuring a topological non-trivial SSH quantum phase, with a very narrow bandgap due to the proximity to the point of topological transition, in-gap zero-energy edge-states and electronic transformation of the π-conjugated polymers.

O 7.10 Mon 13:00 TRE Ma

Tuning topological phase transition and pi-conjugation of 1D pentacene polymers by their length — •Héctor González-Herrero[1], Bruno de la Torre[1], Adam Matěj[1], Shayan Edalatmanesh[1], Nazario Martín[2], David Écija[2], and Pavel Jelínek[1] — [1]Regional Centre of Advanced Technologies and Materials. Palacký University, 78371 Olomouc, Czech Republic. — [2]IMDEA Nanociencia.28049, Madrid, Spain.

The recent study of ethynylene-bridged polyacene polymers has shown the possibility to tune band gap by proximity of the topological phase transition [1]. In the specific case of pentacene polymers situated near the phase transition, a small bandgap of 350 meV and the appearance of edge-states have been reported. This behavior is attributed to a topological transition from trivial to non-trivial phases. However, minimum length required for a polymer to exhibit this transition is not clear.

Theoretical analysis based on total energy DFT simulations predicts that while dimer and trimer pentacene wire adopts aromatic pi-conjugation, longer wires exhibits quinoid ?-conjugation with presence of characteristic zero bias edge states. Motived by this observation, we have grown short pentacene chains in order to study the impact of their length in the final properties of the polymer. Using STM and AFM techniques we will characterize the electronic and structural properties trying to find the key parameters for the topological phase transition to take place and benchmark the theoretical prediction.

[1] B. Cirera et al arXiv:1911.04414.

O 7.11 Mon 13:15 TRE Ma

Nanoribbons with Non-Alternant Topology from Fusion of Polyazulene: Carbon Allotropes Beyond Graphene — •Qitang Fan[1], Daniel Martin-Jimenez[2], Daniel Ebeling[2], Claudio K. Krug[1], Lea Brechmann[3], Corinna Kohlmeyer[3], Gerhard Hilt[3], Wolfgang Hieringer[4], André Schirmeisen[2], and J. Michael Gottfried[1] — [1]Department of Chemistry, Philipps University Marburg, Germany — [2]Institute of Applied Physics, Justus Liebig University Gießen, Germany — [3]Institute of Chemistry, Carl von Ossietzky University Oldenburg, Germany — [4]Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Various two-dimensional carbon allotropes with nonalternant topologies, such as pentaheptites, have been proposed. Predictions indicate that these metastable carbon polymorphs possess unusual (opto)electronic properties. However, none of these materials has been achieved experimentally due to synthetic challenges. Here, by using on-surface synthesis, nonalternant phagraphene and tetra-penta-hepta graphene nanoribbons have been obtained by dehydrogenative C-C coupling of polyazulene chains. These chains were formed in a preceding reaction step via on-surface Ullmann coupling of 2,6-dibromoazulene. Low-temperature scanning probe microscopies with CO-functionalized tip and DFT calculations have been used to elucidate their structural properties. The proposed synthesis of nonalternant carbon nanoribbons from fusion of synthetic line defects may pave the way for the preparation of novel 2D carbon allotropes.

O 7.12 Mon 13:30 TRE Ma

CO ligation to Ru tetraphenylprorphyrins on Ag(111) — •Peter Knecht[1], Joachim Reichert[1], Peter Deimel[1], Peter Feulner[1], Felix Haag[1], Francesco Allegretti[1], Manuela Garnica[1], Martin Schwarz[1], Willi Auwärter[1], Paul Ryan[2], David A. Duncan[2], Ari P. Seitsonen[3], Johannes V. Barth[1], and Anthoula C. Papageorgiou[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]Diamond Light Source, UK — [3]Chemistry Department, ENS Paris, France

For the creation of novel materials and devices, inspiration is frequently sought in nature. Porphyrin molecules are macrocyclic compounds of biological origin, which incorporate a large fraction of the chemical elements. Their versatile properties stimulated widespread application to surface functionalisation.[1] In biology, the binding of small molecules to metal centres of porphyrins determines many vital functions. For Ru tetraphenyl porphyrins (Ru-TPP), CO is determined to have an unusually high ligation energy (1.9 eV).[2] Here we study the effect of the porphyrin surface environment on this ligation for Ru-TPP on Ag(111). We use scanning tunnelling microscopy to find a cis-carbonyl ligation[3] at low temperatures and an axial ligation at higher temperatures, which is also examined with temperature programmed desorption. We correlate the axial binding to conformational and electronic changes, investigated by density functional theory, X-ray photoemission and X-ray standing waves.

1) *Nat. Chem.* **2015**, *7*, 105; 2) *Phys. Chem. Chem. Phys.* **2018**, *20*, 11730; 3) *Nat. Chem.* **2011**, *3*, 114.

O 8: Ultrafast Electron Dynamics I: Surfaces and Interfaces (joint session O/MA)

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

O 8.1 Mon 10:30 TRE Phy

Electron dynamics of surface states in momentum space on Cu and Au — •Lukas Hellbrück, Tobias Eul, Martin Aeschlimann, and Benjamin Stadtmüller — Department of Physics and Research Center Optimas, University of Kaiserslautern, Germany

For the development of nanoscale electronic and spintronic devices, it is critical to understand electronic dynamics in solid states systems and at interfaces. Of particular interest is the correlation between the energy and momentum dissipation mechanisms of the hot carriers and the band structure of the material.

In this work, we employ time-resolved two photon momentum microscopy [1] with monochromatic radiation of about 4.6eV to access the electron dynamics in the excited state energy range of typical noble metal surfaces. From these data, we can extract momentum dependent quasi-particle lifetimes of the electrons, providing insight into momentum dependent scattering processes in these materials.

We focus on the (111) and (110) low-index copper and gold surfaces. These surfaces yield a variety of different states in the unoccupied band structure ranging from resonant and off-resonant bulk transitions to Shockley surface states and image potential states. For these different types of states, we observe lifetime differences of several femtoseconds, which points to a complex momentum dependent lifetime of the electrons, even for simple single crystalline materials.

[1] F. Haag et al., Rev. Sci. Instr. 90, 103104 (2019)

O 8.2 Mon 10:45 TRE Phy

Above-threshold multiphoton photoemission from noble metal surfaces — •Marcel Reutzel[1,2], Andi Li[2], and Hrvoje Petek[2] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, USA

Exciting solid surfaces with intense femtosecond laser pulses prompts electrons of the interrogated material to respond in highly non-linear manner, as is evident in the emission of high-order harmonic radiation and photoelectrons with kinetic energies well above that of the driving photons (above threshold photoemission, ATP). In the solid state, the optical field interacts with the electronic eigenstates defined by the Coulomb potential of a periodic crystal, as well as with its many-body screening response.

In this contribution, we probe the nonlinear photoelectric responses of the pristine silver surfaces in (111) and (110) crystal orientation using interferometrically time-resolved multi-photon photoemission spectroscopy. First, we study the coherent electron dynamics leading to non-resonant coherent mPP of the occupied Shockley surface band of Ag(111). We characterize and benchmark the two-dimensional Fourier transform (2D-FT) spectra based on the photoemission order m and the coherences induced in the sample (m = 2-6) [Phys. Rev. X 9, 01104545 (2019)]. Second, we show that ATP can be used to probe deep points in the Brillouin zone, namely the surface state of Ag(110) at the $\bar{\mathrm{Y}}$-point, that is otherwise hidden below the photoemission horizon in lowest order of mPP.

O 8.3 Mon 11:00 TRE Phy

Interfacial carrier and phonon dynamics in nanostructured metal/2D-semiconductor plasmonic heterostructures — •Tommaso Pincelli[1], Thomas Vasileiadis[1], Shuo Dong[1], Samuel Beaulieu[1], Maciej Dendzik[1], Daniela Zahn[1], Sang-Eun Lee[1], Hélène Seiler[1], Yinpeng Qi[1], Patrick Xian[1], Julian Maklar[1], Emerson Coy[2], Niclas Müller[3], Yu Okamura[3], Stephanie Reich[3], Martin Wolf[1], Laurenz Rettig[1], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]NanoBioMedical Centre, Adam Mickiewicz University, Poznan, Poland — [3]Freie Universität Berlin, Berlin, Germany

Noble metal nanostructures enhance light absorption in semiconductors to produce plasmons, whose decay couples strongly with the generation of hot carriers and non-equilibrium phonons. We combine the use of time and angle-resolved photoemission spectroscopy and femtosecond electron diffraction to investigate both charge carrier and phonon dynamics in a plasmonic metal/semiconductor heterostructure.

We grow epitaxial Au nanoislands on single-crystalline bulk WSe$_2$. The presence of Au nanostructures causes a shortening of the Σ-exciton lifetime and an accelerated lattice heating of WSe$_2$, which indicate interfacial charge transfer. Furthermore, we observe a non-equilibrium phonon distribution in WSe$_2$ with sub-bandgap optical pumping, demonstrating increased sensitivity of the semiconductor to near infrared frequencies. The corresponding energy transfer scales nonlinearly with the incident laser fluence, owing to plasmonically-enhanced phonon excitation.

O 8.4 Mon 11:15 TRE Phy

Ultrafast hole-transfer in MoSe$_2$/WSe$_2$ revealed by polarisation dependent second-harmonic imaging microscopy — •Jonas Zimmermann, Ulrich Höfer, and Gerson Mette — Fachbereich Physik, Philipps-Universität Marburg, Germany

Charge transfer across heterointerfaces plays a fundamental role for the functionality of electronic devices. 2D heterostructures based on transition metal dichalcogenides (TMDC) with their wide variety of materials and stacking combinations represent a unique opportunity for systematic studies of the interfacial charge-carrier dynamics.

Here, we present results on a MoSe$_2$/WSe$_2$ heterostructure investigated by time-resolved second-harmonic (SH) imaging microscopy. The transient SH-response after resonant optical excitation reveals a delayed filling and an enhanced lifetime for the heterostructure which is absent for the individual monolayers, indicating the formation of interlayer excitons. By careful selection of the polarisation of the probe laser, we are able to enhance the sensitivity to the individual layers in the heterostructure and with that to the charge transfer. Systematic measurements in dependence of the pump photon energy and the probe polarisation exhibit temporal signatures which are attributed to hole transfer from WSe$_2$ to MoSe$_2$ and vice versa with transfer times of a few hundred femtoseconds in both cases.

O 8.5 Mon 11:30 TRE Phy

Electron transfer dynamics in MoS$_2$ imaged by time-resolved momentum microscopy — •Lasse Münster[1], Sarah Zajusch[1], Katsumi Tanimura[2], Jens Güdde[1], Robert Wallauer[1], and Ulrich Höfer[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, Germany — [2]Institute of Scientific and Industrial Research, Osaka University, Japan

We investigate the electron dynamics in the topmost layer of MoS$_2$ after optical excitation above the A-exciton resonance by means of time- and angle-resolved two-photon photoemission with a high harmonic probe. High harmonic generation in krypton is used to produce an almost isolated 7th harmonic of the 400 nm driving laser pulses at a repetition rate of 200 kHz. This is combined with tunable pump pulses in the visible range for resonant excitation. The photoemitted electrons are detected by a momentum microscope with time of flight detection that covers the full photoemission horizon in a single measurement. With a high harmonic probe this results in the imaging of the entire first Brillouin zone in TMDCs.

We observe an instantaneous occupation of the conduction band after optical excitation at all $\overline{\mathrm{K}}$-points followed by an ultrafast transfer to the conduction band minima at $\overline{\Sigma}$. For longer delays the excited electron distribution localizes at these high symmetry points which we attribute to electron cooling. The real-space imaging capability of the momentum microscope allows the restriction of such experiments to micrometer-size regions which opens up the possibility to observe momentum-resolved charge transfer in TMDC heterostructures.

O 8.6 Mon 11:45 TRE Phy

Ultrafast electron dynamics in black phosphorus studied by time-resolved photoemission momentum microscopy — •Maciej Dendzik[1,2], Shuo Dong[1], Tommaso Pincelli[1], Samuel Beaulieu[1], Patrick Xian[1], Helene Seiler[1], Martin Wolf[1], Laurenz Rettig[1], and Ralph Ernstorfer[1] — [1]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14915 Berlin, Germany — [2]KTH Royal Institute of Technology, Electrum 229, 164 40 Kista, Sweden

Black phosphorus (BP) has recently emerged as a promising material due to its highly anisotropic thermal, electronic and optical properties. The high hole mobility together with a band-gap tunable by thickness in the visible to mid-IR range make BP attractive for future applications in opto-electronics. Therefore, detailed information on both the equilibrium and excited-state electronic band structure of BP is of strong interest. Here we present a fs time-resolved study of transient electronic structure of BP in the entire surface Brillouin zone (SBZ) directly imaged with a momentum microscope using a novel setup for XUV time- and angle-resolved photoemission spectroscopy. The measured dispersion is found to be in good agreement with density functional theory calculations. We find that an optical excitation at 800 nm creates a hot-carrier distribution around the SBZ center, which scatters to two other valleys in the conduction band within ca. 15 fs. We further observe a strong linear dichroism in the optical absorption of BP. Interestingly, the inter-valley scattering dynamics are also found to depend on the pump polarization vector direction.

O 8.7 Mon 12:00 TRE Phy

Carrier dynamics in a laser-excited Fe/(MgO)(001) heterostructure from real-time TDDFT — •Elaheh Shomali, Markus Ernst Gruner, and Rossitza Pentcheva — Department of Physics and Center for Nanointegration, CENIDE, University of Duisburg-Essen, Germany

The interaction of a femtosecond optical pulse with a metal/oxide interface has been addressed based on time-dependent density functional theory (TDDFT) in the real-time domain using the Elk code. We systematically studied electronic excitations of a Fe$_1$/(MgO)$_3$(001) heterostructure as a function of laser frequency, peak power density and polarization direction. We find a marked anisotropy in the response to in-plane and out-of-plane polarized light, which changes its character for frequencies lower and higher than the MgO band gap. For laser frequencies between the MgO band gap and the charge transfer gap, interface states resulting from the hybridization of the $d_{3z^2-r^2}$ orbitals of Fe and the p_z orbitals of O at the interface may foster the propagation of excitations into the central layer of MgO. Spin-orbit coupling (SOC) is found to result in a small time-dependent reduction of magnetization only. Finally, we extend our investigation to thicker heterostructures, such as Fe$_3$/(MgO)$_5$(001).

Financial support from the DFG within SFB 1242 (project C02) is gratefully acknowledged.

O 8.8 Mon 12:15 TRE Phy

Local and non-local electron dynamics of Au/Fe/MgO(001) heterostructures analyzed by time-resolved two-photon photoemission spectroscopy — Yasin Beyazit[1], Jan Beckord[1], Ping Zhou[1], Jan Philipp Meyburg[2], Detlef Diesing[2], Manuel Ligges[1], and •Uwe Bovensiepen[1] — [1]University of Duisburg-Essen, Faculty of Physics and Center for Nanointegration (CENIDE), 47048 Duisburg) — [2]University of Duisburg Essen, Faculty of Chemistry, Universitätsstr. 5, 45711 Essen

The ultrafast electron dynamics at interfaces is determined by the competition of local scattering processes and transport effects. Employing femtosecond laser pulses in front and back side pumping of Au/Fe/MgO(001) [1] combined with detection in two-photon photoelectron emission spectroscopy we analyze local relaxation dynamics of excited electrons in buried Fe, injection into Au across the Fe-Au interface, and electron transport across the Au layer at 0.6 to 2.0 eV above the Fermi energy. By analysis as a function of Au film thickness we obtain the electron lifetimes of bulk Au and Fe and distinguish the relaxation in the heterostructure's constituents. We conclude further that electron injection across the epitaxial interface proceeds by electron wavepacket propagation. We also show that the excited electrons propagate through Au in a superdiffusive regime determined by few e-e scattering events. Application of such back side pumping photoelectron spectroscopy to further material systems will be discussed.

Funding by the DFG through CRC 1242 is gratefully acknowledged. [1] Alekhin et al., J. Phys. Condens. Matter 31, 124002 (2019)

O 8.9 Mon 12:30 TRE Phy

Time-resolved nonlinear optical spectroscopy of ultrafast charge transfer at the buried GaP/Si(001) interface — •Gerson Mette[1], Jonas Zimmermann[1], Alexander Lerch[1], Kristina Brixius[1], Jens Güdde[1], Andreas Beyer[1], Michael Dürr[2], Kerstin Volz[1], Wolfgang Stolz[1], and Ulrich Höfer[1] — [1]Fachbereich Physik, Philipps Universität Marburg, Germany — [2]Institut für Angewandte Physik, Justus-Liebig-Universität Giessen, Germany

The ongoing miniaturization increases the contribution of interface processes to electronic device properties. For a microscopic understanding, the dynamics of charge transfer across interfaces are particularly important. However, due to the experimental difficulty to detect and isolate the weak interface signature from the dominant bulk signals, direct experimental information about the ultrafast dynamics at buried interfaces is scarce.

Here, we will show that the experimental challenges can be overcome by optical second-harmonic generation (SHG), a technique which is intrinsically highly interface sensitive. We are investigating the ultrafast charge-carrier dynamics at the buried interface of GaP on Si(001) by time-resolved optical-pump SHG-probe spectroscopy. Photon energy dependent measurements reveal the existence of electronic interface states in the band gap of both materials. Charge carriers excited via these interface states are efficiently injected within a few hundred femtoseconds from the GaP/Si interface into the Si substrate resulting in the build-up of an electric field on a picosecond time scale.

O 8.10 Mon 12:45 TRE Phy

Pump-probe second harmonic spectroscopy of molecule/metal interfaces — Jinghao Chen, Ping Zhou, Uwe Bovensiepen, and •Andrea Eschenlohr — Faculty of Physics, University Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Achieving a microscopic understanding of charge transfer dynamics and the relaxation of optically excited electrons and holes at molecule/metal interfaces requires an interface-sensitive analysis on the respective femtosecond timescales. Second harmonic spectroscopy (SHS) [1] is such an interface-sensitive probe in centrosymmetric materials. We employ a non-collinear optical parametric amplifier in the visible wavelength range (1.9-2.5 eV) for pump-probe SHS with <20 fs pulse duration. A prototypical molecule/metal interface is prepared by adsorption of iron octaethylporphyrin (FeOEP) molecules on Cu(001) [2] and analyzed *in situ* in ultrahigh vacuum. We find a molecule-induced resonance at about 2.2 eV fundamental photon energy in the second harmonic spectrum of one monolayer of FeOEP/Cu(001). At this resonance, we observe a markedly slower relaxation time of the pump-induced changes in SHS compared to the bare Cu(001) surface, which indicates an increased lifetime of the electronic molecular state.

We thank H. Wende, J. Güdde and E. Riedle for valuable experimental advice, and the German Research Foundation for funding via SPP 1840 QUTIF and Sfb 1242.

[1] T. F. Heinz, C. K. Chen, D. Ricard, and Y. R. Shen, Phys. Rev. Lett. **48**, 478 (1982); U. Höfer, Appl. Phys. A **63**, 533 (1996).

[2] H. C. Herper et al., Phys. Rev. B **87**, 174424 (2013).

O 8.11 Mon 13:00 TRE Phy

Dynamics of interfacial electron-hole separation in an organic heterojunction monitored by femtosecond time-resolved X-ray photoelectron spectroscopy — •Friedrich Roth[1], Mario Borgwardt[2], Lukas Wenthaus[3], Johannes Mahl[2], Steffen Palutke[4], Günter Brenner[4], Serguei Molodtsov[1,5], Wilfried Wurth[3,4,6], Oliver Gessner[2], and Wolfgang Eberhardt[3] — [1]Institute of Experimental Physics, TU Bergakademie Freiberg, Leipziger Straße 23, D-09599 Freiberg, Germany — [2]Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA — [3]Center for Free-Electron Laser Science / DESY, D-22607 Hamburg, Germany — [4]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22603 Hamburg, Germany — [5]European XFEL GmbH, Holzkoppel 4, 22869, Schenefeld, Germany — [6]Universität Hamburg, Luruper Chaussee 149, 22761, Hamburg, German

The dynamics of ultrafast photon-to-charge conversion in a copper-phthalocyanine (CuPc)-C$_{60}$ heterojunction is studied by femtosecond time-resolved X-ray photoemission spectroscopy (tr-XPS) at the free-electron laser FLASH. The technique provides site-specific access to electron dynamics and monitors the generation and decay of interfacial charge-transfer (ICT) states after excitation with 775 nm photons. A previously unobserved channel for ICT separation into mobile charge carriers with an efficiency of $22 \pm 7\,\%$ is identified, providing a direct measure of the internal quantum efficiency of the heterojunction for this channel.

O 9: Plasmonics and Nanooptics I: Local Probes and Raman (joint session O/CPP)

Time: Monday 10:30–13:45 Location: WIL A317

O 9.1 Mon 10:30 WIL A317

Light emission from charged Hydrogen-Phthalocyanine molecules on NaCl layers — •Vibhuti Rai[1], Lukas Gerhard[1], Sun Qing[1], and Wulf Wulfhekel[1,2] — [1]Institut für Nanotechnologie, Karlsruher Institut für Technologie, 76344 Eggenstein-Leopoldshafen, Germany — [2]Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Recently, light emission studies from single molecules on insulating layers studied by scanning tunneling microscopy (STM) has had made considerable progress. However, many fundamental aspects of light emission remain unclear. In this report, we used a home build STM[1] with high light collection efficiency to investigate the light emission from single Hydrogen-Phthalocyanine (H_2Pc) molecules thermally evaporated onto bi- and trilayers of NaCl on Au(111) surface. For the first time we have observed light emission from both charged and neutral H_2Pc molecules and mapped the spatial dependence of light emission. We find that the photon yield of the charged species is significantly higher than the neutral one and that the tautomerization of the charged H_2Pc molecule is reflected in the energy and spatial distribution of the emitted light. For further understanding of the fundamental processes of light emission we performed detailed current and voltage dependence of light emission spectra from charged H_2Pc molecule.

1. Edelmann et al., Review of Scientific Instruments 89, 123107 (2018).

O 9.2 Mon 10:45 WIL A317

Anti-Stokes Light Scattering in an Electrically Biased Plasmonic Nanojunction — •Shuyi Liu[1], Martin Wolf[1], and Takashi Kumagai[1,2] — [1]Department of Physical Chemistry, Fritz-Haber Institute of the Max-Planck Society, Faradayweg 4-6, 14195 Berlin, Germany. — [2]JST-PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan.

Photon scattering and emission from plasmonic nanostructures have attracted increasing attention but the underlying mechanisms have been debated. [1,2] We report on light scattering from an electrically-biased plasmonic nanocavity, which composed of a Ag tip and Ag(111) surface, using a low-temperature scanning tunneling microscope (STM). It is found that anti-Stokes shifted scattered light is observed occurs when a bias voltage (< 2V) is applied to the junction. By observing the scattering spectra in dependence on the spectral shape of the localized surface plasmon resonance (LSPR) in the STM junction, we revealed that either electronic Raman scattering (ERS) or photoluminescence (PL) dominates the process depending on spectral matching of the LSPR with excitation wavelength. We discuss the possibility that ERS occurs by the interaction of the LSPR with a "gap exciton" in the STM junction. Reference: [1] Mertens et al, Nano Lett. 17, 2568-2574 (2017).[2] Cai et al, Anti-Stokes Emission from Hot Carriers in Gold Nanorods. Nano Lett. 19, 1067-1073 (2019).

O 9.3 Mon 11:00 WIL A317

Broadband measurement of local density of optical states by plasmonic nanofocusing spectral interferometry — •Abbas Chimeh[1], Martin Esmann[2], Anke Korte[1], Jinhui Zhong[1], Nahid Talebi[3], and Christoph Lienau[1] — [1]Universität Oldenburg, Oldenburg, Germany — [2]Centre de Nanosciences et de Nanotechnologies, Paris, — [3]Universität Kiel, Kiel, Germany

The local density of optical states (LDOS) is one of the most fundamental quantities in nanophotonics [1]. Experimental mapping of the LDOS enables to understand how a quantum emitter is coupled to its nanostructred photonic environment. Here, we demonstrate a novel experimental approach to directly measure the LDOS with <10 nm spatial resolution in a broad spectral range. Surface plasmon polaritons (SPPs) propagating along a conical gold taper are adiabatically converted to a local dipole mode at the very apex [2], which can locally excite and detect the optical states around single gold nanoparticles. Integration of an inline interferometer in this plasmonic nanofocusing taper allows us to extract amplitude a phase of local light scattering spectra of gold nanoparticles and quantify line broadenings and spectral shifts induced by tip-sample coupling [3]. We show that, in the limit of weak tip-sample coupling, this measurements directly probe the projected local density of optical states of the plasmonic system.

[1] R. Carminati et al., Surf. Sci. Rep. 70, 1 (2015) [2] M. Esmann et al., Nature Nanotechnol. 6, 6040 (2019) [3] M. Esmann et al., Nanophotonics, in press (2020)

O 9.4 Mon 11:15 WIL A317

Spatial and spectral mode mapping of a Sb_2S_3 nanodot by broadband interferometric homodyne scanning near-field spectroscopy — Jinxin Zhan[1], Wei Wang[2], Jens Brauer[1], Lukas Schmidt-Mende[2], Christoph Lienau[1], and •Petra Gross[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]University of Konstanz, Konstanz, Germany

We present and demonstrate a novel approach towards broad-bandwidth scattering-type near-field scanning optical spectroscopy based on homodyne mixing and on rapid acquisition of spectra facilitating tip-modulated spectroscopy. We aim at a fast and spectrally resolved near-field measurement of plasmonic and dielectric nanostructures. The weak, broad-bandwidth near field is amplified above the background by homodyne mixing using a Michelson interferometer, and spectral interferograms over a >150 nm bandwidth are recorded. For rapid acquisition of complete spectra, we use a monochromator and a line camera with 210-kHz readout rate. The near-field spectra obtained after demodulation show supreme background suppression.

We apply this new method to the characterization of Sb_2S_3 semiconductor nanodots fabricated by electron beam lithography. Sb_2S_3 recently became attractive as photovoltaic material, and patterning the surface of a thin film with nanodots of the same material is a strategy to achieve light trapping. Here, we present spatially and spectrally resolved measurements of waveguide-like modes that are excited by below-bandgap illumination. These constitute a practical mechanism for improved below-bandgap absorption in Sb_2S_3 thin film solar cells.

O 9.5 Mon 11:30 WIL A317

Polarization-sensitive near-field optical nanoscopy for investigating optical phonon anisotropies at mid-infrared to THz wavelengths — •Lukas Wehmeier[1], Tobias Nörenberg[1], Thales V. A. G. de Oliveira[1,2], J. Michael Klopf[2], Susanne C. Kehr[1], and Lukas M. Eng[1,3] — [1]Technische Universität Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany — [3]ct.qmat, Dresden-Würzburg Cluster of Excellence - EXC 2147, Technische Universität Dresden, Germany

Polarization-sensitive techniques, such as ellipsometry, are of essential value when investigating optically anisotropic (low-dimensional) materials. Yet, polarization is often neglected in scattering scanning near-field optical microscopy (s-SNOM) and spectroscopy. In a first attempt towards quantitative nano-ellipsometry, we demonstrate here the phonon-enhanced resonant near-field excitation when using both p- and s-polarized incident photons. Notably, we find their near-field responses to be on the same order of magnitude [1]. We apply this s-SNOM mimic for inspecting a broad set of crystalline perovskite materials, i.e. $BiFeO_3$, $PbZrTiO_3$, $SrTiO_3$, and $LiNbO_3$. Their phonon resonances are easily excited by our setup, making use here of the broad tunability range of the free-electron laser FELBE at Dresden-Rossendorf, Germany [1,2]. Hence, we are able to resonantly excite specific phonons, i.e. a single type of vibronic bonding within the crystal in our s-SNOM setup [2].

[1] L. Wehmeier et al., Phys. Rev. B 100, 035444 (2019).

[2] L. Wehmeier et al., Appl. Phys. Lett., submitted (2019).

O 9.6 Mon 11:45 WIL A317

Single-molecule vibrational signature and redox-states probed with STM-Induced Fluorescence Microscopy — •Benjamin Doppagne, Michael C. Chong, Etienne Lorchat, Stephane Berciaud, Michelangelo Romeo, Hervé Bulou, Alex Boeglin, Fabrice Scheurer, and Guillaume Schull — Institut de Physique et Chimie des Matérieux de Strasbourg, 67034 Strasbourg, France

Infrared, Raman and fluorescence spectroscopies are powerful methods to obtain precise information regarding the chemical structure or environment of an organic system. In this presentation, I report the use of a STM to obtain the fluorescence spectrum of a single Zinc-Phthalocyanine molecule, to go beyond the limitations commonly observed in conventional optical techniques. We have shown that in such configuration, it is possible to obtain optically an accurate vibrational signature of the probed molecule with a sub-molecular resolution, without light excitation. This technique has allowed us to obtain, for the first time, the fluorescence spectrum of a charged single molecule. Comparison between fluorescence spectra of the neutral and the charged species shows that these latters exhibit different vibrational signatures. Thanks to this identification, we performed a complete optical monitoring of the redox state of a single molecule with STM-Induced Fluorescence Microscopy.

O 9.7 Mon 12:00 WIL A317

Optical tracking of a tautomerization process with STM-Induced Fluorescence Microscopy — •Benjamin Doppagne[1], Tomas Neuman[2], Ruben Soria Martinez[1], Luis E. Parra Lopez[1], Hervé Bulou[1], Michelangelo Romeo[1], Stephane Berciaud[1], Fabrice Scheurer[1], Javier Aizpurua[2], and Guillaume Schull[1] — [1]Institut de Physique et Chimie des Matérieux de Strasbourg, 67034 Strasbourg, France — [2]Center for Materials Physics, San Sebastian 20018, Spain

Optical spectroscopies are powerful techniques to obtain precise information regarding the chemical structure or the environment of organic molecules. Therefore, gathering the optical signal from a single molecule represents the ultimate limit in terms of chemical analysis and provide a way to probe its local environment. In this presentation, I report recent results, where we used a STM to induce fluorescence emission from a single H2Pc molecule. Two different emission lines, which are relative to each tautomer of the molecule are observed in the STM-Induced fluorescence spectrum. Spatial mapping of these fluorescence lines coupled with a theoretical model using the concept of plasmonic picocavity, where the light is confined by the last atoms of the tip within volumes of the order of 1 nm3, allowed us to obtain optical images of the two tautomers. Thanks to this identification, real-time optical tracking of the tautomerization process is carried out, providing the tautomers lifetimes. This result shows that STM-Induced single-molecule fluorescence experiments constitute a complete optical microscopy technique at the atomic scale.

O 9.8 Mon 12:15 WIL A317

Compensating for electrostatically-induced artifacts in scanning near-field optical microscopy — •Tobias Nörenberg[1], Susanne C. Kehr[1], and Lukas M. Eng[1,2] — [1]Institute of Applied Physics, Technische Universität Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, Technische Universität Dresden, Germany

Nanotechnology and modern material sciences demand reliable local probing techniques with nanometer resolution. In particular, scattering-type scanning near-field optical microscopy (s-SNOM) is a well-established method that is sensitive to the local optical response of a sample, yielding a wavelength-independent lateral resolution on the order of ∼10 nm. Nevertheless, local variations of the electric potential at the sample surface may dramatically affect the tip-sample interaction, thereby introducing artifacts in both optical near-field signal and topography.

Here, we present a comprehensive experimental study investigating the mentioned artifacts for different sample systems, i.e. metals (Au), semiconductors (Si), and insulators (SiO_2). By combining s-SNOM with Kelvin-probe force microscopy (KPFM) we firstly fully compensate for these errors, while secondly also being able to measure such local potentials. Optical, topographic, and electronic information hence become well separated and quantified.

O 9.9 Mon 12:30 WIL A317

Tip-Enhanced Raman Scattering of CdSe-CdS Nanoplatelets on Plasmonic Substrates — •Ilya Milekhin[1], Mahfujur Rahaman[1], Tatyana Duda[2,3], Ekaterina Rodyakina[2,3], Kirill Anikin[2,3], Roman Vasiliev[4], Volodymyr Dzhagan[5], Alexander Milekhin[2,3], Alexander Latyshev[2,3], and Dietrich RT Zahn[1] —

[1]Semiconductor Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]A.V. Rzhanov Institute of Semiconductor Physics RAS, Novosibirsk, Russia — [3]Novosibirsk State University, Novosibirsk, Russia — [4]Department of Material Science, Moscow State University, Moscow, Russia — [5]V.E. Lashkaryov Institute of Semiconductor Physics, Kiev, Ukraine

We present the results on a gap-plasmon tip-enhanced Raman scattering (TERS) study of core-shell CdSe-CdS nanoplatelets (NPs) deposited on periodic arrays of Au nanodisks which serve as plasmonic substrates. The fabrication of Au nanodisks with a diameter of 110 nm and a height of 50 nm on Si substrates covered with a 77 nm of SiO2 was performed by electron beam lithography. NPs with a characteristic size of 100x30x3 nm were deposited onto the plasmonic substrate using the Langmuir-Blodgett technique. We observe a remarkable Raman enhancement of the phonon modes of CdSe and CdS from NPs located in the plasmonic gap between Au nanodisks and TERS tip. Gap-mode TERS imaging was performed at 638 and 785 nm excitation and allowed us to visualize the near field distribution of the gap-plasmon with relative TERS contrast of 30. A phonon response of the single NP was achieved with a spatial resolution of 2 nm.

O 9.10 Mon 12:45 WIL A317

The influence of size and shape of tip and substrate in gap-mode tip-enhanced Raman spectroscopy — •lu he, mahfujur rahaman, teresa i. madeira, and d.r.t. zahn — Semiconductor physics, University of technology Chemnitz, Germany

Tip-enhanced Raman Spectroscopy (TERS) utilizes the confined electric field in the vicinity of a metal tip. The typical spatial resolution is around 2 nm[1] and even sub-nanometer can be achieved[2,3]. Many factors play a role in the TERS technique[4]. Our simulation focuses on the comparison of the two configurations. The first one consists of various tip radii with thin film while the second one consists of a constant tip radius with various radii of spherical substrates in a metal-metallic gap-mode TERS system using the finite element method (FEM). An unusual shift in the first case is observed. An improved expression of the above approximation is obtained for the second case.

O 9.11 Mon 13:00 WIL A317

Probing the Local Generation and Diffusion of Active Oxygen Species on a Pd/Au Bimetallic Surface by Tip-Enhanced Raman Spectroscopy — Hai-Sheng Su[1], •Jin-Hui Zhong[2,1], and Bin Ren[1] — [1]State Key Laboratory of Physical Chemistry of Solid Surfaces, iChEM, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China. — [2]Institute of Physics, Carl von Ossietzky University, Oldenburg 26129, Germany

In this contribution, we discuss the application of tip-enhanced Raman spectroscopy (TERS) to image local atomic site-specific electronic and catalytic properties of bimetallic Pd monolayer/Au(111) [1] and Pt nanoisland/Au(111) surface [2]. The high spatial resolution (<3 nm) of TERS allows us to reveal distinct properties of surface atoms that correlate to the catalytic properties. We further probe the local generation and diffusion of OH radicals on a Pd monolayer/Au(111) bimetallic catalyst surface [3]. The reactive OH radicals can be catalytically generated from hydrogen peroxide (H2O2) at the active Pd step edge site and could diffuse to both the Au and Pd surface sites to induce oxidative reactions, with a diffusion length estimated to be about 5.4 nm. The results suggest the capability of TERS, as a plasmon-enhanced nanoscopy, to in-situ study catalysis with unprecedent spatial resolution and rich molecular identity. [1] J.-H. Zhong, B. Ren*, et al., Nat. Nanotech., 2017, 12, 132. [2] H.-S. Su, J.-H. Zhong*, B. Ren*, et al., Angew. Chem. Int. Ed. 2018, 57, 13177. [3] H.-S. Su, J.-H. Zhong*, B. Ren*, et al., submitted.

O 9.12 Mon 13:15 WIL A317

Strong surface plasmon localization in gold nanosponges probed by plasmonic nanofocusing spectroscopy — •Anke Korte[1], Abbas Chimeh[1], Jinhui Zhong[1], Dong Wang[2], Peter Schaaf[2], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität Oldenburg, Germany — [2]Technische Universität Ilmenau, Germany

Porous gold nanosponges, percolated with a three-dimensional network of 10 nm sized ligaments, recently emerged as promising substrates for plasmon-enhanced spectroscopy. Experimental and theoretical studies suggest surface plasmon localization in small hot-spots. To probe the existence of such hot-spots, we have first used scattering-type scanning near-field optical microscopy with homodyne detection of the scattered signal from individual nanosponges to reveal such strong spatially and spectrally confined modes. By recording local near-field scattering spectra, high quality factors of 40 for individual hot-spots are demonstrated. More recently, we combined this method with plasmonic nanofocusing, where surface plasmon polaritons propagate along the shaft of a conical gold taper and form an isolated nano light source. This removes unwanted background since hot-spot modes are locally excited just by the nano-localized tip dipole field, resulting in a highly improved signal-to-noise-ratio and a simplified image interpretation. This advanced technique is used to investigate the coupling behaviour between such hot-spot modes and small quantum emitters, which were deposited inside the pores of a nanosponge.

O 9.13 Mon 13:30 WIL A317

Resonant, plasmonic enhancement of alpha-6T molecules encapsulated in CNTs — •Sören Wasserroth[1], Sebastian Heeg[1,2], Niclas Mueller[1], Patryk Kusch[1], Uwe Hübner[3], Etienne Gaufrès[4], Nathalie Tang[4], Richard Martell[4], Aravind Vijayaraghavan[2], and Stephanie Reich[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]The University of Manchester, Manchester, UK — [3]Leibniz IPHT, Jena, Germany — [4]Université de Montréal, Montréal, Canada

Surface-enhanced and resonant Raman scattering are widely used techniques to enhance the Raman intensity by several orders of magnitude. SERS uses plasmonic near-fields to enhance the Raman scattering process, whereas electronic transitions are the origin of the enhancement in resonant Raman scattering. Typical Raman reporters in SERS are molecules; in SERS experiments, the intrinsic resonance of the molecules is often ignored. We present a wavelength dependent Raman study of sexithiophenes encapsulated in carbon nanotubes. To distinguish between the intrinsic resonance and plasmonic enhancement we investigate different tube bundles with and without plasmonic near field. The filled nanotubes are placed precisely in a gold dimer gap by dielectrophoretic deposition. Polarization dependent Raman measurements confirmed the alignment of the molecules within the nanotubes and the influence of the plasmonic near-field. By tuning the excitation wavelength, we were able to determine the intrinsic molecular resonance and observed a strong redshift towards the plasmon resonance of maximum Raman intensity under plasmonic enhancement.

O 10: Oxides I: Growth and Characterization

Time: Monday 10:30–13:45 Location: WIL B321

O 10.1 Mon 10:30 WIL B321

Growth, reconstruction and electronic band structure of ultrathin cuprous oxide Films on Ru(0001) — •Nicolas Braud[1], Jan Ingo Flege[2], Enrique G. Michel[3], Paolo Moras[4], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Applied Physics and SemiconductorSpectroscopy, BTU Cottbus-Senftenberg, Germany — [3]Departemento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, Spain — [4]Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Italy

Cuprous oxide Cu_2O is a p-type direct semiconductor and is expected to play an important role in optoelectronics, solar technologies and in photoelectrochemistry due to its band gap of 2.17 eV and an optical gap of 2.62 eV which fit in the solar spectrum.

Here we present angle resolved photelectron spectroscopy investigations of thin two dimensional cuprous oxide films. All the samples were characterized allong the ΓM and the ΓK direction in a photon range between 75 and 125 eV.

Depending on the oxide thickness we observe three different phases by LEED and LEEM. After the oxidation of Cu/Ru(0001) in low oxygen partial pressure of 3×10^{-6} mbar at 400°, the surface exhibits a rectangular $(3 \times 2\sqrt{3})$ reconstruction. Increasing the oxygen partial pressure up to 3×10^{-5} mbar leads to a $(2\sqrt{7} \times 2\sqrt{7})$R19.1°reconstructed hexagonal $Cu_2O(111)$-like film. An oxygen pressure of 3×10^{-6} mbar leads to a (2 × 2) reconstruction. For these phases we also observed differences in the electronic band strucuture.

O 10.2 Mon 10:45 WIL B321

Epitaxial growth of wurtzite CoO(0001) on Au(111) and conversion into rocksalt CoO(001) — •Maximilian Ammon[1], Lutz Hammer[1], Sara Baumann[1], Andreas Raabgrund[1], Tilman Kisslinger[1], Josef Redinger[2], and M. Alexander Schneider[1] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg — [2]Institut für Angewandte Physik & CMS, TU Wien

Wurtzite (w-)CoO is a semiconducting [1] and antiferromagnetic [2] material. We establish the preparation parameters for the epitaxial growth of closed w-CoO films on Au(111) of several nanometer thickness. A LEED-IV analysis ($R_p = 0.112$) proves the structure to be w-CoO ($a = 3.26$ Å, $c = 5.22$ Å) with small relaxations in the 1. surface layer only. DFT calculations based on hybrid functionals or LDAU schemes reproduce all measured geometrical parameters very well.

We used STS and DFT to study the electronic properties of these w-CoO films. Films with a thickness of 15 bilayers (BL) ≈ 4 nm exhibit a bandgap of 1.8 ± 0.2 eV around E_F as measured by STS that is comparable to the optical bandgap quoted in literature [1]. We observe a reduction of the bandgap with decreased film thickness.

Annealing of w-CoO(0001) films to 600°C induces a phase transition to closed rocksalt (rs-)CoO(001) films. Experiments with ultrathin films (≤ 4 BL) show that this conversion results in films of homogeneous thickness corresponding to three cubic lattice constants of rs-CoO (≈ 1.2 nm).

[1] Wang et al., Chem. Commun. **54**, 13949 (2018)

[2] Roca et al., Small **14**, 1703963 (2018)

O 10.3 Mon 11:00 WIL B321

Structural and electronic properties of single-layer CoO_2 — •Ann-Julie Holt[1], Marco Bianchi[1], Jonathan Fernandez[2], Yu Zhang[3], Davide Curcio[1], Paolo Lacovig[4], Sahar Pakdel[1], Nicola Lanata[1], Jeppe Lauritsen[2], Silvano Lizzit[4], Philip Hofmann[1], and Charlotte Sanders[3] — [1]Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark — [2]Department of Chemistry, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Aarhus, Denmark — [3]Central Laser Facility, Oxfordshire, UK — [4]Elettra - Sincrotrone Trieste S.C.p.A., Trieste, Italy.

Single-layer transition metal dichalcogens are among the most actively investigated material systems of the past several years and increased attention is now being directed to the oxygen-based members of this family. In particular, CoO_2 is predicted to manifest intrinsic two-dimensional ferromagnetism and is a potential corrosion-resistant catalyst in the oxygen evolution reaction.

Here, we present an experimental study of single-layer CoO_2, obtained from a newly developed synthesis method for epitaxially fabricating stable, rotationally aligned single-layer CoO_2 on Au(111) (*e.g.*,[1]). The material structure is studied through scanning tunneling microscopy, low energy electron diffraction, and X-ray photoelectron diffraction. The electronic dispersion is characterised by the use of angle-resolved photoelectron spectroscopy, revealing a metallic behaviour. A structural model of the material is established, and the electronic structure is related to density functional theory calculations.
[1] *ACS Nano* **9** (2015) 2445

O 10.4 Mon 11:15 WIL B321

Strongly strained VO_2 thin film growth — •Simon Fischer[1], Jan Ingo Flege[2], Michael Foerster[3], Lucia Aballe[3], Andrea Locatelli[4], Tevfik Onur Menteş[4], Jens Falta[1], and Jon-Olaf Krisponeit[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus, Germany — [3]ALBA Synchrotron Light Facility, Barcelona, Spain — [4]Elettra Sincrotrone Trieste, Italy

The semiconductor-metal transition temperature of VO_2 strongly shifts as a result of strain applied along the rutile c axis, making it relevant for various switching applications such as smart coatings and sensors. In the past this has been demonstrated, for instance, through the application of epitaxial strain on TiO_2 substrates.

We extend this tailoring approach by utilizing the much larger lattice mismatch of 8.78 % occurring in the VO_2/RuO_2 system for orientations where the c axis lies in-plane. Depositing vanadium oxide by atomic oxygen-supported reactive MBE on an oxidized Ru(0001) template, we have grown VO_2 thin films on single domain RuO_2 islands with varying orientation. Locally resolved electron spectroscopy was used to ascertain the correct stoichiometry of the grown VO_2 films on all template island types. Low energy electron diffraction reveals the VO_2 films to grow indeed fully strained on $RuO_2(110)$ but fully relaxed on $RuO_2(100)$.

Hence, the presented template allows simultaneous access to a remarkable strain window ranging from bulk-like structures to massively strained regions.

O 10.5 Mon 11:30 WIL B321

Growth and Characterization of Calcium-Molybdate Thin Films on Mo(001) — Maike Lockhorn[1], Sergio Tosoni[2], Gianfranco Pacchioni[2], and •Niklas Nilius[1] — [1]Institute of Physics, Carl von Ossietzky University Oldenburg, Germany — [2]Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Italy

Ca-Mo mixed oxide films were grown on a Mo(001) surface and characterized by various surface science techniques and DFT. Several highly crystalline phases were observed with rising annealing temperature, before the mixed oxide decays to binary MoOx. The stoichiometry of the low-temperature phase was determined to CaMo3O6, and resembles a CaMo5O8 bulk structure. A corresponding DFT model consists of alternating flat-lying and upright-standing Mo octahedrons, separated by Ca2+ ion rows. As the Ca and O content decreases upon heating, the central Mo units grow in size and the film evolves through distinct (3x3), (4x4) and (6x6) reconstructions. This leads also to an increasing metallicity of the film, as probed with STM conductance spectroscopy. Our work presents an easy approach towards crystalline ternary oxide films that exploits the inter-diffusion of substrate atoms into a suitable binary oxide.

O 10.6 Mon 11:45 WIL B321

Detecting Tiny Cation Nonstoichiometry in Complex Oxide Films — •Michele Riva, Giada Franceschi, Michael Schmid, and Ulrike Diebold — IAP, TU Wien, Austria

The rise of semiconductor-based electronics has gone hand in hand with the technological advancements allowing to reproducibly prepare materials with exceptionally small concentration of defects. A similar control of defects and composition is the key to making all-oxide electronics a reality, allowing to fully exploit the multitude of functionalities of these materials. Precise tuning of the oxide composition, however, requires the development of reliable tools to detect cation nonstoichiometry with extreme sensitivity: We develop an unconventional method based on STM that pushes down this detection limit by at least one order of magnitude [1].

We take advantage of the well-controlled surface reconstructions of $SrTiO_3(110)$, and use the established relation between those reconstructions and the surface composition to assess the cation excess deposited in PLD-grown $SrTiO_3(110)$ films. We demonstrate that a $< 0.1\%$ change in cation non-stoichiometry is detectable by our approach, and show that, for thin films that accommodate all the non-stoichiometry at the surface, our method has no fundamental detection limit.

[1] Phys. Rev. Mater. **3**, 043802 (2019)

O 10.7 Mon 12:00 WIL B321

Non-stoichiometry segregation in perovskite oxides and its role for film growth — •Giada Franceschi, Michael Schmid, Ulrike Diebold, and Michele Riva — TU Wien, Institute of Applied Physics, Wiedner Haupstrasse 8-10/E134, 1040, Vienna, Austria

Achieving atomically flat and stoichiometric films of complex multi-component oxides is crucial for integrating these materials in emerging technologies. While pulsed laser deposition (PLD) can in principle produce these high-quality films, growth experiments often result in rough surfaces and nonstoichiometric compositions. To understand the cause, we follow the growth at an atomic level from its early stages as a function of the growth conditions, using atomically resolved STM. We investigate the growth of $SrTiO_3(110)$ and $La_{0.8}Sr_{0.2}MnO_3(110)$ films. Both accumulate small non-stoichiometries introduced during growth at the surface. As a result, their surface structure evolves along phase diagrams of surface structure vs. composition.[1] This can produce dramatic effects on the surface morphology: If two surface reconstructions with different sticking properties develop and coexist during growth, pits can form, degrading the surface morphology.[2] Moreover, if the introduced non-stoichiometry is too large to be accommodated by the surface via a change in its structure, ill-defined oxide clusters nucleate and grow, eventually dominating the surface morphology. We show our approach to grow films with thickness of tens of nanometers showing atomically flat surfaces, and with stoichiometry control within 0.1%.[1]
[1] PRMater. 3, 043802 (2019) [2] PRResearch 1, 033059 (2019)

O 10.8 Mon 12:15 WIL B321

Fundamental asymmetry in the electronic reconstruction of polar $LaMnO_3/LaAlO_3$ vs. $LaAlO_3/LaMnO_3$ thin films on $SrTiO_3(001)$ — •Benjamin Geisler and Rossitza Pentcheva — Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg

Interface polarity plays a key role in oxide heterostructures. Here we explore its effect on the electronic reconstruction in polar $LaMnO_3/LaAlO_3$ and $LaAlO_3/LaMnO_3$ thin films on $SrTiO_3(001)$ and show that the materials sequence fundamentally impacts the mechanism. [1] First-principles calculations including a Coulomb repulsion term reveal that for $(LaMnO_3)_n/(LaAlO_3)_2/SrTiO_3(001)$, the electronic reconstruction is triggered already at $n = 2$, and we observe the formation of a two-dimensional electron gas (2DEG) at the $SrTiO_3(001)$ interface with enhanced Ti $3d$ occupation compared to the $(LaAlO_3)_4/SrTiO_3(001)$ case. Interestingly, in the reversed $(LaAlO_3)_m/(LaMnO_3)_3/SrTiO_3(001)$ system, charge transfer from the surface sets in at $m = 3$, but compensation occurs in the manganate and no 2DEG is formed at the $SrTiO_3(001)$ interface. For lower $m = 2$, no charge transfer is observed at all, highlighting the pivotal role of the materials sequence and thickness. These findings suggest more general design principles of the electronic reconstruction in polar oxide thin films on a nonpolar substrate.

Funding by the DFG within TRR 80 (G3) is acknowledged.

[1] B. Geisler, P. Reith, H. Hilgenkamp, and R. Pentcheva, in preparation

O 10.9 Mon 12:30 WIL B321

Temperature-dependent SXRD from a two-dimensional oxide quasicrystal — •Sebastian Schenk[1], Stefan Förster[1], Marc de Boissieu[2], and Wolf Widdra[1,3] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Universite Grenoble Alpes, CNRS, SIMaP, 38402 St Martin d Heres, France — [3]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

Two-dimensional oxide quasicrystals (OQC) are mono-atomically high ternary oxide layers with 12-fold rotation symmetry forming spontaneous on Pt(111) [1,2]. Here we report on studies of the structural dynamics of the prototypical example of the $BaTiO_3$-derived OQC using surface X-ray diffraction (SXRD) at the SIXS beamline, Soleil. In contrast to periodic systems, temperature-induced changes in the diffraction pattern of OQCs occur not only due to the excitation of phonons (Debye-Waller factor) but also due to additional excitations, called phasons [3]. Both will cause a redistribution of intensity from the Bragg peaks to the diffuse background and will be discussed for temperature-dependent SXRD data in the range from 300 to 1300K. In this way, a separation of frozen-in phason flips and dynamically excited phasons is possible. In addition, changes of the shape of the most intense [1110] diffraction peaks are explained by frozen-in phason flips.

[1] S. Förster et al., Nature **502**, 215 (2013)

[2] S. Förster et al., Phys. Status Solidi B, doi: 10.1002/pssb.201900624, (2019)

[3] M. de Boissieu et. al., PRL **95**, 105503 (2005)

O 10.10 Mon 12:45 WIL B321

Oxide quasicrystal formation on Pd(111) — •Friederike Wührl[1], Oliver Krahn[1], Stefan Förster[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle(Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle(Saale), Germany

The discovery of a quasicrystalline phase in ultrathin films of $BaTiO_3$ (BTO) on Pt(111) opened a new field of research on ternary oxides on metal substrates. Its observation was the first example for spontaneous formation of an aperiodic dodecagonal structure at the interface to a periodic crystal. So far oxide quasicrystals (OQC) have been found only on the surface of Pt(111) [1]. Here we report on the first OQC on an alternative substrate, namely Pd(111). Pd(111) has a 1% reduced lattice parameter as compared to Pt(111). LEED and STM data show several long-range-ordered wetting layer structures between 3D $BaTiO_3(111)$ islands after heating the film under UHV conditions. The diffraction spots of the BTO-islands show a Moiré pattern. The wetting layer structures finally converge at a temperature of 960 K to 1000 K into two domains of dodecagonal OQC's, which are rotated by ±5° against the high symmetry directions of the substrate. This dodecagonal structure coexist with another wetting layer structure. Surprisingly, the characteristic length of the newly discovered BTO-derived OQC is reduced according to the smaller lattice parameter.

[1] S. Förster *et al.*, Phys. Status Solidi B, doi: 10.1002/pssb.201900624, (2019)

O 10.11 Mon 13:00 WIL B321

Large-Scale Quasicrystal Approximants in the $SrTiO_3/Pt(111)$ System — •Oliver Krahn[1], Sebastian Schenk[1], Stefan Förster[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

The recent discovery of two-dimensional oxide quasicrystals (OQC) draws attention to aperiodic structure formation from perovskite materials on Pt(111) [1,2]. On the atomic level, the OQC generates an aperiodic self-similar tiling consisting of triangles, squares and rhombes with Ti atoms at the vertices and equal edge lengths. Periodically repeated patches of a quasicrystal are known as approximants.

In this talk, we present low-temperature scanning tunneling microscopy and spectroscopy data of the largest unit cell approximant known so far in 2D systems. Its unit cell is commensurate with a superstructure matrix of $\begin{pmatrix} 16 & 0 \\ 9 & 18 \end{pmatrix}$ with respect to Pt(111) and covers an area of 44.3 Å × 43.2 Å. The cell contains 48 Ti atoms that occupy the vertices of 48 triangles, 18 squares and 6 rhombes. These tiling elements are furthermore decorated with 48 Sr and 120 O atoms assuming a stoichiometry of 1:1:2.5 as determined for a related small unit cell approximant [3]. This adds up to a 2D unit cell containing 216 atoms.

[1] S. Förster et al., Nature **502** (2013)

[2] S. Förster, O. Krahn et al., Phys. Status Solidi B, doi: 10.1002/pssb.201900624 (2019)

[3] S. Förster et al., Phys. Rev. Lett. **117** (2016)

O 10.12 Mon 13:15 WIL B321

Bulk and Interface Characteristics of $Ni_xCu_{1-x}O_y$ - An Alternative Inorganic Hole Transport Material Systems with Widely Tunable Optoelectronic Properties — •Lucas Bodenstein-Dresler[1], Adi Kama[2], Johannes Frisch[1], Claudia Hartmann[1], Anat Itzhak[2], Regan Wilks[1], Gary Hodes[2], David Cahen[2,3], and Marcus Bär[1,4,5] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [2]Bar-Ilan University — [3]Weizmann Institute of Science — [4]Friedrich-Alexander-Universität Erlangen-Nürnberg — [5]Helmholtz-Institute Erlangen-Nürnberg for Renewable Energy

Halide perovskite (HaP) solar cells have reached efficiencies of over 25% being now primarily limited by the interfaces between the HaPs absorber and the charge carrier transport layers (TL). Especially organic TL employed in standard HaP solar cells, like PEDOT:PSS or Spiro-OMeTAD, are potentially sources of degradation. Alternative inorganic ternary metal oxide (MO) hole TLs (HTL) promise better stability. Furthermore, their optoelectronic properties can be tuned, allowing for deliberate HaPs/HTL interface tailoring. One possible HTL MO is $Ni_xCu_{1-x}O_y$, which we studied as a combinatorial NiO - Cu_2O 72 x 72 m^2 material library produced by pulsed laser deposition by photoelectron spectroscopy (XPS) to reveal composition-dependent chemical/electronic surface characteristics. In our presentation, the XPS analysis will be correlated to complementary crystal structure and optical bulk properties, to arrive at a complete picture of the $Ni_xCu_{1-x}O_y$ system and allow first steps towards the tailoring of such.

O 10.13 Mon 13:30 WIL B321

Surface diffusion of precursors in area-selective Atomic Layer Deposition — •Daniel Anders[1], Philip Klement[1], Jörg Schörmann[1], Christian Heiliger[2], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I and Center for Materials Research, Justus Liebig University Giessen, Germany — [2]Institute of Theoretical Physics, Justus Liebig University Giessen, Germany

Bottom-up nanofabrication by area-selective Atomic Layer Deposition (ALD) is expected to become a key technology in the fabrication of sub 5-nm semiconductor-devices. ALD eliminates conventional top-down alignment errors by limiting the deposition to specific areas. Surface diffusion of precursors becomes important as precursors may adsorb to no-growth areas and diffuse towards growth areas leading to previously unconsidered phenomena.

Here we show the impact of precursor surface diffusion in area-selective ALD of TiO2 on SiO2. We find strongly increased growth rates on substrates with pattered poly(methyl methacrylate) masks and a non-uniform topography. We apply a kinetic Monte-Carlo simulation model for the growth process based on different diffusion coefficients on different surfaces. The numerical results agree excellently with the experimental observations and allow us to deduce the different diffusion lengths. This work facilitates the understanding of surface diffusion processes in area-selective deposition, and enables the control of area-selective deposition on small scales.

O 11: 2D Materials I: Electronic Structure, Excitations, etc. (joint session O/CPP/HL)

Time: Monday 10:30–13:45 Location: WIL C107

Invited Talk O 11.1 Mon 10:30 WIL C107

A microscopic view of graphene quantum Hall edge states with STM and AFM measurements — •Joseph A. Stroscio — NIST, Gaithersburg, MD 20899, USA

2D heterostructed devices with electrostatic pn junction boundaries provide a convenient geometry for the examination of Quantum Hall edge states with microscopic probes. In this talk I will review our work in circular and rectangular geometries to examine the quantum Hall edge states which form in high magnetic field using scanning tunneling microscopy (STM) and atomic force microscopy (AFM) measurements. In circular graphene pn junctions a concentric series of compressible and incompressible rings form due to electron interactions, and show single electron charging when probed by scanning tunneling spectroscopy. In a rectangular Hall bar geometry defined by pn junction boundaries, the compressible strips form the topological protected edge states in the quantum Hall effect. For the graphene Hall bar device, we utilize simultaneous AFM, STM, and quantum transport measurements at mK temperatures. The Kelvin probe force microscopy (KPFM) mode of AFM detects the chemical potential transitions when Landau levels are being filled or emptied as a function of back gate potential. In particular, symmetry breaking states can be resolved at filling factors ν = *1 inside the N=0 Landau level manifold, showing the lifting of the graphene four-fold degeneracy due to spin and valley. With KPFM we can map the dispersion of the Landau levels across the quantum Hall edge boundary as a function of density and spatial position, including resolving the ν = *1 edge modes.

O 11.2 Mon 11:00 WIL C107

Energy dissipation on suspended graphene quantum dots — •Alexina Ollier[1,2], Marcin Kisiel[1], Urs Gysin[1], and Ernst Meyer[1] — [1]Department of Physics, University of Basel,Klingelbergstr. 82, 4056 Basel, Switzerland — [2]Swiss Nanoscience Institute, Klingelbergstrasse 82, 4056 Basel

Here we report on a low temperature (T=5K) measurement of striking singlets or multiplets of dissipation peaks above graphene nanodrums surface. The stress present in the structure leads to formation of few nanometer sized graphene quantum dots ribbons (GQDRS) and the observed dissipation peaks are attributed to tip-induced charge state transitions in quantum-dot- like entities. The dissipation peaks strongly depend on the external magnetic field (B=0T-2T), the behavior we attributed to crossover from quantum dot carrier confinement to the confinement by magnetic field.

O 11.3 Mon 11:15 WIL C107

The edge morphology and electronic properties of ballistic sidewall zig-zag graphene nanoribbons on SiC (0001) — •T.T.Nhung Nguyen[1], H. Karakachian[2], J. Aprojanz[1], U. Starke[2], A. Zakharov[3], C. Polley[3], and C. Tegenkamp[1] — [1]TU Chemnitz, Germany — [2]Max Planck Institute, Germany — [3]MAX IV Lab, Sweden

Epitaxial graphene nanoribbons grown on SiC(0001) mesa structures were shown to reveal ballistic transport at room temperature. The subsequent improvement of preparation parameters allows us to fabricate large scale zig-zag type ribbons with 40nm in widths with a pitch size down to 200 nm. We analyzed the electronic structure of the ribbons and their edges by ARPES and STM/STS. Indeed, ARPES reveals clearly the Dirac cone from the ribbon. The Fermi energy coincides with the Dirac point. This finding is corroborated by STS, revealing an elastic tunneling gap of around 130meV. STM shows that the zigzag edge merges into the SiC substrate. Exactly at the position of this edge, a metallic state is seen at 0V. The gradual decrease of its intensity within 3nm comes along with a peak splitting. Moreover, the valence and conduction band states reveal close to the edge a larger gap of around 300 meV. We assign these findings to a hybridization of the zig-zag GNR edge with SiC. Furthermore, we propose that the ballistic transport is rather mediated by a 1D interface state rather than by a GNR edge state. The interface state mimics massive particles, which is consistent with the energy positions of electron transmission peaks found in GNR nanoconstrictions of various lengths.

O 11.4 Mon 11:30 WIL C107

Attosecond-fast current control at graphene-based interfaces — •Tobias Boolakee, Christian Heide, Heiko B. Weber, and Peter Hommelhoff — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

Epitaxially grown monolayer graphene on bulk n-doped silicon carbide (SiC) forms a Schottky contact with remarkable electronic and optical properties. We show that charge transfer across the graphene-SiC solid-state interface takes place within (300 ± 200) attoseconds (1 as = 10^{-18} s), which is the fastest charge transfer observed across a solid-state interface [1]. To reveal the attosecond dynamics, we apply femtosecond laser pulses and use saturable absorption in graphene as an intrinsic clock to determine how long an excited state stays excited before charge transfer and thermalization depopulate this state. Recent experimental results and a simple theoretical modelling based on rate equations and on a quantum mechanical model will be presented [2,3].

[1] Heide, C. et al. accepted in Nat. Photon.

[2] Higuchi, T. et al. Nature **550**, 224–228 (2017).

[3] Heide, C. et al. New J. Phys. **21** (2019).

O 11.5 Mon 11:45 WIL C107

Sideband generation & pseudospin-flip excitations in graphene using tr-momentum microscopy — •Marius Keunecke[1], David Schmitt[1], Christina Möller[1], Davood Momeni Pakdehi[2], Hendrik Nolte[1], Wiebke Bennecke[1], Marie Gutberlet[1], Matthijs Jansen[1], Marcel Reutzel[1], Klaus Pierz[2], Daniel Steil[1], Hans Werner Schumacher[2], Sabine Steil[1], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen. I. Physikalisches Institut, 37077 Göttingen, Germany — [2]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

The coherent control of quantum states is a promising route towards new emerging phases in solids. One of these phases are the so called Floquet-Bloch states, created by a periodic driving laser. Other light-matter coupled states (Volkov states) arise close to the surface of a solid and are understood as a final state dressing by the laser light. In graphene, the driving by circularly polarized light is predicted to open up a bandgap at the dirac point and thus creating a Floquet topological insulator [1]. In our experiment, the electronic bandstructure of ML graphene on SiC (0001) is mapped during photo-excitation using a momentum microscope in combination with a 1 Mhz femtosecond HHG lightsource (26.6 eV). Different pump wavelengths and polarizations are used to disentangle the excited states dynamics and the sideband generation at high momenta. We will discuss the nature of the generated sidebands and the photoinduced anisotropic hot carrier distributions. [1] M. A. Sentef et al., Nat. Commun. 6, 7047 (2015)

O 11.6 Mon 12:00 WIL C107

Melting the low temperature gap in monolayer VSe_2, in time resolved ARPES — •Deepnarayan Biswas[1,2], Alfred Jones[1], Paulina Majchrzak[1,3], Klara Volckaert[1], Charlotte Sanders[1,3], Igor Marković[2], Federico Andreatta[1], Akhil Rajan[2], Yu Zhang[3], Gabriel Karras[3], Tsung-Han Lee[4], Chang-Jong Kang[4], Byoung Ki Choi[5], Richard Chapman[3], Adam Waytt[3], Emma Springate[3], Jill Miwa[1], Philip Hofmann[1], Phil D. C. King[2], Young Jun Chang[5], Nikola Lanata[1], and Søren Ulstrup[1] — [1]Aarhus University, Denmark — [2]University of St Andrews, UK — [3]Central Laser Facility, UK — [4]Rutgers University, USA — [5]University of Seoul, Republic of Korea

The group V transition metal dichalcogenide VSe_2 shows a charge density wave (CDW) transition at 110 K with $(4 \times 4 \times 3)$ charge ordering in its bulk form. In contrast, recent experiments on monolayer (ML) VSe_2 have shown an enhanced transition at $\sim$ 140 K with very different charge ordering. Moreover, this transition is accompanied by a full gapping of the Fermi surface. Here, we have used time and angle resolved photoelectron spectroscopy (TR-ARPES) to understand the electron dynamics in ML VSe$_2$ above and below the transition temperature. We have also modelled the ARPES intensity using a modified BCS self energy and density functional theory calculated bare bands. We find the gapped phase vanishes upon pumping and takes unusually long time to recover (more than 10 ps). This behaviour points toward a hot electron relaxation bottleneck coupled with an electronic phase transition in this sample.

O 11.7 Mon 12:15 WIL C107

Time-dependent momentum distributions of bright and dark excitons in bulk WSe2 — •Shuo Dong[1], Samuel Beaulieu[1], Dominik Christiansen[2], Maciej Dendzik[1], Tommaso Pincelli[1], Rui Patrick Xian[1], Julian Maklar[1], Malte Selig[2], Andreas Knorr[2], Martin Wolf[1], Laurenz Rettig[1], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Transition metal dichalcogenide semiconductors feature exceptional optoelectronic properties. The investigation of excited states in k-space provides access to optically-bright and dark states on equal footing. Here, we perform the momentum-resolved excited-state mapping in the entire first Brillouin zone of bulk WSe2 using time-resolved momentum microscopy. Upon resonant excitation of band gap, the bright excitons with trARPES signal in the K valleys rapidly scatter to finite-momentum dark excitons in the Σ valleys. We analyze the shape and size of momentum distribution of the excited state. Under the plane wave final state approximation, the Fourier transform of photoemission signal yields real-space image of excitonic wave function. Combined with a microscopic theoretical description of exciton dynamics, the momentum-resolved valley carrier distribution provides information of fundamental exciton properties, like size, binding energy and exciton-phonon coupling.

O 11.8 Mon 12:30 WIL C107

Sub-picosecond photo-induced displacive phase transition in two-dimensional MoTe$_2$ — •Bo Peng[1,2], Hao Zhang[2], Heyuan Zhu[2], Bartomeu Monserrat[1], and Desheng Fu[3] — [1]TCM Group, Cavendish Laboratory, University of Cambridge, United Kingdom — [2]Department of Optical Science and Engineering, Fudan University, China — [3]Department of Optoelectronics and Nanostructure Science, Shizuoka University, Japan

Photo-induced phase transitions (PIPTs) provide an ultrafast, energy-efficient way for precisely manipulating the topological properties of transition-metal ditellurides, and can be used to stabilize a topological phase in an otherwise semiconducting material. By first-principles calculations, we demonstrate that the PIPT in monolayer MoTe$_2$ from the semiconducting 2H phase to the topological 1T' phase can be driven purely by electronic excitations. The photo-induced electronic excitation changes the electron density, and softens the lattice vibrational modes. These pronounced softenings lead to structural symmetry breaking within sub-picosecond timescales, which is far shorter than the timescale of a thermally driven phase transition. The transition is predicted to be triggered by photons with energies over 1.96 eV, corresponding to an excited carrier density of 3.4×10^{14} cm^{-2}, which enables a controllable phase transformation by varying the laser wavelength. Our results provide insight into the underlying physics of the phase transition in 2D transition-metal ditellurides, and show an ultrafast phase transition mechanism for manipulation of the topological properties of 2D systems.

O 11.9 Mon 12:45 WIL C107

Understanding electron beam damage in 2D materials from first-principles calculations: Effects of chemical etching and electronic excitation — •Silvan Kretschmer[1] and Arkady V. Krasheninnikov[1,2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Applied Physics, Aalto University School of Science, Aalto, Finland

Two-dimensional (2D) materials are routinely characterized nowadays in the transmission electron microscope (TEM). The high-energy electron beam in TEM can create defects in the target, and as the influence of defects on materials properties is expected to be stronger in systems with reduced dimensionality, understanding defect production in 2D materials is of particular importance. Irradiation-induced defects can appear through three mechanisms, namely ballistic or knock-on damage (1), ionization and electronic excitations (2) and beam-induced chemical etching (3). Only the first channel is well understood, while observations of defects formation in 2D transition metal dichalcogenides below the knock-on threshold point out that other mechanism should be important. Here we investigate the role of beam-induced chemical etching and electronic excitations in defect production by using ab-initio molecular dynamic simulations and advanced first-principles simulation techniques based on the Ehrenfest dynamics combined with time-dependent density-functional theory. We demonstrate that the adsorption of small beam-induced radicals and electronic excitations dramatically lower the displacement threshold.

O 11.10 Mon 13:00 WIL C107

Interaction of highly charged ions with single, bi- and trilayer graphene — •Anna Niggas[1], Janine Schwestka[1], Sascha Creutzburg[2], Benjamin Wöckinger[1], Tushar Gupta[3], Bernhard C. Bayer-Skoff[3], Friedrich Aumayr[1], and Richard A. Wilhelm[1,2] — [1]TU Wien, Institute of Applied Physics, Vienna, Austria — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [3]TU Wien, Institute of Materials Chemistry, Vienna, Austria

The interaction of highly charged ions (HCIs) with surfaces has been in the focus of many groups over the last decades. Recently, the rise of 2D materials has provided access to study the neutralisation dynamics of HCIs as they have not reached their equilibrium charge state inside atomically thin materials yet.

In our experiment, we use Xe ions (Xe^{1+} to Xe^{44+}) with energies in the range of 1-400 keV as projectiles and we then record the exit charge states of the ions after transmission through 2D materials. Additionally, we are able to determine the energy loss during the interaction through time of flight measurements, the yield and energy of emitted secondary electrons and forward sputtered target atoms in coincidence.

We now focus especially on the dependence of the neutralisation process on the thickness of the target. Thus, we employ single, bi- and trilayer graphene to mimic graphite with adjustable thickness. In order to ensure that this target structure is not affected by contaminations, it is crucial to implement cleaning procedures. Possible *in-situ* techniques and their effects will also be discussed in this context.

O 11.11 Mon 13:15 WIL C107

Neutralization of ions transmitted through graphene and MoS$_2$ monolayers — •Sascha Creutzburg[1,7], Janine Schwestka[2], Anna Niggas[2], Heena Inani[3], Anthony George[4], Lukas Madauss[5], Stefan Facsko[1], Jani Kotakoski[3], Marika Schleberger[5], Andrey Turchanin[4], Pedro L. Grande[6], Friedrich Aumayr[2], and Richard A. Wilhelm[1,2] — [1]HZDR, Ion Beam Center, Dresden, Germany — [2]TU Wien, Institute of Applied Physics, Vienna, Austria — [3]University Vienna, Faculty of Physics, Vienna, Austria — [4]Friedrich Schiller University Jena, Institute of Physical Chemistry, Germany — [5]University Duisburg-Essen, Faculty of Physics and CENIDE, Germany — [6]Federal University of Rio Grande do Sul, Porto Alegre, Brazil — [7]TU Dresden, Germany

Ion irradiation is a widely used technique for material modification. The use of ion irradiation for defect engineering in 2D materials requires a high sensitivity of energy deposition in the surface during the ion's impact. Ions of high charge states (e.g. Xe^{30+}) deposit their potential energy of up to tens of keV in shallow surface depths triggering nanostructure formation. In fact, nanostructure formation in 2D materials, like carbon nanomembranes or MoS$_2$, due to the impact of Xe ions of charge states larger than 28 was observed. In contrast, no nanostructures on graphene were found, even after irradiation with Xe^{40+} ions. Here, we investigated the ion's neutralization during the transmission through freestanding graphene and MoS$_2$ monolayers. We deduce the lost energy of the ions (kinetic and potential) in experiment and put our results into context of nanostructuring.

O 11.12 Mon 13:30 WIL C107

Ab-initio Exciton-polaritons: Cavity control of two-dimensional Materials — •Simone Latini[1], Enrico Ronca[1], Hannes Hübener[1], Umberto De Giovannini[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free Electron Laser Science, 22761 Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth avenue, New York NY 10010

We put forward a novel way of controlling the optical features of two-dimensional materials by embedding them in a cavity. The cavity light-matter interaction leads to the formation of exciton-polaritons, mixed states of matter and light. We demonstrate a reordering and mixing of bright and dark excitons leading to the direct optical observation of the latter. In type II van-der-Waals heterostructure, we show that the cavity provides control on the stabilization of inter- over intralayer excitons. Our theoretical predictions are based on a newly developed non-perturbative many-body framework that involves the ab-initio solution of the coupled quantized electron-photon Schrödinger equation in a quantum-electrodynamics plus Bethe-Salpeter approach. Within this framework we are able to investigate exciton-polariton states and predict their dispersion and response in a strong cavity light-matter coupling regime. Our method lends itself to the investigation of more complex polaritonic, so called phonoriton, a mixture of excitons, phonons and photons. In particular we were able to identify elusive phonoritonic spectral features observed in a state-of-the-art pump and probe experiment.

O 12: Focus Session: Topological Phenomena in Synthetic Matter II (joint session DS/O)

Time: Monday 11:15–12:15 Location: CHE 89

Invited Talk O 12.1 Mon 11:15 CHE 89

Atom-by-atom engineering of topological states of matter — •Cristiane Morais Smith — ITP Utrecht University, the Netherlands

Feynman's original idea of using one quantum system that can be manipulated at will to simulate the behavior of another more complex one has flourished during the last decades in the field of cold atoms. More recently, this concept started to be developed in nanophotonics and in condensed matter. In this talk, I will discuss a few recent experiments, in which 2D electron lattices were engineered on the nanoscale. The first is the Lieb lattice [1,2], and the second is a Sierpinski gasket [3], which has dimension $D = 1.58$. The realization of fractal lattices opens up the path to electronics in fractional dimensions. Finally, I will show how to realize topological states of matter using the same procedure. We investigate the robustness of the zero modes in a breathing Kagome lattice, which is the first experimental realization of a designed electronic higher-order topological insulator [4]. Then, we investigate the importance of the sample termination in determining the existence of topological edge modes in crystalline topological insulators. We focus on the breathing Kekule lattice, with two different types of termination [5]. In all cases, we observe an excellent agreement between the theoretical predictions and the experimental results. [1] M.R. Slot et al., Nature Physics 13, 672 (2017). [2] M. R. Slot et al., Phys. Rev. X 9, 011009 (2019). [3] S.N. Kempkes et al, Nature Physics 15, 127(2019). [4] S.N. Kempkes et al., Nature Materials 18, 1292 (2019). [5] S. E. Freeney, ArXiv: 1906.09051. .

Invited Talk O 12.2 Mon 11:45 CHE 89

Topological Insulator Lasers — •Mordechai Moti Segev — Technion - Israel Institute of Technology

The fundamentals of topological insulator lasers will be explained, based on the foundations of topological physics and challenges of reconciling topologically-protected transport and non-Hermiticity. The applications in lasers physics and the recent progress will be described.

O 13: 2D Materials (joint session CPP/O)

Time: Monday 11:30–12:15 Location: ZEU 255

O 13.1 Mon 11:30 ZEU 255

Voltage-dependent quantitative analysis of electron-dose-limited resolution for imaging two-dimensional covalent organic framework — •Baokun Liang[1], Haoyuan Qi[1,2], Hafees Sahabudeen[2], Xinliang Feng[2], and Ute Kaiser[1] — [1]Central facility for Electron Microscopy, Group of Electron Microscopy of Materials Science, University of Ulm, 89081 Ulm, Germany — [2]Department of Chemistry and Food Chemistry & Center of Advancing Electronics Dresden, Dresden University of Technology, 01062 Dresden, Germany

Two-dimensional covalent organic framework (2D COF) are promising candidates for organic electronics and next-generation energy storage. However, due to electron irradiation damage, high resolution (HR) TEM imaging of 2D COFs remains challenging, posing a substantial limitation on the structural elucidation of these organic 2D materials. Therefore, it is necessary to unravel the correlation between total electron dose and achievable specimen resolution for specific specimens. To investigate the relationship between total electron dose and achievable specimen resolution, we performed a dose-series analysis with 2D COF in electron diffraction mode under different acceleration voltages (300, 200, 120, 80 kV). With accumulating electron dose, the higher-order reflections gradually vanish, representing the degradation of specimen resolution. For quantitative analysis, the intensity of reflections within a specific resolution band was analyzed. Our method offers a quick and straightforward determination of dose-related specimen resolution under different voltages. These results lay the foundation for the HRTEM imaging of beam sensitive 2D COFs.

O 13.2 Mon 11:45 ZEU 255

Solvent interactions with two-dimensional materials: A computational investigation of the dispersion of graphene monolayers in commonly-used solvents. — •Urvesh Patil and Nuala Caffrey — School of Physics & CRANN, Trinity College, Dublin 2

Maintaining stable dispersions of two-dimensional (2D) materials is a prerequisite for several applications. The stability of dispersion, i.e., the ability of a solvent to maintain an adequate concentration of suspended flakes over time, depends strongly on the interaction between the 2D material and the chosen solvent. In order to identify the optimal solvent for a particular 2D material it is imperative to determine this interaction on the atomic scale. Here, we use density functional theory (DFT) combined with solvent models and molecular dynamics (MD) to study the interaction of graphene and MoS2 with solvent molecules such as NMP, cyclopentanone and toluene. Using DFT, we show that isolated solvent molecules interact via a van der Waals (vdW) interaction with pristine monolayers, with negligible charge transferred between them. MD calculations show that distinct solvation shells form around the 2D layer; the first solvation shell is formed as a result of vdW interaction irrespective of the polarity of solvent. This then interacts with rest of the solvent via a combination of both electrostatic and vdW forces. We show that the formation of this solvation shell is always favourable, and determine the relationship between the free energy of interaction and the experimental concentration of graphene in solution. Finally, we suggest a simple rule for mixing solvents that can be used to improve the 2D layer concentration in solution.

O 13.3 Mon 12:00 ZEU 255

Relation between topology and electronic structure of 2D polymers — •Maximilian A. Springer[1,2], Tsai-Jung Liu[2], Agnieszka Kuc[1], and Thomas Heine[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Resource Ecology, Research Site Leipzig, Permoserstrasse 15, 04318 Leipzig, Germany — [2]TU Dresden, Faculty of Chemistry and Food Chemistry, Bergstrasse 66c, 01062 Dresden, Germany

New 2D materials open access to a whole new world of compounds and properties. Graphene monolayer is such a material, since it has special electron transport features due to its honeycomb topology. Apart from the honeycomb net, there are many more 2D topologies which promise a manifold of new properties, e.g. the kagomé or the Lieb lattice. As recently shown in the case of the kagomé net, 2D polymers (covalent organic frameworks) can be designed in a way that their geometric and electronic structure match the desired topology [Y. Jing, T. Heine, J. Am. Chem. Soc. 2019, 141, 2, 743-747]. We investigate electronic properties including topological signatures of different 2D nets using a tight-binding approach. Based on these findings, we want to propose new 2D polymers with the desired structures and new properties using density-functional theory.

O 14: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions II (joint session O/HL/CPP/DS)

Time: Monday 15:00–17:30 Location: GER 38

O 14.1 Mon 15:00 GER 38

Satellites in optical and loss spectra — •Pier Luigi Cudazzo — Faculty of Science, Technology and Communication, RU Physics and Materials Science, Campus Limpertsberg, Université du Luxembourg, 162 A, avenue de la Faïencerie, L-1511 Luxembourg

Coupling of excitations leads to intriguing effects on the spectra of materials. We propose a cumulant formulation for neutral electronic excitations which opens the way to describe effects such as double plasmon satellites or exciton-exciton and exciton-phonon coupling. Our approach starts from the GW plus Bethe-Salpeter approximation to many body perturbation theory which is based on a quasiparticle picture, and it adds coupling of excitations through a consistent inclusion of dynamically screened interactions. This requires to consider scattering contributions that are usually neglected. The result is formulated in a way that highlights essential physics, that can be implemented as a post processing tool in first principles codes, and that suggests which kind of materials and measurements should exhibit strong effects. This is illustrated using a model.

O 14.2 Mon 15:15 GER 38

The XPS limit within the one-step model of photoemission: temperature and photon energy effects — •Laurent Nicolaï[1], Vladimir Strocov[2], Juraj Krempaský[2], Federico Bisti[2], Jürgen Braun[3], Hubert Ebert[3], Charles Fadley[4], Ajith Kaduwela[5], Nicholas Pike[6,7], Matthieu J. Verstraete[7], and Ján Minár[1] — [1]Univiversity of West Bohemia, Plzeň, Czech Rep. — [2]Paul Scherrer Institut, Villigen, Suisse — [3]Ludwig-Maximilians-Universität, Germany — [4]Berkeley, California, USA — [5]University of California, USA — [6]University of Oslo, Norway — [7]Université de Liège & European Theoretical Spectroscopy Facility, Belgium

Angle-Resolved Photoemission Spectroscopy (ARPES) is the method of choice for characterising the electronic structure of a given material. A complete understanding of the experimental spectra requires theoretical analyses as well. However, the development of theoretical tools in order to reproduce experimental conditions remains, to this day, a challenge. Using the one-step model of photoemission[1] as implemented in the SPRKKR package[2], our calculations incorporate temperature- and phonon energy-dependent effects via inclusion of both bulk[3] and surface phonons. We also investigate the photon energy range over which the Angle-Integrated PhotoEmission (AIPES) spectra can be compared to the corresponding Weighed Density of States (WDOS).

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O 14.3 Mon 15:30 GER 38

Ab Initio Linear and Pump-Probe Spectroscopy of Naphthalene Crystals — •Alan Lewis[1] and Tim Berkelbach[2,3] — [1]MPSD, Hamburg, Germany — [2]Columbia University, New York City, USA — [3]Flatiron Institute, New York City, USA

Linear and non-linear spectroscopies are powerful tools used to investigate the energetics and dynamics of electronic excited states of both molecules and crystals. While highly accurate ab initio calculations of molecular spectra can be performed relatively routinely, extending these calculations to periodic systems is challenging. Here, we present calculations of the linear absorption spectrum and pump-probe two-photon photoemission spectra of the naphthalene crystal using equation-of-motion coupled-cluster theory with single and double excitations (EOM-CCSD). Molecular acene crystals are of interest due to the low-energy multi-exciton singlet states they exhibit, which have been studied extensively as intermediates involved in singlet fission. Our linear absorption spectrum is in good agreement with experiment, predicting a first exciton absorption peak at 4.4 eV, and our two-photon photoemission spectra capture the behavior of multi-exciton states, whose double-excitation character cannot be captured by current methods. The simulated pump-probe spectra provide support for existing interpretations of two-photon photoemission in closely-related acene crystals such as pentacene.

O 14.4 Mon 15:45 GER 38

All-electron real-time TDDFT implementation with Ehrenfest molecular dynamics — •Ronaldo Rodrigues Pela[1,2] and Claudia Draxl[1,2] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [2]European Theoretical Spectroscopy Facility (ETSF)

Linearized augmented planewaves with local-orbitals (LAPW+lo) are arguably the most precise basis set to represent Kohn-Sham states. When employed within real-time time-dependent density functional theory (RT-TDDFT), they promise ultimate precision achievable for exploring the evolution of electronic excitations in time scales ranging from attoseconds to picoseconds. In this work, we present the implementation of RT-TDDFT in the full-potential LAPW+lo code exciting [1]. For relaxing the nuclear degrees of freedom, we include Ehrenfest molecular dynamics [2]. We benchmark our implementation by analyzing the electric current density and the ion dynamics of Si, C, SiC, and two dimensional BN under the exposure to laser pulses. We compare our results with those obtained using the octopus code [3] and find a satisfactory level of agreement.

References

[1] A. Gulans et al. J. Phys.: Condens. Matter **26**, 363202 (2014).

[2] G. Kolesov et al. J. Chem. Theory Comp. **12**, 466 (2015).

[3] X. Andrade et al. Physical Chemistry Chemical Physics **17**, 31371 (2015).

O 14.5 Mon 16:00 GER 38

Ab initio study of nonradiative recombination for defects in MoS2 via multiphonon emission — •Simone Manti[1], Lukas Razinkovas[2], Audrius Alkauskas[2], and Kristian Thygesen[1] — [1]Computational Atomic-scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, Kongens Lyngby, Denmark — [2]Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania

Carrier capture at point defects determines the lifetime of charge carriers and is therefore a very important process for both electronic and opto-electronic devices. The general theory of nonradiative recombination via the so-called multiphonon emission is rather well established, but most studies to date have mainly focused on the description in bulk materials. In this work, we investigate nonradiative carrier capture for a prototypical 2D material, molybdenum disulphide MoS2. Multiphonon emission is governed by (i) electron-phonon coupling between the band edge states and defect states and (ii) the change in the defect geometry upon carrier capture. Our results provide a preliminary description for nonradiative electron capture at sulphur vacancies in monolayer MoS2. In particular, we reveal the important role of the Jahn-Teller effect on the capture process.

O 14.6 Mon 16:15 GER 38

Phonon-induced electronic relaxation in a strongly correlated system: the Sn/Si(111) $(\sqrt{3} \times \sqrt{3})$ adlayer revisited — •Peter Kratzer and Maedeh Zahedifar — Faculty of Physics, University Duisburg-Essen

The ordered adsorbate layer Sn/Si(111) $(\sqrt{3} \times \sqrt{3})$ with coverage of one third of a monolayer is considered as a realization of strong electronic correlation in surface physics. Our theoretical analysis shows that electron-hole pair excitations in this system can be long-lived, up to several hundred nanoseconds, since the decay into surface phonons is found to be a highly non-linear process. We combine first-principles calculations with help of a hybrid functional (HSE06) with modeling by a Mott-Hubbard Hamiltonian coupled to phononic degrees of freedom. The calculations show that the Sn/Si(111) $(\sqrt{3} \times \sqrt{3})$ surface is insulating and the two Sn-derived bands inside the substrate band gap can be described as the lower and upper Hubbard band in a Mott-Hubbard model with U=0.75eV. Furthermore, phonon spectra are calculated with particular emphasis on the Sn-related surface phonon modes. The calculations demonstrate that the adequate treatment of electronic correlations leads to a stiffening of the wagging mode of neighboring Sn atoms; thus, we predict that the onset of electronic correlations at low temperature should be observable in the phonon spectrum, too. The deformation potential for electron-phonon coupling is calculated for selected vibrational modes and the decay rate of an electron-hole excitation into multiple phonons is estimated, substantiating the very long lifetime of these excitations.

O 14.7 Mon 16:30 GER 38

Spectral properties of the interacting homogeneous electron gas — •Tommaso Chiarotti[1], Nicola Marzari[1], and Andrea Ferretti[2] — [1]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Centro S3, CNR–Istituto Nanoscienze, 41125 Modena, Italy

Despite its simplicity, the interacting homogeneous electron gas (HEG) is a paradigmatic test case in the study of the electronic structure of condensed matter. Beside being a model for valence electrons in simple metals, it also provides the basic ingredients for key electronic-structure theories. Here, we propose to study it with many-body perturbation theory (MBPT) using one shot, partial self-consistent, and full self-consistent GW, and analyze the description of its spectral function. For this, a novel numerical implementation of MBPT for the 3D non-relativistic HEG has been developed, with a special focus on the treatment of the full-frequency dependence of the Green's function and self-energies. Results for a broad range of densities (going from r_s from 1 to 10) are presented with particular attention to the calculated density-of-states and the spectral potential.

O 14.8 Mon 16:45 GER 38

Multipole Polarizabilites of Positronium and Its Interaction with Atoms and Molecules — •Jorge Charry, Dmitry Fedorov, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

Positron – the antiparticle of the electron – has many intriguing fundamental properties and it is also useful in many applications for probing matter. Besides electron-positron annihilation, metastable states of atomic and molecular systems involving binding between electrons and positrons are of great interest [1]. In addition, electrons and positrons can form positronium (Ps) atoms and even larger clusters. The polarization of positron by a residual ion is one of possible mechanisms for the formation of bound states for positron-based chemistry [2]. An accurate description of the polarizability of Ps and its bound state with atoms and molecules is essential to understand such interactions. Here, we extend the direct transition-matrix approach, proposed by Kharchenko to determine the multipole polarizabilities of the hydrogen atom [3], to the case of finite nuclear mass. The obtained analytical results, which are in agreement with our numerical calculations performed by means of the molecular orbital based method [4], show that Ps has unique properties in comparison to other normal atoms. Our results shed light into the fundamental interactions between matter and antimatter. [1] Gribakin *et al.*, Rev. Mod. Phys. **82**, 2557 (2010); [2] Bromley and Mitroy, J. Phys.: Conf. Series **199**, 012011 (2010); [3] Kharchenko, Annal. Phys. **355**, 153 (2015); [4] Reyes *et al.*, Int. J. Quant. Chem. **119**, 1 (2019)

O 14.9 Mon 17:00 GER 38

Energy gap closure of crystalline molecular hydrogen with pressure — •Vitaly Gorelov[1], Markus Holzmann[2,3], David M. Ceperley[4], and Carlo Pierleoni[5,1] — [1]Maison de la Simulation, CEA-Saclay, Gif-sur-Yvette, France — [2]Univ. Grenoble Alpes, CNRS, LPMMC, Grenoble, France — [3]Institut Laue-Langevin, Grenoble, France — [4]Department of Physics, University of Illinois Urbana-Champaign, USA — [5]Department of Physical and Chemical Sciences, University of L'Aquila, L'Aquila, Italy

We study the gap closure with pressure in Phases III and IV of molecular crystalline hydrogen. Nuclear quantum and thermal effects are considered from first principles with Coupled Electron Ion Monte Carlo. The fundamental electronic gaps are obtained from grand-canonical Quantum Monte Carlo methods properly extended to quantum crystals. Nuclear zero point effects cause a large reduction in the gap ($\sim 2eV$). As a consequence the fundamental gap closes at 530GPa for ideal crystals while at 360GPa for quantum crystals. Since the direct gap remains open until ∼450GPa, the emerging scenario is that upon increasing pressure in phase III (C2/c-24 crystal symmetry) the fundamental (indirect) gap closes and the system enters into a bad metal phase where the density of states at the Fermi level increases with pressure up to ∼450GPa when the direct gap closes. Our work partially supports the interpretation of recent experiments in high pressure hydrogen.

O 14.10 Mon 17:15 GER 38

Using the powerful electronic structure theory to identify single photon emitters in h-BN. — •Sajid Ali — CAMD, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

In recent years two-dimensional Van Der Walls material h-BN have gained a considerable interest due to the discovery of single photon emission (in both visible and UV region) from the colour centres in this material. This emission is bright, owing to the natural proximity of the centres to the surface, showing promise for high quantum efficiency applications, linearly polarized and strain tuneable. However, the exact chemical nature of the emitting centres is still unknown.

Here, we have performed first principle calculations to obtain observables that can be directly compared with electron paramagnetic resonance (EPR), Optically Detected Magnetic Resonance (ODMR), photoluminescence spectroscopy (PL) and Raman spectroscopy techniques performed on these h-BN emitters. We identify, based on the comparison of our calculations with the experimental data, the defect centres responsible for single photon emission from hexagonal boron nitride.

O 15: Organic Molecules on Inorganic Substrates II: Mainly Porphyrins

Time: Monday 15:00–18:00 Location: REC C 213

Invited Talk O 15.1 Mon 15:00 REC C 213

Molecular nanostructures on metals vs. graphene: towards preserving functional properties — •Meike Stöhr — Zernike Institute for Advanced Materials, University of Groningen, Netherlands

To preserve the (functional) properties of either individual adsorbates or well-ordered molecular assemblies upon adsorption on solid surfaces, the molecule substrate interactions have to be generally relatively weak. This can be achieved by introducing a decoupling layer between (metallic) surface and molecules. Among others, thin insulating layers of either NaCl or hBN have been shown to be very useful to this end. The chemical inertness and the low density of states near the Fermi level also make graphene a good choice as a buffer layer to decouple adsorbed molecules from the underlying (metallic) substrate. For two different organic molecules, the changes in both structural and electronic properties will be discussed [1]. On the other hand, instead of turning off the molecule substrate interactions, enhancing the intermolecular interactions is another possibility for preserving the adsorbates' properties. This could be shown on the basis of charge-transfer interactions [2] as well as utilizing molecular coverage [3].

[1] J. Li et al., J. Phys. Chem. C 120 (2016) 18093 ; N. Schmidt et al., Chem. Eur. J. 25 (2019) 5065 ; J. Li et al., J. Phys. Chem. C 123 (2019) 12730. [2] K. Müller et al., Small 15 (2019) 190174. [3] B.D. Baker et al., J. Phys. Chem. C 123 (2019) 19681.

O 15.2 Mon 15:30 REC C 213

On-surface synthesis of porphyrin tetramers — •Eduardo Corral-Rascon, Alexander Riss, Yang Bao, and Willi Auwärter — Physics Department E20, Technical University Munich, Germany

Covalently coupled porphyrins [1,2,3] hold great promise for molecular electronics, optoelectronics, gas sensing and light-harvesting. Furthermore, the electronic conjugation [4] might lead to antiaromatic behavior [3] and additionally offers ways to fabricate spin-coupled nanoarchitectures via introduction of metal centers into the porphyrin cores. Here we present the synthesis of porphyrin tetramers possessing a cyclooctatetraene (COT) moiety at the center of the molecules adsorbed on a Ag(100) surface. Bond-resolved atomic force microscopy (AFM) and scanning tunneling microscopy (STM) were used to characterize the coupling and the emerging electronic properties. In particular, we have investigated how the chemical structure affects the electronic conjugation throughout the molecule.

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[2] Bischoff, A. et al. *Angew. Chem.* **2018**, 130, 16262

[3] Nakamura, Y. et al. *J. Am. Chem. Soc.* **2006**, 128, 4119
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O 15.3 Mon 15:45 REC C 213

Electronic Fingerprint of a Tetraphenylporphyrin on MgO — •Silviya Ninova[1] and Michel Bockstedte[1,2,3] — [1]Paris-Lodron-Universität Salzburg, Austria — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg — [3]Johannes-Kepler Universität Linz, Austria

Porphyrin-substrate hybrid systems are the building blocks in a series of materials, such as the organic light-emitting diodes, chemical sensors, dye-sensitized solar cells and solar-energy conversions. Understanding and correctly describing the way molecules interact with the substrate upon adsorption hold the key to the prediction and improvement of the present-day devices.

Recently, distinct features were observed in the photoemission spectra of Co(II)-tetraphenylporphyrin on MgO/Ag(100) related to the molecular monolayer and film[1]. Here we investigate the structural and electronic changes the molecule undergoes upon deposition on the substrate in the framework of hybrid density-functional theory and beyond it. Our simulations of adsorption at different terrace and low-coordinated surface sites give an insight into the underlying distinct interactions and electronic features.

[1] Franke *et al.*, *Physical Chemistry Chemical Physics*, 2017, 19, 11549-11553

O 15.4 Mon 16:00 REC C 213

Oxidation-State Tuning and Supramolecular Mixed-Valence Phases: Nickel(II) Porphyrin on Ag(111) — •Jan Herritsch, Qitang Fan, Marie Albus, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

Porphyrin complexes are of exceptional importance in the field of surface functionalization. The reactivity and selectivity towards gas molecules depends crucially on the active central atom. Here, we report on the influence of the adsorbate interaction on the electronic structure of a nickel porphyrin (NiOEP) monolayer on coinage metal surfaces studied by XPS and STM. Due to the size mismatch between the small low-spin d8 nickel(II) cation and the larger central cavity of the porphyrin macrocycle, the metal center shows a labile oxidation state which depends on the interaction with the metal surface. On the reactive Cu(111) surface, NiOEP forms a long-range ordered structure in which nickel centers are uniformly reduced, according to XPS. On less reactive Ag(111), NiOEP forms a mixed-valent adsorbate phase in which the Ni centers occur in two different oxidation states. The two separate peaks in the Ni 2p XP spectrum indicate that about 40 % of the Ni centers are reduced. STM shows a superstructure with an ordered arrangement of the metal centers in different oxidations states. Analysis of misaligned metastable domains reveals that the registry with the substrate is critical for obtaining the mixed-valence superstructure. On the most inert Au(111) surface, the oxidation state of the Ni centers remains unaffected by adsorbate interactions.

O 15.5 Mon 16:15 REC C 213

Exciton control in single-molecule fluorochromes — •Jiří Doležal[1,2], Pablo Merino[3,4], Pingo Mutombo[1], Pavel Jelínek[1] und Martin Švec[1] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [3]Instituto de Ciencia de Materiales de Madrid, CSIC, Sor Juana Inés de la Cruz 3, E28049, Madrid, Spain — [4]Instituto de Física Fundamental, CSIC, Serrano 121, E28006, Madrid, Spain

Plasmonic picocavities in highly defined environment of ultrahigh vacuum and cryogenic temperatures represent ideal testbeds for investigation of the photophysical properties of single-molecule photon emitters and to explore fundamental aspects of their luminescence. In this work, we studied two structural analogs with distinct electronic properties using a photon-scanning probe microscope: CuPc and ZnPc molecules adsorbed on NaCl / Ag(111) substrates. For the CuPc, we determine how its exact adsorption configuration and coupling to the substrate affect the S1 exciton energy and lifetime. For the ZnPc molecule, two competing excitons [1] are mapped in the real-space with submolecular resolution. Both phenomena are discussed in a broader context of ab-initio simulations and additional experimental evidence available from the atomic force and electron tunneling channels of the microscope.

[1] Doppagne B, Chong MC, Bulou H, Boeglin A, Scheurer F, Schull G. Electrofluorochromism at the single-molecule level. Science 2018;361:251-5.

O 15.6 Mon 16:30 REC C 213

Thermal stability and conformational changes of a catalytically active metal/organic interface — •H. Sturmeit[1], I. Cojocariu[2,6], A. Cossaro[3], A. Verdini[3], L. Floreano[3], C. Africh[3], A. Sala[3,4], G. Comelli[3,4], S. Moro[4], M. Stredansky[3,4], M. Corva[3,4], E. Vesselli[3,4], M. Jugovac[2], P. Puschnig[5], C. M. Schneider[2,6], V. Feyer[2,6], G. Zamborlini[1], and M. Cinchetti[1] — [1]TU Dortmund, Germany — [2]Forschungszentrum Jülich, Germany — [3]CNR-IOM, Lab. TASC, Italy — [4]Physics Department, University of Trieste, Italy — [5]Institut für Physik, Karl-Franzens-Universität Graz, Austria — [6]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Germany

Porphyrin molecules are widely employed as building blocks in photovoltaics, heterogeneous catalysis, gas sensing and the emerging field of on-surface magnetochemistry. When deposited on metal electrodes, they can undergo surface-induced chemical changes, such as partial dehydrogenation, dehydrocyclization or intramolecular structural modifications of their macrocycle. These changes alter their electronic structure and thus their reaction properties essentially. We demonstrate the high thermal stability of catalytically active Ni(I)TPP up to 350°C on a Cu electrode. Photoelectron tomography supported by photoemission and vibronic spectroscopy, and STM measurements prove that, below the fragmentation temperature, the adsorbed porphyrins do not experience any chemical modification, but undergo a conformational modification, while preserving the stability of the reactive Ni(I) ion. This is crucial for the re-activation of saturated catalytical sites.

O 15.7 Mon 16:45 REC C 213

CoTPP molecules deposited on passivated Fe-(100)-p(1x1)O: a molecular orbital tomography study — •David Janas[1], Henning Sturmeit[1], Iulia Cojocariu[2], Vitaliy Feyer[2], Stefano Ponzoni[1], Giovanni Zamborlini[1], and Mirko Cinchetti[1] — [1]Experimentelle Physik VI, TU Dortmund, 44227 Dortmund, Germany — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany

In order to enhance the performances of molecular spintronic devices, a detailed knowledge of the physical properties at the interface is fundamental [1]. In this context molecular orbital tomography (MOT), which combines ab-initio calculations and angle-resolved photoelectron spectroscopy (ARPES), stands out as a powerful and reliable tool to unravel the orbital structure of molecular thin films at metal/organic interfaces [2]. In our work we apply MOT to investigate the interaction of paramagnetic molecules, namely CoTPP, on the passivated Fe-(100)-p(1x1)O surface. Recently, it was shown that the interactions at this interface lead to an emergent magnetic ordering of the molecular layer. Here, we use MOT to further characterize this intriguing system. In particular, we precisely determine the energy level alignment at the interface, the nature of the frontier orbitals, and the azimuthal orientation of the CoTPP molecules with respect to the substrate.

[1] Cinchetti, M., Dediu, V. & Hueso, L. Activating the molecular spinterface. Nature Mater 16, 507-515 (2017) doi:10.1038/nmat4902

[2] Puschnig, P. et al. Reconstruction of molecular orbital densities from photoemission data. Science 326, 702-706 (2009)

O 15.8 Mon 17:00 REC C 213

Electronic and magnetic properties of phtalocyanine molecules on rare-earth noble-metal surfaces — •Laura Fernandez[1], Rodrigo Castrillo[2], Khadiza Ali[2], Maxim Ilyn[2], Michele Gastaldo[3], Miguel Angel Valbuena[4], Marcos Paradinas[3], Aitor Mugarza[3], and Frederik Schiller[2,5] — [1]Universidad del Pais Vasco, San Sebastian, Spain — [2]Centro de Física de Materiales and Material Physics Center, San Sebastian, Spain — [3]Catalan Institute of Nanoscience and Nanotechnology, Bellaterra, Spain — [4]IMDEA Nanociencia, Cantoblanco, Spain — [5]Donostia International Physics Center,San Sebastian, Spain

Here we explore new spin textured interfaces by using as a substrate non-conventional magnetic surface- confined alloys, which contains rare earths (RE) atoms and Au. The broad number of possible RE atoms used for the preparation of such alloys provides an attractive platform to optimize and tune magnetic metal-organic interfaces with many different spin textures. We focus on the growth of CuPc on different 2D surface compounds like GdAu2, HoAu2, and the paramagnetic YbAu2. For the study of the electronic properties we use X-ray and angle resolved photoemission spectroscopy, while the magnetic properties of the systems were investigated by X-ray magnetic circular dichroism. We observe similar electronic interaction of CuPc on these surfaces, with variation depending on the valence of the RE atom. From the magnetic point the different RE atom of the substrate induce different magnetic interactions with the the CuPc molecule.

O 15.9 Mon 17:15 REC C 213

Real-space engineering the optoelectronic properties of single molecules — •Tzu-Chao Hung, Brian Kiraly, Julian Strik, Alexander Khajetoorians, and Daniel Wegner — Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, The Netherlands

While optical properties of light-emitting molecules are mostly studied via luminescence spectroscopy, several recent studies revealed a fundamental lack of understanding luminescence on the single-molecule level. Intermolecular and environmental interactions can have a significant impact on the optoelectronic properties but are hardly controllable in ensemble measurement. We combine STM/STS and atomic manipulation to study the STM-induced light emission of single molecules and molecular assemblies. Using zinc-phthalocyanine (ZnPc) molecules on ultrathin NaCl films, we demonstrate how the emission yield, energy shift and resolution of luminescence spectra change by anchoring ZnPc to a step edge or by assembling molecules into chains. This not only allows us to understand and disentangle the impact of intermolecular and molecule-substrate coupling on exciton lifetimes, but ultimately permits high-resolution vibronic spectroscopy providing a chemical fingerprint of single molecules. Furthermore, utilizing the tautomerism of H2Pc, which can be manipulated by the tunneling current, we study how to fine-tune dipole-dipole coupling, toward sub-molecular design of the spectroscopic response.

O 15.10 Mon 17:30 REC C 213

Vibrational excitation mechanisms in tunneling spectroscopy beyond the Franck-Condon model. — •Gaël Reecht, Nils Krane, Christian Lotze, and Katharina J. Franke — Freie Universität, Berlin, Germany

Since two decades, scanning tunneling spectroscopy (STS) is used to study vibrations of individual molecules on surface, either via inelastic tunneling spectroscopy (IETS) or vibronic spectroscopy. In the latter cases, experimental results were generally explained within the Franck-Condon picture, which treats vibronic excitations within the Born-Oppenheimer approximation and derives the excitation probabilities from an overlap integral of initial and final state. However this model cannot justify any spatial dependence of vibronic excitations. Here we study with low temperature STM, large organic molecules (thiophene derivative and phthalocyanine) on single layer MoS_2 on Au(111). The van der Waals layer acts as an efficient decoupling layer from the metal substrate and provides exceptional energy resolution of a few meV, which gives access to the rich vibronic signature of the investigated molecules. To explain the complete excitation model, spatially and energetically, we show that the Franck-Condon picture has to be combined with a vibration-assisted process, which perturbs the molecular wave functions, and therefore its overlap with the tip wave function. Using DFT calculations of the molecule in gas phase, our simple model reproduces the experimental spectra at arbitrary position of the STM tip over the molecule in great detail.

O 15.11 Mon 17:45 REC C 213

Direct observation of long-range surface-mediated molecule-molecule hybridization — Marina Castelli[1], •Jack Hellerstedt[1], Cornelius Krull[1], Spiro Gicev[2], Lloyd CL Hollenberg[2], Muhammad Usman[2], and Agustin Schiffrin[1] — [1]School of Physics and Astronomy, Monash University, Clayton VIC 3800 Australia — [2]Centre for Quantum Computation and Communication Technology, Faculty of Science, University of Melbourne, VIC 3010, Australia

Metalated phthalocyanines are robust and versatile molecular complexes, whose properties can be tuned by changing its functional groups and central metal atom. Magnesium phthalocyanine (MgPc) is structurally close to the chlorophyll molecule responsible for photosynthesis in bio-organisms. Here we studied the electronic structure of MgPc on Ag(100) via low-temperature scanning probe microscopy (STM/STS/ncAFM) and density functional theory (DFT). Our ncAFM and STS data show that a single isolated MgPc molecule exhibits a flat four-fold symmetric morphology with doubly degenerate, partially populated lowest unoccupied molecular orbitals (LUMOs). Adjacent MgPc's (3 nm or less) show a lift of LUMO degeneracy and symmetry reduction. We explain this interaction by a two-step hybridization process: MgPc orbitals hybridize with Ag(100), forming molecule-surface orbitals with enhanced spatial extension that hybridize in turn with neighboring molecules. Distance-dependent analysis of the resulting symmetry reduction allows us to quantitatively describe the nature of this long-range surface-mediated interaction.

O 16: Nanoscale Heterogeneous Catalysis

Time: Monday 15:00–18:15 Location: TRE Ma

O 16.1 Mon 15:00 TRE Ma

Nickel and Platinum Clusters in Methanol Photocatalysis on Rutile Titania — •Moritz Eder, Carla Courtois, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

We investigate the role of metal clusters in the photocatalytic alcohol conversion on an n-type semiconductor single crystal surface. It is known that small platinum clusters enable the desorption of molecular hydrogen from the surface, preventing catalyst deactivation and making alcohol photoconversion truly catalytic. This work focuses on the role of nickel clusters in methanol chemistry on reduced a titania(110)surface. Strong parallels to the thermal reactivity of platinum are evident, and the photochemistry is still governed by the semiconductor. However, catalyst deactivation is observed. Its likely causes are discussed with respect to certain pre-treatments.

O 16.2 Mon 15:15 TRE Ma

Hydrogenation of small organic molecules on size-selected Pd-clusters supported on MgO — •Kevin Bertrang, Maximilian Krause, Marian David Rötzer, Andrew Scott Crampton, and Ueli Heiz — Technische Universität München, Lichtenbergstr. 4, D-85748 Garching, Germany

Heterogeneous catalysis on size-selected clusters supported on metal-oxide films opens up a huge pallet of potential catalysts. The unique, non-scalable particle size dependency down to differences of only one atom lead to unique chemical and physical proprieties reflected by drastic changes in chemical activity and selectivity. Cluster-size portrays only one of a manifold of tunable variables. Properties of the support (i.e. metal-oxide thin films grown on metal single crystals) influence the cluster charge: film thickness, acidity and reducibility, (local) crystal work function, interface interactions. Control of these quantities allows to induce drastic changes in a catalyst's performance. Beside activity the selectivity of a catalyzed reaction is a fundamental concept in heterogeneous catalysis. Great emphasis is put on tailoring catalytic systems to stir their selectivity towards chemically desirable products. In this regard we studied the ripening of size-selected supported Pd_n-clusters ($n \leq 30$) and the adsorption properties of acrolein, crotonaldeyhde and prenal on MgO by means of electronic (UPS, MIES) and vibrational (IRRAS) spectroscopy. Further, the activity and selectivity towards the hydrogenation of small organic molecules is investigated by means of pulsed molecular beam reactive scattering and temperature programmed desorption.

Invited Talk O 16.3 Mon 15:30 TRE Ma

Nanotuning via local work function control: Ethylene hydrogenation on supported Pt nanoclusters — •Ueli Heiz[1], Marian D. Rötzer[1], Maximilian Krause[1], Andrew S. Crampton[1], Bokwon Yoon[2], and Uzi Landman[2] — [1]Lehrstuhl für Physikalische Chemie, Catalysis Research Center & Chemistry Department, Technische Universität München, Lichtenbergstraße 4, 85748 Garching, Germany — [2]School of Physics, Georgia Institute of Technology, Atlanta, GA 30332-0430, USA

Prevention of blocking and deactivation of the hydrogenation of unsaturated hydrocarbons resulting from carbonaceous coke formation is a major challenge. Here we demonstrate experimentally and theoretically that the activity, selectivity, specificity and deactivation of size-selected platinum clusters can be controllably tuned by manipulating the local electronic density of the catalyzing Pt cluster via appropriate choice of the support system. We show that along with interfacial particle-to-support bonding effects, electron transfer and charge balance on the supported sub-nanometer metal clusters, controlling the catalysts activity, can be tuned by the local work function of the catalysts support. Control of this materials property was demonstrated through synthesis of ultra-thin amorphous silica, a-SiO2, films on single crystals with differing work-functions, Pt(111) or Mo(211), serving as supports for the active sub-nanometer cluster component. The new catalytic control factor introduced here, akin to support-doping, allows steering of the chemical catalytic activity and may be used to inhibit undesirable catalyst poisoning and coke formation.

O 16.4 Mon 16:00 TRE Ma

Palladium nanoparticles supported on sapphire (0001): Decomposition of metastable palladium carbide under LOHC and under inert gas atmosphere — •Ralf Schuster[1], Manon Bertram[1], Henning Runge[2], Simon Chung[2], Vedran Vonk[2], Heshmat Noei[2], Yaroslava Lykhach[1], Andreas Stierle[2], and Jörg Libuda[1] — [1]Interface Research and Catalysis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen — [2]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22607 Hamburg

Surface carbon species can be formed by unselective decomposition during heterogeneously catalyzed dehydrogenation of liquid organic hydrogen carriers (LOHCs). These species may diffuse into the bulk of the catalyst, forming a metal carbide phase. For palladium, however, the carbide phase is metastable with respect to palladium and graphite. Therefore, we studied the stability of palladium carbide on sapphire-supported Pd nanoparticle model catalysts. Two different particle sizes were investigated under reaction conditions (500 K, 1 bar) by high-energy grazing incidence X-ray diffraction. For small particles and low gas flow rate, the carbide formed is stable in LOHC atmosphere but decomposes under pure argon. Increasing the gas flow rate results in immediate decomposition of the carbide even in the presence of LOHC. Studies on bigger particles at low gas flow rate show a different behavior. Here, the carbide is stable in the presence of LOHC only for a limited amount of time before it decomposes in further contact with the LOHC.

O 16.5 Mon 16:15 TRE Ma

Coupled Cluster Embedding of Metal Nanoparticles — •Wilke Dononelli — Department of Physics and Astronomy, Aarhus University, Denmark

In a recent study, we calculated CCSD(T) adsorption energies on metal nanoparticles (NPs) of varying sizes [1]. We were able to show that it is possible to calculate adsorption energies and activation barriers for different sizes of NPs at the CCSD(T) level of theory by using ONIOM as a QM/QM* embedding scheme and discussed the results with respects to full CCSD(T) and DLPNO-CCSD(T) energies for small 13 atom coinage metal NPs [2]. Another way of calculating energies at higher levels of theory is using either the method of increments (see e.g. ref [3]) or a simpler similar approach (without usage of localized molecular orbitals from an all electron calculation) the many body expansion (MBE). The advantage of using a MBE is that the estimated total energy can be calculated from a pre-calculated database or can be estimated e.g. with neural networks [4]. In our new approach we are trying to use a MBE in the framework of the before mentioned QM/QM* embedding scheme [1] in order to overcome some problems related to neglecting the overall electronic structure of a system when using the MBE.

References [1] W. Dononelli and T. Klüner; Faraday Discuss. 208, 105 (2018) [2] R. Arrigo et. al, Faraday Discuss. 208, 147 (2018) [3] E. Voloshina, Phys. Rev. B 85, 045444 (2012) [4] K. Yao, J. E. Herr and J. Parkhill, J.Chem.Phys. 146, 014106 (2017)

O 16.6 Mon 16:30 TRE Ma

Cluster superlattice membranes — Tobias Hartl[1], •Moritz Will[1], Sophia Dellmann[1], Davor Čapeta[2], Virgínia Boix de la Cruz[3], Rajendra Singh[4], Daniel Scheinecker[4], Paolo Lacovig[5], Silvano Lizzit[5], Jani Kotakoski[4], Marko Kralj[2], Jan Knudsen[3], Thomas Michely[1], and Pantelis Bampoulis[1] — [1]II. Physikalisches Institut, University of Cologne — [2]Institut za fiziku, Zagreb — [3]MAX-IV Lab, Lund — [4]Faculty of Physics, University of Vienna — [5]ELETTRA Sincrotrone, Trieste

We demonstrate the fabrication of a free-standing material consisting of a dense array of perfectly ordered and similar-sized metal nanoclusters sandwiched between sp2/sp3-hybridized carbon and graphene, highly stable under reaction conditions. The nanometer-thick membrane is prepared by conformal embedding of pre-formed Ir cluster arrays on graphene/Ir(111) with elemental carbon in ultra-high vacuum and subsequent ex situ transfer from the Ir(111) crystal by the hydrogen bubbling method. High resolution transmission electron microscopy of the free-standing membrane confirms the perfect order and crystallinity of the encapsulated metal clusters, with super-lattice constant of 2.51nm and Ir nearest-neighbor distance of 2.5A. The approach presented in this study can be extended to different cluster materials and sizes. It paves the way for synthesizing cluster membranes with tunable functionalities which have potential applications in optoelectroncis, nanomagnetism and catalysis.

O 16.7 Mon 16:45 TRE Ma

Shape-controlling effects of hydrohalic and carboxylic acids in TiO_2 nanoparticle synthesis — Kai Sellschopp[1], Wolfgang Heckel[1], Johannes Gäding[1], Clemens Schröter[2], Andreas Hensel[2], Tobias Vossmeyer[2], Horst Weller[2], Stefan Müller[1], and •Gregor Vonbun-Feldbauer[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology — [2]Institute of Physical Chemistry, University of Hamburg

Shape-controlled synthesis of nanoparticles (NP), here titania (TiO_2), is paramount for various fields from catalysis to materials design. In thermodynamic equilibrium, the NP shape is governed by the stability of competing surface facets which also determine characteristics of NPs such as the reactivity or the mechanical properties of assembled NPs. Combing density functional theory (DFT) calculations with experimental techniques such as TEM, we studied the influence of various adsorbates on the NP shape during synthesis. This effort allowed the identification of mechanisms stabilizing different facets and the detailed characterization of the NPs which shows the agreement between computational and experimental work. Investigating the effects of variations in the physical conditions and chemical environments, e.g. via changes in the chemical potentials, highlights potentials for new synthesis routes and NP shapes.

O 16.8 Mon 17:00 TRE Ma

Ru/TiO_2 catalysts in the CO_2 methanation: chemical nature of Ru nanoparticles investigated by operando X-ray absorption spectroscopy — •Joachim Bansmann, Ali Abdel-Mageed, Shilong Chen, Klara Wiese, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, Albert-Einstein-Allee 47, D-89081 Ulm, Germany

The CO_2 methanation (known as Sabatier reaction) is an important catalytic process for the conversion of CO_2 to methane in H_2 rich gas mixtures over Ni and Ru catalysts and has recently gained increasing interest due to its application in the power-to-gas technology.

In this contribution, we concentrate on the physical and chemical properties of Ru nanoparticles on Ru/TiO_2 catalysts in the CO_2 methanation using TiO_2 (P90) supports. The catalysts were investigated at the ID 24 beamline at the ESRF (Grenoble) using operando X-ray absorption spectroscopy (XAS) at the Ru K edge in a CO_2 reformate gas mixture at atmospheric pressure (15.5% CO_2, balance H_2) at 190C. Additionally, we applied a stepwise increase in the temperature up to 350C in the reaction gas mixture in order to activate the catalysts followed by measurements at 190C. XANES data showed a very high content of metallic Ru species during the activation period. The effect of the activation step on the activity and deactivation of the catalyst will be discussed based on simultaneously recorded IR/GC data. Furthermore, the results will be compared to recently obtained operando XAS in the CO methanation over Ru/TiO_2 catalysts used in our group.

O 16.9 Mon 17:15 TRE Ma

Nanoscale surface chemistry of Au-based catalysis studied by field emission techniques — Luc Jacobs[1], Thierry Visart de Bocarmé[1], Austin Akey[2], David Bell[2], and •Cédric Barroo[1,2] — [1]Université Libre de Bruxelles — [2]Harvard University

To improve the efficiency of binary catalysts, it is crucial to understand the surface composition/reactivity relationships. Here, we studied the AuAg system exhibiting high activity and selectivity for deNOx and selective oxidation reactions. The catalytic performance of AuAg is attributed to the presence of traces of silver allowing to provide adsorbed atomic oxygen, the key factor for activity/selectivity on gold surfaces. To do so, we used field ion microscopy (FIM), field emission microscopy (FEM) and atom probe tomography (APT). APT is used to characterize the structure of nanoporous gold catalysts and to study the non-homogeneous distribution of Ag within the 3D-structure. The size of a single ligament corresponds to ~50nm and can be modelled by sharp tips. Such samples are analyzed with atomic-scale resolution by FIM to study the structure before and after reaction; but also by FEM to observe the structure-reactivity relationships during the ongoing process. N2O+H2 was selected for its ability to provide atomic oxygen at the surface, and the experiments provide insights into the local reactivity of the sample: within a very strict temperature range, we can study the relative reactivity of different crystallographic orientations. Further experiments were performed during O2+H2 and CH3OH+O2 reactions. These results prove the relevance of field emission techniques to study the catalytic activity of alloys.

O 16.10 Mon 17:30 TRE Ma

In situ SEM as surface-sensitive tool to study catalytic reactions — •Cédric Barroo[1], Zhu-Jun Wang[2], and Marc Willinger[2] — [1]Université Libre de Bruxelles — [2]ETH Zurich

Non-equilibrium reactions are observed in a variety of reactive systems, including at the surface of catalytic materials. Probing such reactions and their dynamics during the ongoing processes remains challenging due to the scarcity of techniques allowing for in situ experiments. Here we report the observation and analysis of nonlinear behaviours during NO2+H2 on Pt catalysts using in situ environmental scanning electron microscopy (ESEM), a technique sensitive to the variations of work function due to the presence of adsorbates. The ESEM instrument allows to study samples with various morphologies, allowing to bridge the materials-gap, and can be used with gas pressures up to tens of Pa. Experiments during the NO2 hydrogenation were performed on Pt single crystals and on Pt foils, and several types of nonlinear behaviours were observed, mainly in the form of spiral patterns. Different brightness levels can be distinguished on a single propagating wave, sign of different surface adsorbate composition. These patterns were observed on regions as large as 100 *m and over a wide range of pressures: from 10-3 to 20 Pa. ESEM can be used to observe similar phenomena over different pressure conditions, allowing to, somewhat, bridge the pressure-gap; but also analysing the same reaction on single crystal and foils: it is then possible to study the various reaction behaviors, the structure sensitivity of the reaction, the spillover between different facets, and how the presence of boundaries affects the reactivity.

O 16.11 Mon 17:45 TRE Ma

Molecular Dynamics Simulations of Silver Tarnishing — •Gabriele Saleh[1,3], Chen Xu[2], and Stefano Sanvito[3] — [1]Istituto Italiano di Tecnologia, Via Morego 30, Genova 16163 Italy — [2]Nokia Bell Labs, 600 Mountain Avenue, Murray Hill, NJ, USA — [3]a School of Physics, AMBER and CRANN institute, Trinity College Dublin, College Green, Dublin 2, Ireland

Silver is broadly adopted in electronics, although its tendency to degrade by reacting with the environment (Ag tarnishing) represents a severe limitation. Ag is easily tarnished by sulphur compounds, even at ppb concentrations, but hardly reacts with O2, despite thermodynamics predicts both sulphide and oxide to form favorably at ambient conditions[1]. The reactivity disparity is thus to be sought in the reaction dynamics, that is the focus of this contribution. We performed extensive Molecular Dynamics (MD) simulations of Ag/S and Ag/O reactions by employing reactive force fields (ReaxFF [2]). We unearth the different mechanisms of silver oxidation and sulphidation[3], thereby explaining why the latter but not the former takes place. The influence of various defects on Ag reactivity is also considered. Ab initio calculations are performed to confirm and further rationalize the MD findings. Additionally, our results recover (and explain) a number of experimental results from literature. Importantly, for this study we developed new ReaxFF force fields that was extensively tested against ab initio results. [1] P. Patnaik *Handbook of Inorganic Chemicals* [2] A.C.T. van Duin et al., J. Phys. Chem. A 105, 9396 (2001) [3] G. Saleh et al., Angew. Chem. 58, 6017 (2019)

O 16.12 Mon 18:00 TRE Ma

Water-Gas Shift Activity on Au-Clusters Supported over TiO2(110) Surface: The Role of Planar Versus Non-Planar Au-Clusters — •Bhumi Baraiya[1], Venu Mankad[2], and Prafulla Jha[1] — [1]Department of Physics, Faculty of Science, The M. S. University of Baroda, Vadodara-390002, Gujarat, India — [2]Department of Physics, School of Technology, GITAM, Hyderabad Campus, Hyderabad -502329, Telangana, India

Water-gas shift (WGS) reaction over transition metal nanoclusters supported on reducible oxides achieved noticeable attention by the surface scientists due to its great potential to improve catalytic activity compared to conventional catalysts. The two key factors for this reaction is a matter of intense debate, (1) the adsorption strength of carbon monoxide (CO) and (2) the dissociation of water (H2O). Herein, we have adopted dispersion-corrected density functional theory (DFT-D2) calculations to investigate WGS activity for the production of hydrogen (H2) over planar and non-planar Au clusters supported over TiO2(110) rutile surface. In quest of the most preferable site for co-adsorption, we studied adsorption energetics of H2O, CO and carboxyl (COOH) intermediate over various sites of Au over TiO2(110) rutile surface. Strong metal*support interactions stabilize Au-clusters which favor the formation of COOH through the dissociation of O*H bonds. The neighboring edges of non-planar Au-cluster are more suitable for CO and H2O adsorption for the formation of COOH by lowering the energy barrier below 0.5 eV compared to planar Au-clusters.

O 17: Solid-Liquid Interfaces I: Reactions and Electrochemistry

Time: Monday 15:00–17:45 Location: TRE Phy

O 17.1 Mon 15:00 TRE Phy

Hydration layers at the graphite-water interface: Attraction or confinement? — Hagen Söngen[1], Ygor Morais Jaques[2], Lidija Zivanovic[2], Sebastian Seibert[1], •Ralf Bechstein[1], Peter Spijker[2], Hiroshi Onishi[3], Adam S. Foster[2,4], and Angelika Kühnle[1] — [1]Physical Chemistry I, Bielefeld University, Germany — [2]COMP Centre of Excellence, Department of Applied Physics, Aalto University, Helsinki, Finland — [3]Department of Chemistry, Kobe University, Japan — [4]Division of Electrical Engineering and Computer Science, Kanazawa University, Japan

Water molecules at solid surfaces typically arrange in layers. The physical origin of the hydration layers is usually explained by (1) the attraction between the surface and the water and/or (2) the confinement of water due to the presence of the surface. While attraction is specific for the particular solid-solvent combination, confinement is a general effect at surfaces. A differentiation between the two effects is critical for interpreting hydration structures. At the graphite-water interface, the solid-solvent attraction is often considered to be negligible. Nevertheless, we observe hydration layers using three-dimensional atomic force microscopy at the graphite-water interface. We use Monte Carlo simulations to explain why confinement alone could cause the formation of hydration layers. With molecular dynamics simulations, we show that at ambient conditions, there is a significant graphite-water attraction which is pivotal for the formation of layers at the graphite-water interface.

[1] H. Söngen et al., Physical Review B, 100 (2019) 205410

O 17.2 Mon 15:15 TRE Phy

Novel methods to simulate the electrode - electrolyte interface: New approach, old charging methods — •Sudarshan Vijay[1], Georg Kastlunger[1], Hendrik Heenen[1], Joseph Gautheir[2], Henrik Kristoffersen[1], and Karen Chan[1] — [1]CatTheory, Department of Physics, Technical University of Denmark — [2]SUNCAT Center for Interface Science and Catalysis, Department of Chemical Engineering, Stanford University

A major challenge preventing complete mechanistic understanding of reactions at the metal | solution interface is determining ab-initio barriers at constant driving force. Current state of the art methods require calculations to be done at different unit cell sizes and with explicit treatment of the electrolyte. More recently, hybrid continuum charge - explicit solvent models have been developed which account for solvent effects at lower computational expense. Furthermore, it has been suggested that the effective surface charge is the descriptor for activity of reactions occurring at the electrode-electrolyte interface [1]. In this work, we develop methods that can be readily used to simulate electrochemical processes accurately and at minimal computational cost.

This novel procedure is applied to two contemporary electrochemical test cases. First, we compute potential dependent kinetics for the electrochemical Hydrogen Evolution Reaction. Second, we explain the experimentally observed [2] change in peak position for hydroxide adsorption with cation size on Platinum stepped surfaces.

1. Gauthier et al. J. Chem. Theory Comput. 2019 2. Angew.Chem.2017,129,15221-15225

O 17.3 Mon 15:30 TRE Phy

Solvation at metal/liquid interfaces: A benchmark of computational methods — •Hendrik H. Heenen[1], Joseph Gauthier[2], Thomas Ludwig[2], Henrik H. Kristofferson[1], and Karen Chan[1] — [1]Department of Physics, Technical University of Denmark — [2]Department of Chemical Engineering, Stanford University

Recently, the application of continuum solvation methods in DFT simulations has surged in studies of solid/liquid interfaces, specifically when treating electrochemical systems. These continuum solvation models mimic the mean solvent response, effectively relying on parameters derived from solvation energies of molecules in bulk solution. To date, it is unclear how well these methods perform at the solid/liquid interface where directional solvent interactions such as hydrogen bonds may differ from the bulk solution. In this work, we evaluate continuum solvation methods for the metal/liquid interface by benchmarking against *ab-initio* molecular dynamic simulations. This technique presents the most accurate representation for solvation energies at interfaces, which cannot yet be assessed experimentally [1]. Our benchmark includes a variety of adsorbates solvated by water on the Pt(111), Au(111), Cu(111), and Cu(211) surface. We find that continuum solvation methods capture solvation energies for weakly solvated adsorbates adequately, but are unable to account for the impact of hydrogen bonding and competitive water adsorption. We quantify these contributions to the resultant binding energies and propose estimations of appropriate corrections.

[1] O.M. Magnussen, A. Groß, J. Am. Chem. Soc. **141**, 4777 (2019)

Invited Talk O 17.4 Mon 15:45 TRE Phy

Tales of 1000 and 1.2 electrons: Grand Canonical Simulations of Electrified Interfaces using Implicit Solvation Models — •Nicolas G. Hörmann — Chair of Theoretical Chemistry and Catalysis Research Center, Technische Universität München, Germany

In this talk I will present an overview over recent developments in simulation strategies of electrochemical interfaces using hybrid QM/continuum models. In these approaches, grand canonical (GC) interface energies are derived by varying the total number of electrons in the system [1] and by self-consistently including the energy contributions from solvent and electrolyte through an appropriate mean-field (implicit solvation) description. GC calculations allow to determine a wide range of electrochemical observables that are inaccessible by traditional calculations at zero-net-charge – typically referred to as the *Computational Hydrogen Electrode* (CHE) approach. Examples discussed in the talk are non-trivial shifts of electrosorption peaks with pH, non-integer electrosorption valencies or potential-induced surface reconstructions of metallic electrodes. In this context, I will also elaborate on the general limitations of the prevalent CHE method and show how it originates from a low-order Taylor expansion of the GC energetics. Likewise, inherent accuracy limitations of the GC method and of implicit solvation models in general will also be assessed, and possible improvements presented, e.g. using hybrid models with explicitly treated interfacial water [2].

[1] N.G. Hörmann, *et al.*, J. Chem. Phys. 150, 041730 (2019). [2] N.G. Hörmann *et al.*, npj Computational Materials 5, 100 (2019).

O 17.5 Mon 16:15 TRE Phy

Electrochemical Interfaces Getting Real - Theoretical Modeling of Transition States at Applied Electrode Potential — •Simeon D. Beinlich, Nicolas G. Hörmann, and Karsten Reuter — Technische Universität München, Germany

Based on recent improvements in the field of computational modeling of electrochemical interfaces, we present a method that explicitly incorporates the influence of an applied electrode potential on reaction transition states.

Commonly, transition state calculations at electrified solid-liquid-interfaces are performed at zero-net-charge conditions without including electric field and double-layer effects. Under reaction conditions, however, the energetics is influenced by charge-exchange with the electrode which acts as a thermodynamic bath for the electronic degrees of freedom. Using an implicit solvation scheme in combination with a grand canonical description of the system [1], we provide an approach that is able to accurately model processes at electrochemical interfaces with the electrode potential included explicitly in the simulations.

[1] N.G. Hörmann, O. Andreussi, N. Marzari, J. Chem. Phys. 150, 041730 (2019)

O 17.6 Mon 16:30 TRE Phy

Electrochemical N_2 reduction: How nature does it & what we can learn from it — •Vanessa J. Bukas and Jens K. Nørskov — Department of Physics, Technical University of Denmark

Electrochemical conversion of molecular N_2 into ammonia (NH_3) is a key goal in our quest toward global sustainability. Catalyzing this reaction, however, faces the formidable task of breaking the stable $N\equiv N$ bond, while simultaneously suppressing the parasitic hydrogen evolution reaction (HER). As a result, all attempts to realize such a technology have so far been hindered by invariably large (>1 V) overpotentials and low (∼1%) selectivity. Remarkably, the enzyme nitrogenase overcomes these limitations and selectively reduces atmospheric N_2 under ambient conditions to provide NH_3-based fertilizer directly into the soil. Guided by recent experimental evidence of a structurally dynamic cofactor [1], we present here a molecular-level mechanism of the biologic N_2 fixation from first-principles calculations [2]. The proposed mechanism shows that the enzyme is catalytically activated/deactivated through site-specific ligand exchange in order to drive the most difficult steps of the reaction. In the meantime, rate-limiting electron transfer prevents the reaction from evolving via a series of coherently-coupled proton-electron transfers which, in turn, kinetically suppresses the competing HER. Based on this insight, we propose revised strategies for designing the next generation of solid catalysts for electrochemical NH_3 production.

[1] Sippel *et al.*, Science **359**, 1484-1489 (2018)
[2] Bukas and Nørskov, ChemRxiv (2019)

Invited Talk O 17.7 Mon 16:45 TRE Phy

Electrochemical microcalorimetry - measuring the entropy of electrochemical reactions — •Rolf Schuster — Karlsruhe Institute of Technology, Institute of Physical Chemistry, Karlsruhe, Germany

Electrochemical reactions are accompanied by heat transfer between the electrode/electrolyte interface and its surrounding. In electrochemical systems the reversible part of the exchanged heat is directly correlated with the entropy changes in the interface. This gives access to the reaction entropy of the electrochemical processes, including the charge transfer itself as well as non-Faradaic side processes like coadsorption or solvent reordering. The reaction entropy, as a thermodynamic quantity, provides complementary information, e.g., to the charge vs. potential relation, as usually probed by conventional electrochemical methods. We study heat effects during electrochemical surface reactions with minute conversions down to about 1% of a monolayer. This allows for monitoring of the reaction entropy as a function of the electrode potential, for example, during hydrogen adsorption on Pt or underpotential Cu-deposition on Au. After a general introduction, we will present examples for entropy changes upon adsorption processes and double layer charging on Au(111) and discuss the effect of configurational entropy of the adlayer. Time-resolved studies of the heat evolution during Cu-bulk deposition will demonstrate the implications from heat measurements on the reaction steps of this complex reaction.

O 17.8 Mon 17:15 TRE Phy

Microcalorimetric investigation of silver deposition from silver cyanide complexes — •Franziska Karcher, Marco Schönig, and Rolf Schuster — Institute of Physical Chemistry, Karlsruher Institute of Technology, 76131 Karlsruhe, Germany

Electrochemical silver deposition from cyanide containing solutions is of great technical importance. However, the detailed mechanism of this reaction is still controversially discussed in the literature. Here we study the deposition and dissolution process of silver in 0.01 M $KAg(CN)_2$ electrolyte with different concentrations of KCN by electrochemical microcalorimetry. Measuring the reversibly exchanged heat during an electrochemical reaction enables the determination of the reaction entropy, which, in turn, allows conclusions on the reaction mechanism.

The results show that in solutions with additional KCN the silver deposition takes place by direct reduction of the $[Ag(CN)_2]^-$-complex after the dissociation of the predominant $[Ag(CN)_3]^{2-}$-complex. Based on the microcalorimetric measurements the reduction of an adsorbed species seems unlikely. In solutions with low or no additional KCN the formation of a passivating surface layer on the Ag-electrode is detectable. From determination of its formation entropy we conclude that this surface layer consists of solid AgCN.

O 17.9 Mon 17:30 TRE Phy

Entropy change during specific anion adsorption on Au(111) — •Marco Schönig and Rolf Schuster — Karlsruhe Institute of Technology, Germany

The understanding of specific adsorption is of fundamental importance for the description of the electrochemical double-layer(EDL). We used electrochemical microcalorimetry to investigate the specific adsorption of anions (Cl-,Br-, I-) on Au(111) from different electrolytes. Thereby we measure the reversibly exchanged heat during the anion adsorption/desorption process, which is directly correlated with the reaction entropy of the half cell reaction [1]. For all electrolytes we found negative reaction entropy for the adsorption process, with a distinct minimum around half coverage. We provide an interpretation of the data on the basis of a lattice gas model considering adsorbed ions and solvent molecules. [1]K. Bickel, K.D. Etzel, V. Halka and R. Schuster, Electrochim. Acta 2013, 112,801. *

O 18: Plasmonics and Nanooptics II: Ultrafast and Nonlinear Phenomena (joint session O/CPP)

Time: Monday 15:00–18:00 Location: WIL A317

Invited Talk O 18.1 Mon 15:00 WIL A317

Probing Nanophotonic Modes and Optical Phase Shaping of Electron Beams in Ultrafast Transmission Electron Microscopy — •Armin Feist — IV. Physical Institute, University of Goettingen, 37077 Göttingen, Germany

Ultrafast transmission electron microscopy (UTEM) combines the versatile imaging, diffraction and spectroscopy capabilities of state-of-the-art TEM with femtosecond temporal resolution achieved by a laser-pump/electron-probe scheme [1,2]. The novel applications of UTEM include the study of coherent inelastic electron-light scattering (IELS) at laser-excited nanostructures [3,4].

Here, I will briefly introduce the UTEM methodology and show recent results of the Göttingen UTEM instrument, which features high coherence electron pulses generated from nanoscale field emitter tips [2]. Besides nanometer mapping of chiral optical near-fields and local plasmonic modes, IELS enables the transverse and longitudinal phase control of the free-electron wavefunction [4,5], with applications for coherent electron beam splitters and generating attosecond electron pulse trains. Furthermore, the phase-matched interaction of electrons with optical whispering gallery modes (WGMs) enables a strongly enhanced coupling and traces the ring-down of a dielectric microresonator [6].

[1] A. H. Zewail, Science **328**, 187 (2010). [2] A. Feist *et al.*, Ultramicroscopy **176**, 63 (2017). [3] Barwick *et al.*, Nature **462**, 902 (2009). [4] A. Feist *et al.*, Nature **521**, 200 (2015). [5] K. E. Priebe *et al.*, Nat. Photonics **11**, 793 (2017). [6]. O. Kfir *et al.*, arXiv:1910.09540 (2019).

O 18.2 Mon 15:30 WIL A317

Time-resolved and spatially-resolved mode dynamics within a plasmonic nanoslit cavity investigated by coherent two-dimensional nanoscopy — Sebastian Pres[1], Daniel Friedrich[2], Daniel Fersch[1], Enno Krauss[2], Bernhard Huber[1], Victor Lisinetskii[1], •Matthias Hensen[1], Bert Hecht[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Recently, we revealed the impact of off-resonant eigenmodes on the local field dynamics of plasmonic hot-spots within a single nanoslit cavity with a spatial and temporal resolution of 10 nm and 20 fs, respectively, by combining photoemission electron microscopy and interferometric two-pulse sequences [1]. Here, we extend the excitation scheme of the nanoslit cavity to a three-pulse sequence using an LCD-based pulse shaper to perform two-dimensional spectroscopy with unprecedented spatial resolution [2]. Due to the nonlinearity of the photoelectron emission process higher-order signals are easily disclosed. These results are supported by quantum dynamical simulations in which the plasmonic nanoslit is modelled as a quantized harmonic oscillator instead of classical fields. Detecting such signal contributions will be helpful in future experiments to reveal the impact of many-body interactions in molecular or solid-state systems with nanometer resolution.

[1] M. Hensen et al., *Nano Lett.* 19, 4651 (2019)

[2] B. Huber et al., *Rev. Sci. Intrum.* 90, 113103 (2019)

O 18.3 Mon 15:45 WIL A317

Coherent two-dimensional nanoscopy on coupled plasmonic nanostructures — •Lysanne Monika Dietrich[1], Daniel Friedrich[2], Jessica Meier[2], Enno Krauss[2], Daniel Fersch[1], Raphael Wichary[1], Victor Lisinetskii[1], Matthias Hensen[1], Bert Hecht[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]NanoOptics & Biophotonics Group, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Two-dimensional (2D) nanoscopy combines the femtosecond time resolution of coherent 2D spectroscopy with nanoscale selectivity: Instead of measuring optical diffraction-limited light fields, we detect photoemitted electrons with a spatial resolution < 5 nm utilizing aberration-corrected photoemission electron microscopy (AC-PEEM) [1]. Since 2D spectroscopy provides direct insights into couplings between single system constituents, we investigate coupled plasmonic nanostructures (i.e. "dolmen" structures) as a model system [2,3] to demonstrate the additional spatial resolution. We complement our experimental findings by simulated 2D spectra using the local response function as retrieved from finite-difference time-domain (FDTD) method.

[1] B. Huber et al., *Rev. Sci. Instrum.*, **90**, 113103 (2019).

[2] H. Yu et al., *ACS Nano*, **10**, 10373-10391 (2016).

[3] J.-S. Huang et al., *Nano Lett.*, **10**, 2105-2110 (2010).

O 18.4 Mon 16:00 WIL A317

THz streaking spectroscopy for mapping the transformation from far-fields to nanostructure near-fields — •Felix Sommer and Georg Herink — Physikalisches Institut EP VIII, Universität Bayreuth

Field-driven experiments at the nanoscale require the precise characterization of local ultrafast transients. We apply THz near-field streaking spectroscopy [1,2] to metallic nanotips to map the enhanced near-field at the apex.

The local waveforms are critical to various emerging ultrafast instruments for nanoscopic imaging and spectroscopy. The transformation of focused far-fields to nanoscale near-fields sensitively depends on either the individual nano- and macroscopic geometry and structure, involving effects of antenna resonances, plasmon excitations and excitation geometries [3,4]. In order to study the THz-response in the time-domain, we developed an optimized near-field streaking setup based on a strong-field THz source and present experimental data on the THz-waveform transformation.

[1] Wimmer et al., Nat. Phys. 10, 432-436 (2014).

[2] Wimmer et al., APL 111(13), 131102 (2017).

[3] Talebi et al., ACS nano 9(7), 7641-7648 (2015).

[4] Schröder et al., PRB 92(8), 085411 (2015).

O 18.5 Mon 16:15 WIL A317

Tunable strong coupling — •Daniel Friedrich, Benedikt Schurr, Heiko Gross, and Bert Hecht — NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany

Using a scanning plasmonic nano resonator we have shown recently how to achieve tunable strong coupling to colloidal CdSe quantum dots at ambient conditions. The developed system provides an elegant method to tune the coupling strength and can also be used as high resolution optical microscope. [1]

In the presentation we highlight the possibility to establish strong coupling with different kinds of emitters that can be placed on any (transparent) substrate. The emitters include a variety of colloidal semiconductor nanoparticles and platelets as well as TMDCs.

[1] H. Groß et al., Science Adv. 4, 3, eaar4906 (2018)

O 18.6 Mon 16:30 WIL A317

Strong coupling in planar metamaterials — •Manuel Gonçalves[1], Hayk Minassian[2], and Armen Melikyan[3] — [1]Ulm University, Ulm, Germany — [2]A. Alikhanyan National Laboratory (YerPHI), Yerevan, Armenia — [3]Russian-Armenian University, Yerevan, Armenia

Strong coupling is a regime of matter-radiation interaction in a resonant cavity where both the decay rate of the excited state of the matter and the loss rate of the radiation in the cavity are smaller than the coupling strength of matter with radiation. This is a special case of modified spontaneous emission. Fast decay of excited matter state and large cavity loss lead to the more probable Purcell enhancement of spontaneous emission. However, there is strong coupling beyond the quantum optical realm. In classical systems an interaction regime of coupled resonators with similar properties to the quantum case can be produced.

We show how coupled planar optical resonators can be fabricated and present their optical properties. For some configurations the classical analogue of the quantum strong coupling is achieved. Furthermore, higher degrees of interaction between resonators can be achieved and an analogy with the ultrastrong coupling regime of quantum optical systems can be established.

O 18.7 Mon 16:45 WIL A317

Quantum Coherent Interference Paths in Interaction of Single-Electron Wavepackets with Light — •Nahid Talebi[1] and Christoph Lienau[2] — [1]Institute für Experimentelle und Angewandte Physik, Christian Albrechts Universität zu Kiel, D-24118 Kiel, Deutschland — [2]Institut für Physik and Center of Interface Science, Carl von Ossietzky Universität Oldenburg, D-26111 Oldenburg, Germany

Ultrafast coherent processes imposed by laser beams into a traveling electron wavepacket in an electron microscope modulate the phase and amplitude of the electron wavefunction (Near-Field Mediated Electron-Light Interactions, Springer Nature, Switzerland (2019)). As a result, electrons can be either accelerated (Nat. Phys. 14 121-5 (2018)), or diffracted (Proc. Camb. Phil. Soc. 29 297-300 (1923)). Particularly the latter, the so-called Kapitza-Dirac effect (KDE), is within the scope of current work. Here, with the aid of first-principle numerical calculations, we describe the physics of KDE. Moreover, we generalize the KDE into a combination of standing-wave and travelling-wave platforms (New J. Phys. 21 093016 (2019)). We show that by virtue of such generalizations, novel quantum-coherent interference paths are formed. Two competing parts of the interaction Hamiltonian, i.e., photon-absorption and emission processes as well as ponderomotive potential, contributes to these interference effects. These interference paths can be controlled by means of either laser or electron wavepacket parameters. Our investigations open up new directions in the domain of matter-wave interferometry.

O 18.8 Mon 17:00 WIL A317

Strong-Field Angle-Resolved Plasmoemission Spectroscopy — •Pascal Dreher, David Janoschka, Jan-Henrik Herrig, Michael Horn-von Hoegen, and Frank-J. Meyer zu Heringdorf — Faculty of Physics, University of Duisburg-Essen, Germany

Photoemission in strong fields has received a lot of attention in the past and the coherent interaction of electrons with the field after the emission process has been revealed, i.e. using plasmonic near-field enhancement at nanotips. The behavior of electrons within the solid, however, can as well become dominated by the influence of strong fields, and the respective electron dynamics is expected to be fundamentally different from the electronic equilibrium. Clarifying the dominant interaction processes in this case ultimately requires electronic state resolution as well as precise control over the exact field.

We combine nanofocusing of femtosecond surface plasmon polariton (SPP) pulses on flat surfaces with photoemission electron microscopy to achieve angle-resolved plasmoemission spectroscopy (ARPLES) in the strong-field regime. The emission of electrons from the Au(111) Shockely surface state into SPP-dressed electron final states by the absorption of up to seven SPP quanta is observed. The ponderomotive energy that the emitted electrons acquire within the strong plasmonic nanofocus is determined and provides us with a direct measure for the transient SPP field strength in the focus point.

O 18.9 Mon 17:15 WIL A317

Nonlinear plasmon-exciton coupling enhances sum-frequency generation from a Au/ZnO nanohybrid — •Jin-Hui Zhong[1], Jan Vogelsang[2], Jue-Min Yi[1], Dong Wang[3], Lukas Wittenbecher[2], Sara Mikaelsson[2], Anke Korte[1], Abbas Chimeh[1], Cord L. Arnold[2], Peter Schaaf[3], Erich Runge[3], Anne L'Huillier[2], Anders Mikkelsen[2], and Christoph Lienau[1] — [1]Carl von Ossietzky University, 26111 Oldenburg, Germany — [2]Lund University, SE-221 00 Lund, Sweden — [3]Technische Universität Ilmenau, 98693 Ilmenau, Germany

Nanohybrids of plasmon/quantum emitter system can dramatically enhance coherent harmonic generation, often resulting from the coupling of fundamental plasmonic fields to higher-energy, electronic or excitonic transitions of quantum emitters. The ultrafast optical dynamics of such hybrids have been rarely explored. Here, we study those dynamics by interferometrically probing nonlinear optical emission from individual porous gold nanosponges infiltrated with zinc oxide (ZnO) emitters. Few-femtosecond time-resolved photoelectron emission microscopy reveals multiple long-lived localized plasmonic hot spot modes at the surface of single nanosponges, resonant in a broad spectral range. The hot spot near-field couples to the ZnO excitons, enhancing sum-frequency generation, and boosting resonant excitonic emission. The quantum pathways of the coupling are further uncovered from a two-dimensional spectrum correlating fundamental plasmonic excitations to nonlinearly driven excitonic emissions.

O 18.10 Mon 17:30 WIL A317

fluctuation-modulated third harmonic deep ultraviolet emission from randomly disordered Si nanograss — •Juemin Yi[1], Dong wang[2], Jinhui Zhong[1], Peter Schaaf[1], Erich Runge[3], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität, Institut für Physik and Center of Interface Science, 26129 Oldenburg — [2]TU Ilmenau, Institut für Werkstofftechnik und IMN MacroNano, 98693 Ilmenau — [3]TU Ilmenau, Institut für Physik und IMN MacroNano, 98693 Ilmenau

It is well known that Si nanograss or black Si greatly enhances light absorption in a broad spectral range and thus is of relevance for solar cell application. Very little is known about their nonlinear optical properties. For that, we have utilized a broadband and few-cycle ultrafast laser to generate coherent third harmonic (TH) emission from randomly disordered Si nanograss. The TH signal is two-order-of-magnitude stronger than that from bulk Si surfaces. For individual hot spots, the TH enhancement even reaches a factor of the order of 1000. A statistical analysis of the TH intensity fluctuations demonstrates that multiple light scattering within the randomly disorder medium is the cause of those fluctuations. A phase-locked and collinear pulse pair excitation proves the coherent nature of the deep ultraviolet emission. The interferometric frequency-resolved autocorrelation (IFRAC) microscopy shows that the deep ultraviolet pulse is around 10fs. Our findings identify random Si nanograss as the most promising candidates for generating ultrashort deep ultraviolet pulses.

O 18.11 Mon 17:45 WIL A317

Electron-Driven Photon-Sources for Spectral Interferometry using Electron Microscopes — Nika van Nielen[3], Mario Hentschel[2], Harald Giessen[2], Albert Polman[3], and •Nahid Talebi[1] — [1]Institute für Experimentelle und Angewandte Physik, Christian Albrechts Universität zu Kiel, D-24118 Kiel, Deutschland — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [3]Center for Nanophotonics, AMOLF, Science Park 104, 1098 XG Amsterdam, The Netherlands

Electron beams can inelastically interact with matters, and as a result, photons are emitted to the far-field. Mechanisms of electron-induced radiations are numerous, covering Cherenkov radiation, transition radiation, and plasmon-induced radiation, to name a few (Rev. Mod. Phys. 82, 209 (2010)). Here, we report on metamaterial- and photon-sieve-based structures for tailoring the electron-induced emission (Nature communications 10 (1), 599 (2019)). By engineering the dispersion of the interface optical modes, radiation relaxation channels for the plasmon polaritons supported by our engineered thin film are formed, leading to an enhanced electron-induced radiation. We also particularly emphasize on the generation of chiral light using plasmonic chains of nanohole arrays. Moreover, we outline our efforts towards realization of combined electron-photon spectroscopy techniques for investigating nanooptical systems in electron microscopes, using electron-driven photon sources (Scientific Reports 6, 33874 (2016)).

O 19: 2D Materials II: Electronic Structure, Excitations, etc. (joint session O/CPP/HL)

Time: Monday 15:00–18:15 Location: WIL C107

O 19.1 Mon 15:00 WIL C107

Unfolding and analysis of a defect band structure using doped MoSe$_2$ and MoS$_2$ — •Stefan Rost, Christoph Friedrich, Irene Aguilera, Beata Kardynal, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We investigate substitutional doping of chromium and phosphorus in MoSe$_2$ and MoS$_2$ monolayers, as they are promising candidates for single photon emission. The systems are characterized by density-functional-theory (DFT) studies of structural relaxation, projected density-of-states, and band structure, all calculated with the Jülich FLAPW code family (www.flapw.de). Different sizes of super-cells are necessary to calculate the doped system depending on the strength of interaction between the dopants. The super-cells contain between 3×3 and 5×5 monolayer unit cells. Compared to the pristine material, the band structure of the defect system is backfolded in **K**-space, which complicates a straightforward interpretation, in particular for low doping concentrations. We have implemented a method for unfolding the bands obtained from the super-cell calculation. The resulting band structure resembles the one of the pristine material, but it contains additional information about the defect system, which, in this sense, can be regarded as a perturbed host system. – The authors gratefully acknowledge the computing time granted through JARA-HPC on the supercomputer JURECA at Forschungszentrum Jülich, (project cjpgi10) as well as the support through „Integration of Molecular Components in Functional Macroscopic System“ initiative of VW Stiftung.

O 19.2 Mon 15:15 WIL C107

Geometry, electronic structure, and bonding of single-domain h-BN on Pt(110) — •Marco Thaler[1], Dominik Steiner[1], Alexander Menzel[1], Florian Mittendorfer[2], and Erminald Bertel[1] — [1]Physikalische Chemie, Universität Innsbruck, Österreich — [2]Institut für Angewandte Physik, TU Wien, Österreich

Recently we reported single-domain growth of hexagonal Boron Nitride (h-BN) on Pt(110)[1]. This is a peculiar system, where the substrate adapts to the h-BN adlayer by forming a (1xn) missing-row reconstruction (n = 5 or 6). The bandstructure was investigated by angle-resolved UV photoemission (ARPES) and is very similar to that of a free-standing h-BN monolayer except for the appearance of umklapp bands reflecting the periodicity of the Moiré pattern and testifying for the perfect film quality. Binding energies agree with other h-BN/transition metal systems if referenced to the vacuum level. Additionally, we studied the local density of states (LDOS) for differently positioned atoms in the h-BN film by DFT calculations. For N atoms on top of Pt atoms a small LDOS maximum appears at the Fermi level, indicating a weak covalent contribution to the h-BN-Pt bonding. This, the mean h-BN-Pt(110) distance, and the workfunction change place the present system at the borderline between purely dispersive and chemisorptive bonding[2]

[1] Steiner, D., Mittendorfer, F., Bertel, E. ACS Nano 13, 7083-7090(2019)

[2] Bokdam, M., Brocks, G., Kelly, P. J. Phys. Rev. B 90, 085415(2014)

O 19.3 Mon 15:30 WIL C107

Photoinduced band renormalization in the nodal-line semimetal ZrSiSe — •Gianmarco Gatti[1], Alberto Crepaldi[1], Nicolas Tancogne-Dejean[2], Michele Puppin[3], Angel Rubio[2], Majed Chergui[3], and Marco Grioni[1] — [1]Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — [2]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Laboratory of Ultrafast Spectroscopy, ISIC, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

ZrSiSe is a layered material that is classified as a nodal-line semimetal. Its low-energy bandstructure is composed by linearly dispersing surface and bulk bands whose crossing points creates a one-dimensional contour in the momentum space with vanishing density of states close to the Fermi level. We investigate its equilibrium and out-of-equilibrium electronic structure by the means of angle- and time-resolved photoemission spectroscopy and compare the results with ab initio calculations. Our analysis indicates that the dispersion of the Dirac quasiparticle can be correctly reproduced by density functional theory with the inclusion local and non-local electronic correlations. Moreover, we observe a transient renormalization of the bands velocity above the Fermi level under the photoexcitation produced by ultrashort infrared pulses. We associate the microscopic origin of this effect to the increased screening of the non-local Coulomb interaction due to the presence of high-energy and non-thermalized carriers.

O 19.4 Mon 15:45 WIL C107

Micro-focus ARPES on a twisted graphene/hBN field-effect device — •Alfred Jones[1], Ryan Muzzio[2], Davide Curcio[1], Deepnarayan Biswas[1], Jill A. Miwa[1], Philip Hofmann[1], Simranjeet Singh[2], Chris Jozwiak[3], Eli Rotenberg[3], Aaron Bostwick[3], Roland J. Koch[3], Søren Ulstrup[1], and Jyoti Katoch[2] — [1]Aarhus University, Aarhus, Denmark — [2]Carnegie Mellon University, Pittsburgh, Pennsylvania, USA — [3]Advanced Light Source, E. O. Lawrence Berkeley National Laboratory, Berkeley, California, USA

Graphene/ hBN heterostructures are an ideal testing ground for functional 2D devices owing to the atomically smooth surface and weak screening offered by hBN. On top of the record mobilities this structure offers, controlling the twist angle between layers creates a superlattice effect from which exotic electronic properties can occur.

Here, I present a study of the ARPES spectrum of graphene integrated in a device architecture with a hBN dielectric and graphite gate electrode. Micron-scale ARPES based on an X-ray capillary was used to collect the Dirac spectrum at different gate-voltages. A clear, reversible doping effect up to $5*10^{12}$ cm^{-2} is observed, providing access to the doping dependent quasiparticle dynamics in graphene on hBN.

Simultaneous measurements of this gate-dependent Dirac cone dispersion and the electrical resistance of the device enables extraction of electronic mobility and lifetimes. Our approach thereby demonstrates the tantalizing prospect of combining electron transport measurements with a spectroscopic probe of the electronic structure.

O 19.5 Mon 16:00 WIL C107

Final-State Effects in Photoemission from Black Phosphorus — •Charlotte E. Sanders[1], Irene Aguilera[2], Klara Volkaert[3], Deepnarayan Biswas[3], Marco Bianchi[3], and Philip Hofmann[3] — [1]Central Laser Facility, STFC Rutherford Appleton Laboratory, Harwell OX11 0QX, UK — [2]Institute of Energy Research - Photovoltaic, Forschungszentrum Jülich, D-52425 Jülich, Germany — [3]Department of Physics and Astronomy, Aarhus University, 8000-C Aarhus, Denmark

Intrinsically doped bulk black phosphorus, although a van der Waals layered crystal, has nontrivial interlayer interactions and out-of-plane dispersing (k_z) electronic states, with a direct bandgap at the Z point of the three-dimensional (3D) Brillouin zone. The material's 3D character is related to key properties such as the thickness dependence of the bandgap in thin films and the tunability of the bandgap by strain and electric field. Interestingly, studies from angle-resolved photoemission spectroscopy (ARPES) of the k_z dispersion reveal intensity modulations near the Fermi level that are difficult to interpret in terms of the valence band dispersion predicted by theory. They have been attributed to surface-resonant states [1,2]. However, on the basis of density functional theory calculations and ARPES data acquired across a broad photon energy range, we suggest here an alternative interpretation based on final-state effects. The results call attention to the meaning of the free-electron-like final-state assumption and to the limits of its applicability. [1] *PRB* **90** (2014) 085101. [2] *PRB* **93** (2016) 075207.

Invited Talk O 19.6 Mon 16:15 WIL C107

Atomic scale neural circuitry capable of self-adaptation — •Brian Kiraly — Radboud University, Nijmegen, The Netherlands

Driven by the rise of artificial intelligence and its potential for reduced energy consumption, there have been expanded efforts directed toward investigating materials which can perform pattern recognition directly in hardware. This requires a step away from physical systems which show simple bistability, toward complex, stochastic systems, which are inherently tunable. At the moment, however, the state of the art in neuromorphic computing still struggles with fundamental issues, such as scaling or adaptability, often referred to as on-chip learning. In this talk, I will show a ground-breaking example, in which as few as 7 cobalt dopants on the surface of anisotropic semiconducting black phosphorus [1,2] can be utilized for pattern recognition. For this demonstration, we illustrate that controlled coupling between Co atoms [3] leads to a stochastic system which is well described using the concept of a Boltzmann machine. Both probing and reading the system with a scanning tunneling microscope, I will demonstrate how we realize an atomic scale synaptic memory and how the stochastic dynamics adapt and learn, depending on the input stimulus. The main aspects of this work have been carried out in the Scanning Probe Microscopy department at Radboud University. [1] Kiraly, Knol, Volckaert, Biswas, Rudenko, et. al., Phys. Rev. Lett. 123, 216403 (2019). [2] Kiraly, Hauptmann, Rudenko, Katsnelson, Khajetoorians, Nano Lett. 17, 3607 (2017). [3] Kiraly, Rudenko, Weerdenburg, Wegner, Katsnelson, Khajetoorians, Nature Commun. 9, 3904, (2018).

O 19.7 Mon 16:45 WIL C107

Diffusion of magnetic dopants in pristine and defected phosphorene — •Rohit Babar[1] and Mukul Kabir[1,2] — [1]Department of Physics, Indian Institute of Science Education and Research, Pune, India — [2]Centre for Energy Science, Indian Institute of Science Education and Research, Pune, India

The incorporation of transition metal atoms is a robust way to imprint magnetism in non-magnetic 2D materials. In this regard, phosphorene has emerged as a versatile host for spintronic applications. Combining first-principles calculations with kinetic Monte Carlo simulations, we study the binding, magnetism, and diffusion of TM (TM = Cr, Fe, Co) atoms in pristine and defected phosphorene. The TM migration is highly anisotropic and favorable along the zigzag axis due to the puckered structure of phosphorene. While TM adsorption on pristine surface induces a local moment, the TM diffusion is uncontrolled at room temperature. We further show that vacancy defects exert an attractive potential beyond 1 nm and act as trapping centers for magnetic dopants. Our findings will assist in overcoming the practical limitations of surface decoration in phosphorene.

O 19.8 Mon 17:00 WIL C107

Ab-initio structural dynamics of laser-excited graphene — •Sergej Krylow[1], Felipe Valencia Hernandez[2], Bernd Bauerhenne[1], and Martin E. Garcia[1] — [1]University of Kassel, 34132 Kassel, Germany — [2]National University of Colombia, 111321 Bogota, Colombia

We calculate the response of graphene to an ultrafast laser pulse using ab initio density functional molecular dynamics simulations. Our results show a biexponential decay of the Bragg peak intenities of the (100) and (110) peaks. We are able to show that the fast decay is caused by the equilibration between the electrons and a few strongly coupled optical phonons (SCOPs). The slower decay can be attributed to the equilibration of the SCOPs to the other phonon modes. Furthermore, we analyze the decay pathways from the SCOPs to the other phonon modes.

O 19.9 Mon 17:15 WIL C107

Tailoring the opto-electronic response of graphene nanoflakes by size and shape optimization — •Raquel Esteban-Puyuelo[1], Rajat Sonkar[2], Bhalchandra Pujari[2], Oscar Grånäs[1], and Biplab Sanyal[1] — [1]Division of Materials Theory, Department of Physics and Astronomy, Uppsala University, Box-516, SE 75120, Sweden — [2]Centre for Modeling and Simulation, Savitribai Phule Pune University, Ganeshkhind, Pune 411007, India

The long spin-diffusion length, spin-lifetime and excellent optical absorption coefficient of graphene provide a promising platform for building opto-electronic devices as well as spin-based logic in the nanometer regime. We have used time-dependent density functional theory to study how the magnetic structure and optical properties of graphene nanoflakes depend on their size and shape. We optimize the magnetic ground state and the exchange coupling between the edges of the flakes to tailor the external fields needed to switch the magnetic ordering. Finally it's shown that the magnetic state alters the optical response of the flake leading to the possibility of opto-spintronic applications.

O 19.10 Mon 17:30 WIL C107

Electronic and optical properties of two-dimensional magnets (CrI$_3$) and their effects on adjacent material (WSe$_2$/CrI$_3$) — •Marie-Christin Heissenbüttel, Michael Rohlfing, and Peter Krüger — Institut für Festkörpertheorie WWU, Münster, Deutschland

For the development of novel opto-electronic devices the access and manipulation of the spin degree of freedom is of fundamental importance. The recently discovered 2D magnets provide a great opportunity to study the delicate interplay of spin, orbital, charge and lattice degree of freedom and the manipulation of other non-magnetic 2D materials, as for example TMDCs, by proximity effects. In this talk I will demonstrate our results from ab-initio calculations for the magnetic monolayer of chromium triiodide (CrI$_3$). The electronic and optical properties are analyzed as well as the effects of magnetism on the optics of WSe$_2$ within the heterobilayer tungsten diselenide (WSe$_2$) on CrI$_3$ are shown. The investigation of CrI$_3$ by many body perturbation theory (MBPT) within the LDA+GdW approximation reveals a ferromagnetic and insulating behavior and the optical absorption obtained from the solution of the BSE shows large exciton binding energies up to 1.04 eV. Furthermore due to the impact of ferromagnetic proximity effects on the TMDC WSe$_2$ in the heterosystem WSe$_2$ / CrI$_3$ a lifting of the energy degeneracy in the K-valleys of WSe$_2$ is found. Both the electronic band gap at ±K as well as the corresponding excitons in WSe$_2$ are affected.

O 19.11 Mon 17:45 WIL C107

Engineering intrinsic π-magnetism in nanographenes — •Shantanu Mishra[1], Doreen Beyer[2], Kristjan Eimre[1], Shawulienu Kezilebieke[3], Reinhard Berger[2], Oliver Gröning[1], Peter Liljeroth[3], Carlo Pignedoli[1], Xinliang Feng[2], Pascal Ruffieux[1], and Roman Fasel[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — [2]Technical University of Dresden, Dresden, Germany — [3]Aalto University, Espoo, Finland

Among the multitude of properties realized in organic compounds due to the chemical versatility of carbon, magnetism remains one of the most challenging. The electronic structure of polycyclic aromatic hydrocarbons (nanographenes) depends critically on the topology of the underlying π-electron network, which provides a tunable platform to realize all-carbon magnetism at the nanoscale.

Combining rational design principles with on-surface synthesis, we engineer and probe emergent magnetism in elusive magnetic nanographenes, namely, Clar's goblet [1] and extended triangulenes [2], and their covalently-bonded assemblies. Our experimental approach follows low-temperature scanning tunneling microscopy and inelastic electron tunneling spectroscopy, with further insights provided by mean-field and many-body perturbation theory calculations.

[1] S. Mishra et al., Nature Nanotech. (in press)
[2] S. Mishra et al., J. Am. Chem. Soc. 141, 10621 (2019)

O 19.12 Mon 18:00 WIL C107

Theoretical study on the magnetic structure of few-layer TMPS3 — •Tae Yun Kim[1,2,3] and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Gwanak-Gu Hoam-Ro 519 101-1205 — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

Transition metal phosphorus sulfides (TMPS3) are a family of the layered magnetic materials. Due to the layered structure and the rich spectrum of the magnetic structure [1], TMPS3 has been thought to be a good playground for testing two-dimensional magnetism in real world experiments [2]. It was found that the antiferromagnetic order in FePS3 remains down to the monolayer limit [3, 4], which was soon followed by the discovery of two-dimensional ferromagnetism in CrI3 [5] and Cr2Ge2Te6 [6]. More recently, the existence of the magnetic ordering in few-layer TMPS3 has been investigated in experiments [7, 8]. In this contribution, we present an in-depth investigation of the magnetic structure of few-layer TMPS3 based on the results of our first-principles calculations.

[1] R. Brec, Solid State Ionics 22, 3 (1986).
[2] K. S. Burch et al., Nature 563, 47-52 (2018).
[3] X. Wang et al., 2D Materials 3, 031009 (2016).
[4] J.-U. Lee et al., Nano Letters 16, 7433 (2016).
[5] B. Huang et al., Nature 546, 270-273 (2017).
[6] C. Gong et al., Nature 546, 265-269 (2017).
[7] K. Kim et al., Nature Communications 10, 345 (2019).
[8] K. Kim et al., 2D Materials 6, 041001 (2019).

O 20: Oxides II: Structures, Interactions and Reducibility

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

O 20.1 Mon 15:30 WIL B321

From UHV to ambient conditions: Water on In_2O_3(111) — Hao Chen[1,2], Matthias A. Blatnik[1], Francesca Mirabella[1], Giada Franceschi[1], Michele Riva[1], Michael Schmid[1], Jan Čechal[3], Bernd Meyer[4], Ulrike Diebold[1], and •Margareta Wagner[1,3] — [1]Inst. of Applied Physics, TU Wien, Wien, Austria — [2]State Key Laboratory of Catalysis, CAS, iChEM, Dalian Inst. of Chem. Phys., Chin. Acad. of Science, Dalian, China — [3]CEITEC, Brno University of Technology, Brno, Czech Republic — [4]ICMM/CCC FAU Erlangen-Nürnberg, Erlangen, Germany

We study the interaction of water with the In_2O_3(111) surface, employing surface science techniques (TPD, XPS, non-contact AFM and STM as well as DFT calculations). The adsorption is investigated as a function of coverage, i.e., from single water molecules to multilayers, in UHV, at pressures present in the ambient and as a liquid. The saturation coverage at 300 K in UHV is three dissociated molecules per unit cell, visible as propeller-shaped bright protrusions in STM. Their internal structure is revealed by nc-AFM, showing in total six objects: 3 OH groups sharing a surface oxygen and 3 residual hydroxyl groups; TPD shows 3 desorption peaks above 300 K resulting from different desorption barriers for the recombining water molecules. After the interaction with liquid water also molecular water species are found on In_2O_3 (111).

O 20.2 Mon 15:45 WIL B321

Direct Assessment of the Proton Affinity of Individual Surface Hydroxyls with AFM and DFT — •Bernd Meyer[1], Margareta Wagner[2], Martin Setvin[2], Michael Schmid[2], and Ulrike Diebold[2] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg, Germany — [2]Institute of Applied Physics, TU Wien, Austria

The state of protonation/deprotonation of individual surface sites has far-ranging implications in all areas of chemistry. However, common experimental measurements of surface acidity are integral techniques which give only average quantities integrated over the whole surface. Here we show that an OH-functionalized tip of an atomic force microscope (AFM) can be used for quantitative insights into the acidity of individual surface OH groups. The chosen model oxide, In_2O_3(111), offers four types of surface O atoms with distinct properties, each giving rise to a characteristic force–distance curve after protonation. Density-functional theory (DFT) calculations demonstrate a linear correlation between the force minimum and the proton affinity of the surface hydroxyls. By benchmarking the calculations to known proton affinities and $\mathrm{p}K_\mathrm{a}$ values of gas-phase molecules, the force minima provide a direct measure of proton affinity distributions and $\mathrm{p}K_\mathrm{a}$ differences at the atomic scale.

Invited Talk O 20.3 Mon 16:00 WIL B321

Polarons in oxide surfaces — •Cesare Franchini — University of Vienna & University of Bologna

In this talk I shall discuss recent advances in the modelling and simulation of polaron effects in transition metal oxide surfaces by first principles and machine learning approaches: polaron formation and mobility, polaron-induced surface reconstruction, polaron-adsorbates interaction and competition between localized and delocalized carriers in quantum paraelectrics.

arXiv:1902.04183 DOI: 10.1007/978-3-319-50257-1_52-1

O 20.4 Mon 16:30 WIL B321

$ZrO_{2-\delta}$ thin films: Oxygen-deficient, but not reduced — Peter Lackner, Sabrina Mayr, Josef Redinger, Ulrike Diebold, and •Michael Schmid — Institute of Applied Physics, TU Wien, Vienna, Austria

Zirconia (ZrO_2) has a wide range of applications, as an engineering material, in solid-state electrochemistry (gas sensors, solid oxide fuel cells), and as a catalyst support. We have studied thin films ($\approx 5\,\mathrm{ML}$) sputter-deposited in ultrahigh vacuum on metal substrates [1]. As-deposited films are slightly oxygen-deficient, which leads to a pronounced core level shift in x-ray photoelectron spectroscopy (XPS). This is caused by positively charged oxygen vacancies ($V_O^{\bullet\bullet}$) shifting the electrostatic potential [2]. The XPS results indicate a preference for vacancy formation near the interface, in agreement with density functional theory (DFT) calculations. Full oxidation of the films is possible via oxygen spillover from a metal [2]. The positive $V_O^{\bullet\bullet}$s present in the vicinity of the metal support have much lower formation energies than neutral V_Os. Thus, oxygen-deficient films can form on a metal under conditions where bulk ZrO_2 would remain stoichiometric. Due to charge transfer from the $V_O^{\bullet\bullet}$s to the substrate, Zr can retain its preferred 4+ charge state. In other words, the Zr in metal-supported, oxygen-deficient $ZrO_{2-\delta}$ films is not reduced.

[1] P. Lackner et al., Surf. Sci. 679, 180 (2019).

[2] P. Lackner et al., Phys. Chem. Chem. Phys. 21, 17613 (2019).

O 20.5 Mon 16:45 WIL B321

High temperature reduction and reoxidation of cerium oxide on Cu(111) — •Linus Pleines[1], Lars Buss[1,4], Tevfik Onur Menteş[2], Francesca Genuzio[2], Andrea Locatelli[2], Jan Ingo Flege[4], and Jens Falta[1,3] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]ELLETRA Synchrotron Light Source, Basovizza, Italy — [3]MAPEX Center for Materials and Processes, Bremen, Germany — [4]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany

Cerium oxide is of great interest due to its technological importance in various electronic, optical and catalytic applications. The inverse model catalyst cerium oxide on Cu(111) shows a high activity for the production of methanol. For the production of methanol from CO_2 and H_2 oxygen vacancies, e.g. in form of reduced ceria, are necessary. The reduction of ceria may be achieved by exposure to H_2 at elevated temperatures. We studied the interaction of H_2 and CO_2 with cerium oxide islands on a Cu(111) substrate with low-energy electron mircoscopy (LEEM) and x-ray absorption spectroscopy (XAS). From earlier studies the orientation of the CeO_x is known to be decisive for the catalytic activity. In our experiments both orientations are directly compared via growth of (100) and (111) CeO_x islands side by side on the same metal substrate, so that the same conditions prevail during the experiment. At high temperatures, exposure to H_2 leads to partial reduction and exposure to CO_2 leads to complete reoxidation of the cerium oxide. The (100) and (111) orientations show different reduction and reoxidation behaviours.

O 20.6 Mon 17:00 WIL B321

Atomic structure of cubic ceria surfaces: an IR spectroscopic study — Chengwu Yang, •Junjun Wang, Xiaojuan Yu, Alexei Nefedov, Stefan Heissler, Christof Wöll, and Yuemin Wang — Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344, Eggenstein-Leopoldshafen, Germany

Polar surfaces of solid ionic compounds exhibit unique physical and chemical properties but they are intrinsically instable due to a diverging electrostatic energy. A fundamental understanding of the compensation mechanisms is a key but challenging issue. Here, we present an atomic-level picture of the stabilization mechanisms governing the surface polarity compensation of cube-shaped ceria nanoparticles based on a thorough surface science study on polar CeO2(100) single-crystal surfaces using primarily temperature and polarization-resolved infrared reflection absorption spectroscopy (IRRAS). The results obtained by IRRAS in conjunction with high-resolution transmission electron microscopy and density functional theory calculations reveal a multistep scenario for polarity compensation at the polar (100) surface of ceria.

O 20.7 Mon 17:15 WIL B321

Copper Oxidation on Pt(111) - More than a Surface Oxide? — •Alexander Gloystein and Niklas Nilius — Institute of Physics, Carl von Ossietzky University Oldenburg, Germany

LEED, STM and XPS have been used to monitor the growth of copper oxide thin films on a Pt(111) support. At 500 K preparation temperature, a monolayer oxide forms while most of the precipitated copper accumulates as Cu(111) at the Pt interface. Respective films are composed of distorted Cu-O six-rings and resemble the well-known '29' and '44' surface oxides formed via low-pressure oxidation of Cu(111). With increasing temperature, unreacted Cu mixes with the Pt toplayers, resulting in a well-ordered Cu3Pt surface alloy. In response to this substrate modification, the oxide film undergoes an order-disorder transition, in which an increasing number of 5-7 defects are inserted into the Cu-O honeycomb lattice, before it decays into isolated oxide islands. Above 750 K annealing, uniform Cu3O shamrock units that self-assemble into highly crystalline 2sqrt3 domains become the dominant structural element of the film.

O 20.8 Mon 17:30 WIL B321

Ab-initio studies of the (110) surface terminations of rutile VO_2 — •Jakub Planer, Florian Mittendorfer, and Josef Redinger — Vienna University of Technology, 1040 Vienna, Austria

Vanadium dioxide is a promising candidate for fast electronic or optical switching. These applications are based on an insulator-to-metal transition which occurs at 340 K and is accompanied by the structural change from a monoclinic to a rutile phase.

Despite the potential usability of the VO_2, many open questions remain with respect to its surface structure. We will therefore discuss properties of the rutile VO_2 (110) surface under varying oxygen partial pressure, and compare our results to recent experimental findings. Although standard GGA functionals (PBE) offer an appropriate description of the structural properties of the rutile and monoclinic phase, the surface properties such as surface energy or stability of surface reconstructions are not captured well. Advanced functionals such as meta-GGA approaches (SCAN) implemented in the Vienna Ab initio Simulations Package (VASP) thus have been employed to overcome these shortcomings.

It is experimentally found that the VO_2 surfaces contain more oxygen than the bulk. This is in agreement with the previous study focused on the oxygen adsorption on the (110) surface. However, our work shows different oxygen-rich tetrahedral surface terminations that are related to the vanadium pentoxide (001) monolayer, in agreement with the STM results.

O 20.9 Mon 17:45 WIL B321

First-Principles Study of Lithium Oxide Surfaces and Crystallites for Lithium-Oxygen Batteries — •Behnaz Rahmani Didar and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

Li-O_2 batteries are a promising alternative to Li-ion batteries as they theoretically provide the highest possible specific energy density. In this type of battery, O_2 anions produced in the cathode react with Li cations produced from the oxidation of the Li anode, thus forming LiO_2, and more prominently, Li_2O_2, as discharge products. Li_2O_2 is an electronic insulator and its precipitation on the cathode is thought to be the main limiting factor in achieving high capacities. SEM and TEM observations reveal crystallite morphologies of Li_2O_2 compounds, rather than uniform layers covering the electrode surface. The shapes and crystallite morphologies of LiO_2 and Li_2O_2 particles, may all affect the capacity, rechargeability and generally the electrochemistry of the cell. The precise morphologies and their effects, however, remain largely undetermined. We use DFT calculations and *ab initio* thermodynamics to study the stability of these oxide surfaces, and their crystallite morphologies. Surface-state analyses are also employed to gain insight into the electronic structure of these oxides.

O 20.10 Mon 18:00 WIL B321

Structure and properties of Cs ions grown on ZnO/Ag(111) — •Ting-Chieh Hung and Karina Morgenstern — Chair of Physical Chemistry I, Ruhr-University of Bochum, Bochum, Germany

Zinc oxide (ZnO) is a broad direct bandgap semiconductor, which is widely used as a catalyst. Therefore, the properties of ZnO and interaction between ZnO and molecules have been investigated extensively. However, the microscopic views and properties of the adsorbed molecules and ions interacting on ZnO ultrathin layers supported by metal substrates have remain unexplored. To understand the interaction between water molecules and ions on ZnO ultrathin layer, we first investigated the structures and properties of the caesium (Cs) ions grown on ZnO(0001)/Ag(111) model system. From scanning tunneling microscopy (STM) images we found that the Cs ions are grown only on the ZnO layer by following its moiré pattern [1]. Further STM results will be presented in this talk.

[1] Q. Pan et al, Catalysis Letters, 2014, 144(4), 648-655.

O 20.11 Mon 18:15 WIL B321

Hydrogen Atom Scattering at Aluminium Oxide — •Martin Liebetrau and Jörg Behler — Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstraße 6, 37077 Göttingen, Germany

The adsorption of atomic hydrogen is important in many fields, from heterogeneous catalysis via hydrogen storage to nuclear fusion. Here, we report molecular dynamics simulations of high-energy hydrogen atom scattering at the α-Al_2O_3(0001) surface. Employing a high-dimensional neural network potential, which allows us to include the full-dimensional thermal motion of the surface atoms, we are able to calculate a large number of trajectories with the accuracy of density-functional theory at a small fraction of the computational costs. Probing different kinetic energies, surface temperatures and incident angles, we are able to characterize the scattering process in detail.

O 21: Interfaces and Thin Films I (joint session CPP/O/DY)

Time: Monday 16:30–17:15 Location: ZEU 260

O 21.1 Mon 16:30 ZEU 260

In Situ Monitoring Mesoscopic Deformation of Nanostructured Porous Titania Films Caused by Water Ingression — Lin Song[1,2], Monika Rawolle[1], Nuri Hohn[1], Jochen S. Gutmann[3], Henrich Frielinghaus[4], and •Peter Müller-Buschbaum[1,5] — [1]Lehrstuhl für funktionelle Materialien, Physik Department, TU München, 85748 Garching, Germany — [2]Xian Institute of Flexible Electronics, Northwestern Polytechnical University, Xian 710072, Shaanxi, China — [3]Fakultät für Chemie, Universität Duisburg-Essen, 45141, Essen, Germany — [4]JCNS at MLZ, Forschungszentrum Jülich GmbH, 85748 Garching, Germany — [5]MLZ, TU München, 85748 Garching, Germany

Nanostructured porous titania films are used in many energy related applications. We investigate the temporal evolution of the mesoscopic deformation of mesoporous titania films synthesized via block copolymer assisted sol-gel chemistry with in situ grazing incidence small-angle neutron scattering (GISANS) during exposure to water vapor. Two types of mesoporous titania films are compared, which have a different degree of structural stability, depending on the applied annealing temperature in nitrogen atmosphere. Water ingression causes a gradual structure deformation in terms of decreasing center-to-center distances and broadening of the size distribution of the titania nanostructures. Based on the evolution of the mesopore size obtained from in situ GISANS measurements, the results show which type of titania structure is more stable against water infiltration.

O 21.2 Mon 16:45 ZEU 260

In situ GISAXS Investigations of Multi-responsive Block Copolymer Thin Films during Solvent Vapor Annealing — •Florian A. Jung[1], Panayiota A. Panteli[2], Detlef-M. Smilgies[3], Dorthe Posselt[4], Constantinos Tsitsilianis[5], Costas S. Patrickios[2], and Christine M. Papadakis[1] — [1]Physics Department, Soft Matter Group, Technical University of Munich, Garching, Germany — [2]Department of Chemistry, University of Cyprus, Nicosia, Cyprus — [3]Wilson Laboratory, Cornell University, Ithaca, USA — [4]Department of Science and Environment, Roskilde University, Denmark — [5]Department of Chemical Engineering, University of Patras, Greece

Responsive block copolymer thin films are of interest for many applications, e.g. as fast sensors or switchable membranes. In the present work, we investigate a pH and temperature responsive pentablock quaterpolymer in thin films during solvent vapor annealing (SVA). The end blocks are temperature-responsive and hydrophobic while the midblock is pH-responsive and hydrophilic. Structural information was obtained by employing in situ grazing-incidence small-angle X-ray scattering (GISAXS) and by model fitting the obtained 2D patterns. We find that, varying the pH value of the solution for spin-coating as well as the nature of the solvent used for SVA gives the opportunity to tune the structures in a wide range.

O 21.3 Mon 17:00 ZEU 260

Self-assembly of large magnetic nanoparticles in ultrahigh molecular weight linear diblock copolymer films — •Wei Cao[1], Senlin Xia[1], Xinyu Jiang[1], Markus Gallei[2], Matthias

Opel[3], Matthias Schwartzkopf[4], Stephan V. Roth[4,5], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Saarland University, Chair in Polymer Chemistry, 66123 Saarbrücken — [3]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [4]DESY, Notkestrasse 85, 22603 Hamburg — [5]KTH Royal Institute of Technology, FPT, SE-100 44 Stockholm, Sweden

The fabrication of diblock copolymer nanocomposite films that consist of magnetic nanoparticles (NPs) with diameters (D) of more than 20 nm is a challenging task. Herein, ultrahigh molecular weight (UHMW) linear polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) diblock copolymer is spin-coated as a template for the self-assembly of large iron oxide NPs (D = 27 nm), and the morphology of hybrid nanocomposites is governed by the concentration of the iron oxide NPs. The NPs are functionalized with carboxylic acid groups showing an affinity to the PMMA blocks. Due to the rearrangement of the polymer chains for accommodating the NPs, well-ordered spherical nanostructures are readily generated at a NP concentration of 0.5 wt%. Most interestingly, a chain-like network appears inside the hybrid films at a high NP loading. All hybrid films show ferromagnetism at room temperature, proven with a superconducting quantum interference device magnetometer.

O 22: Poster Session - 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction

Time: Monday 18:15–20:00 Location: P1A

O 22.1 Mon 18:15 P1A

Structural and electronic investigations of Blue Phosphorene on Au(111) — •Julian Picker, Maximilian Schaal, Marco Gruenewald, Felix Otto, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

In the last decades a wealth of two dimensional (2D) materials have obtained profound interest in fundamental research and practical applications because of their unique physical properties. A relatively new representative of these kind of materials is semiconducting Blue Phosphorene (BlueP), an allotrope of phosphorus. Theoretically, a buckled honeycomb structure and fascinating properties for optoelectronic applications such as a tuneable band gap size and a high carrier mobility were predicted [1,2]. In our study we observed the growth of BlueP on Au(111) by using molecular beam epitaxy (MBE) as well as the physical properties of this 2D material. The layer deposition was monitored *in-situ* via reflection high-energy electron diffraction (RHEED). Furthermore, we investigated the structural properties in reciprocal space by low-energy electron diffraction (LEED) and in real space by scanning tunneling microscopy with and without a hydrogen functionalised tip (STHM, STM). The electronic structure of the valence and conduction band were investigated by angle-resolved ultra violet photoelectron spectroscopy (ARUPS) and scanning tunneling spectroscopy (STS).

[1] J. L. Zhang *et al.*: Nano Lett. **16**, 4903-4908 (2016).
[2] J. Zhuang *et al.*: ACS Nano **12**, 5059-5065 (2018).

O 22.2 Mon 18:15 P1A

Selective Oxygen Functionalization of the h-BN/Rh(111) Nanomesh — •Marie Freiberger, Florian Späth, Fabian Düll, Philipp Bachmann, Johann Steinhauer, Hans-Peter Steinrück, and Christian Papp — FAU, Erlangen, Germany

2D materials such as hexagonal boron nitride (h-BN) and graphene are interesting due to their electronic properties, as inert template structures or as possible hydrogen storage materials. As a structural graphene analogue, h-BN features a honeycomb structure. The morphology of a supported h-BN layer strongly depends on the underlying crystal surface. In the case of Rh(111), a Moiré pattern evolves, also known as nanomesh, showing pore and wire regions. This strong corrugation makes h-BN/Rh(111), for example, a suitable template for confined metal nanocluster growth. Further modification of h-BN can be achieved via oxygenation or hydrogenation. In the case of the h-BN nanomesh on Rh(111), this is interesting since the pores and wires may show different reactivity towards functionalization.

Herein, we present detailed studies on the adsorption of molecular oxygen on the h-BN nanomesh on Rh(111). The system is investigated in a model approach under ultra-high vacuum conditions. Using synchrotron radiation-based in situ high-resolution X-ray photoelectron spectroscopy (HR-XPS) we are able to provide a deep insight in this system regarding the adsorption behaviour and thermal stability. Oxygenation is performed via a supersonic molecular beam and is found to occur selectively in the pores of h-BN. The adsorbed oxygen species is stable up to 600 K.

O 22.3 Mon 18:15 P1A

Gating monolayer MoS2 by charging its substrate — •Camiel van Efferen, Clifford Murray, Jeison Fisher, Joshua Hall, and Thomas Michely — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

We gate quasi-freestanding monolayer MoS2, grown by molecular beam epitaxy (MBE) on graphene (Gr) on Ir(111) [1], by introducing intercalants between Gr and Ir(111). Using intercalants like Eu and O, we control the position of the Gr Dirac point, allowing us to n- or p-gate the Gr and in turn also the MoS2. Applying a combination of scanning tunneling microscopy and spectroscopy we measure the effects of the gating on the band structure of monolayer MoS2, which has previously been studied using comprehensive scanning tunneling spectroscopy [2]. In ungated MoS2/Gr/Ir(111) a 1D hole gas is found around the 4|4E mirror twin boundaries of MBE-grown MoS2, a consequence of band bending around the charged boundary. We investigate how the band bending and the 1D hole gas are affected by the gating, due to changes in the screening environment and the charge transfer from the substrate. Moreover, as a consequence of gating, we observe also a shift in the periodicity of the confined states in the mirror twin boundaries.

[1] Joshua Hall et al., 2D Materials 5, 025005 (2018)
[2] Clifford Murray et al., Phys. Rev. B 99, 115434 (2019)

O 22.4 Mon 18:15 P1A

When halogene atoms do not guide the selfassembly of GNR precursor molecules — •Christoph Dobner[1], Jacob Teeter[2], Paulo Costa[3], Alexander Sinitskii[2], and Axel Enders[1,3] — [1]Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth — [2]Department of Chemistry, University of Nebraska - Lincoln, Lincoln NE 98588, USA — [3]Department of Physics and Astronomy, University of Nebraska - Lincoln, Lincoln NE 98588, USA

The on-surface selfassembly of the prototypical precursor molecule for graphene nanoribbon synthesis, 6,11-dibromo-1,2,3,4-tetraphenyltriphenylene ($C_{42}Br_2H_{26}$), and its non-brominated analog hexaphenylbenzene ($C_{42}H_{30}$), was investigated as a function of thermal treatment using scanning tunneling microscopy. The "herringbone" reconstructed surface of Au(111) was used for all growth studies, and all experiments have been carried out under ultrahigh vacuum conditions. It is found that for sufficiently high substrate temperatures, there is no halogene-guided selfassembly of the brominated molecules, in stark contrast to the well-known formation of chevron-shaped GNRs from these precursors. Instead, both species, the brominated and non brominated ones, form identical one-dimensional structures consisting of fully planarized and cyclized molecules on the surface. For hexaphenylbenzene, which form non-covalent two-dimensional networks at room temperature, a thermally induced transition of the network structure could be achieved by moderate annealing, which is likely driven by π-bond formation.

O 22.5 Mon 18:15 P1A

Classical molecular dynamics investigation of carbon nanomembranes — •Julian Ehrens and Jürgen Schnack — Universität Bielefeld, PF 100131, D-33615 Bielefeld

Nanometer thin carbon nanomembranes (CNMs) that are made by electron-induced crosslinking of aromatic self-assembled monolayers (SAMs) [1] can not be adequately investigated with regard to their internal structure by experimental means such as X-ray diffraction. Computer simulation is thus a viable method to further investigate the membranes on an atomic level.

We present the extension and continuation of our previous theoretical research with the focus on possible internal structures of carbon nanomembranes. We compare our theoretical estimates of the Young's modulus to the experimental results. For our calculations classical molecular dynamics as implemented in LAMMPS is employed and various ways of obtaining the modulus are presented for different models of membrane formation.

[1] Turchanin et al., Progress in Surface Science, Volume 87, Issues 5-8, May-August 2012, Pages 108-162

O 22.6 Mon 18:15 P1A

Growth and characterization of WS_2 on epitaxial graphene on SiC(0001) — •Adrian Schütze, Philip Schädlich, Constance Schmidt, Florian Speck, Dietrich R. T. Zahn, and Thomas Seyller — Institute of Physics, TU Chemnitz, Chemnitz, Germany

2D materials such as, for example, graphene, hexagonal boron nitride or transition metal dichalcogenides have recently received much interest as building blocks for electronic devices. For a successful integration of these materials, scalable growth methods are essential. Here we investigate the growth of WS_2 by metal organic molecular beam epitaxy (MOMBE) [1] on epitaxial graphene on SiC(0001). In that process $W(CO)_6$ is used as a precursor in conjunction with sulfur vapor produced by decomposition of FeS_2 in a thermal evaporator. Using MOMBE we were able to grow ultra-thin films of WS_2 on epitaxial graphene which were characterized by a combination of X-ray photoelectron spectroscopy (XPS), angle resolved photoemission spectroscopy (ARPES), low-energy electron diffraction and microscopy (LEED, LEEM), atomic force microscopy (AFM) and Raman spectroscopy. The ultra-thin films, which had thicknesses between one and two monolayers, were observed to consist of triangular domains. We discuss the influence of the growth parameters on the structural and electronic properties of the layers.
[1] S. Tiefenbacher et al., Surf. Sci. 318 (1994) L1161.

O 22.7 Mon 18:15 P1A

Growth and characterization of monolayer $MnSe_2$ on Au(111) — •Sebastien Hadjadj, Evangelos Golias, Sangeeta Thakur, Ivar Kumberg, and Wolfgang Kuch — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

During the last couple of years, there is a rising interest in novel two-dimensional magnetic materials. Most recently, several groups have shown that magnetic order in two-dimensional materials can be stable [1, 2]. The case of $MnSe_2$ is interesting, since it has shown magnetic properties at room temperature, making it an ideal candidate for actual applications. However, magnetic order has been reported for $MnSe_2$ grown on GaSe or $SnSe_2$, and the role of the interface in the stabilization of magnetic order is not yet clear. It needs to be ascertained if the magnetic ordering of monolayer $MnSe_2$ is an intrinsic effect of the material or an interface-induced phenomenon. Here we use molecular beam epitaxy to co-deposit Se and Mn on Au(111). Selenium is mounted in an effusion cell and is heated up to evaporate, while manganese is evaporated by electron bombardement. We characterize the films chemically by x-ray and Auger electron spectroscopy as well as structurally by low-energy electron diffraction.

[1] B. Huang et al. "Electrical control of 2D magnetism in bilayer CrI_3", Nature Nanotechnology 13, 544 (2018).

[2] D. J. O'Hara et al. "Room Temperature Intrinsic Ferromagnetism in Epitaxial Manganese Selenide Films in the Monolayer Limit", Nano Letters 18, 3125 (2018).

O 22.8 Mon 18:15 P1A

Growth of transition metal dichalcogenides on hBN — •Ziyang Gan[1], Emad Najafidehaghani[1], Zian Tang[1], Johannes Holler[2], Antony George[1], Kenji Watanabe[3], Takashi Taniguchi[3], Christian Schüller[2], Tobias Korn[4], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, D-07743 Jena, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [3]National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan — [4]Institut für Physik, Universität Rostock', D-18059 Rostock, Germany

Monolayer transition metal dichalcogenides (TMD) have emerged as versatile materials with the potential to be applied in next-generation electronics and optoelectronics devices owing to their attractive physical properties such as direct bandgap, spin-coupled valley degrees of freedom, etc. High quality TMDs can be synthesized by chemical vapor deposition (CVD) on Si substrates. However, the as grown monolayers show poor optical quality due to the detrimental interaction with the dielectric environment of the substrate. It has been shown recently that encapsulation in hexagonal boron nitride (hBN) is crucial to access the intrinsic optical quality of CVD grown monolayer TMDs. This motivates us to develop growth procedures for direct growth of monolayer TMDs on exfoliated and CVD grown hBN layers. The grown TMDs on hBN were characterized using optical microscopy, atomic force microscopy, Raman spectroscopy and photoluminescence spectroscopy to reveal their morphological, structural and optical properties.

O 23: Poster Session - Electron-Driven Processes at Surfaces and Interfaces

Time: Monday 18:15–20:00 Location: P1A

O 23.1 Mon 18:15 P1A

Photoinduced carbon dioxide fixation by means of surface-functionalized silicon quantum dots with aromatic amines — •Oscar A. Douglas-Gallardo[1], Cristián G. Sánchez[2], and Esteban Vöhringer-Martinez[1] — [1]Departamento de Físico-Química, Facultad de Ciencias Químicas, Universidad de Concepción, Chile. — [2]CONICET & Facultad de Ciencias Exactas y Naturales, Universidad Nacional de Cuyo, Padre Jorge Contreras 1300, Mendoza, Argentina.

In the last decade, the search for efficient methods able to capture, store and transform chemically atmospheric CO_2 has become a very dynamic research area. Several environmental issues such as global warming and climate change have been closely associated with the high atmospheric concentrations of this greenhouse gas. Here, a novel molecular system based on the use of surface-functionalized silicon quantum dots (sf-SiQDs) is theoretically explored as a proof of concept to bind CO_2 molecules. Within this scheme, CO_2 trapping is modulated by a photoinduced charge redistribution between the capping molecule and the silicon quantum dots (SiQDs). Chemical and electronic properties of the proposed sf-SiQDs have been studied with the Density Functional Theory (DFT) and Density Functional Tight-Binding (DFTB) approach along with a Time-Dependent model based on the DFTB (TD-DFTB) theoretical framework. Furthermore, a set of structural designs for capping molecules have been considered in order to strengthen the CO_2 binding energy. This study opens a new avenue to improve devices based on the use of sf-SiQDs for photochemically activated CO_2 fixation.

O 23.2 Mon 18:15 P1A

Transmission of radio-frequency voltages to the tunneling junction of a scanning tunneling microscope — •Nafise Kalantari, Thomas Jürgens, Rene Woltmann, Alexander Weismann, Rirchard Berndt, and Manuel Gruber — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Electron spin resonance scanning tunneling microscopy (ESR-STM), as implemented by Baumann et al. [1], requires the application of a constant-amplitude radio frequency voltage at the tunnel junction over a wide range of frequencies (DC-40GHz). The constant amplitude is achieved by tuning the radio-frequency input power to compensate the variation of the transmission of the voltage line as a function of frequency [2]. However, this requires a precise determination of the radio-frequency transmission function. Here, we discuss the upgrade of a low-temperature STM with high-frequency cables and a superconducting magnet. The radio-frequency voltage applied to the tunneling junction has been measured for different frequencies to evaluate the transmission of the voltage line.

[1] S. Baumann, W. Paul, T. Choi, C. P. Lutz, A. Ardavan, A. J. Heinrich, Science 350, 417-420 (2015).

[2] W. Paul, S. Baumann, C. P. Lutz, A. J. Heinrich, Rev. Sci. Instrum. 87, 074703 (2016).

O 24: Poster Session - Electronic-Structure Theory: General

Time: Monday 18:15–20:00 Location: P1A

O 24.1 Mon 18:15 P1A

Surface influence on the electronic properties of GaAs(001) — •Isaac A. Ruiz-Alvarado[1], Alfonso Lastras-Martínez[1], and Milton Muñoz-Navia[2] — [1]IICO, UASLP, San Luis Potosí, México — [2]CONACYT-IFUASLP, San Luis Potosí México

Tailoring materials properties nowadays requires alloying individual properties. Due to its open scientific questions and technological implications, combining Ga and As (GaAs) is a long standing binary system of interest. Recently, the Reflectance Difference Spectroscopy (RDS), has re-emerge as a powerful technique to characterize and monitor the specific in situ growth in surfaces. However, for the system of interest (GaAs), in the literature several possible surface reconstructions are proposed. The physics behind the optical anisotropies related to the surfaces is an open question and not yet resolved with (RDS). Understanding the physics that gives rise to the reconstruction of GaAs (2x4) surface, and its implications in the (RDS), is interesting from a scientific and technological point of view. In this work, we discussed the structural energy landscape of several possible reconstructions in GaAs (2x4) surface. In the framework of a density functional theory using projector-augmented-wave method, with an exchange correlation potential in the form of the generalized gradient approximation (GGA), the electronic structure of the different surface reconstructions (namely α, $\alpha2$, β, $\beta2$ and $\beta3$) are obtained. Our results show that the energy landscape of the surface reconstructions of the GaAs system can be discuss in terms of the layer by layer mobility influence and the dependence in the concentration (As or Ga rich structure).

O 24.2 Mon 18:15 P1A

Complex contour integration in non-equilibrium Green's function formalism — •Jonas Fey[1], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Zentrum für Materialforschung (LaMa), Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

In a previous work we introduced a new method for calculating the electronic density as a partial step in a self-consistent algorithm using Green's functions by calculating a non-equilibrium occupation function for complex-valued energies. In order to calculate the density in the non-equilibrium steady state Keldysh formalism, one needs a high amount of computational effort, since the integration is along the real energy axis. Going to the complex plane allows for less computational effort, but the non-equilibrium occupation function is needed. The calculation of this function worked well for a single step and indicated the possibility to make electronic structure calculations more efficient. The validity for a complete self-consistent calculation remains open. Therefore, we tested the method for different model systems simulating for example a potential barrier or a quantum dot. We investigated the correctness of our results as well as the convergence depending on the number of energy points. Furthermore, we studied analytic properties of the functions used which are crucial for the functionality of our method.

O 24.3 Mon 18:15 P1A

AiiDA workflows in KKR-DFT for high-throughput computations — •Irina Heinz[1], Philipp Risius[1,2], Alexander Fabian[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Zentrum für Materialforschung (LaMa), Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

Magnetic tunnel junctions (MTJs) have seen several industrial applications over the years. Most ab initio descriptions focus on a 1×1 slab of material owing to constraints in computational time. However, supercells are necessary to describe interesting physics resulting from k-scattering. Skyrmionic structures, for example, may modulate tunnel magnetoresistance due to scattering between parts of the Brillouin zone [2]. At finite temperatures, atomic displacement and magnonic excitations are expected to contribute to the intricate effects in MTJs. However, such effects are highly material dependent. We develop workflows using a plugin for the AiiDA framework to automatically calculate transport through supercells of various materials with different types of disorder. This work paves the way for future high-throughput searches for promising material combinations.

[1] Pizzi, Giovanni, et al. "AiiDA: automated interactive infrastructure and database for computational science." *Comp. Mater. Sci.* **111** (2016): 218-230.

[2] Schäfer-Richarz, Jonas Friedrich, et al. "Magnetic tunnel junctions: An efficient way for electrical skyrmion detection investigated by ab initio theory." *Phys. Rev. B*, accepted.

O 25: Poster Session - Focus Sessions: Innovation in Machine learning PRocEsses for Surface Science (IMPRESS)

Time: Monday 18:15–20:00 Location: P1A

O 25.1 Mon 18:15 P1A

Recovering molecular configurations during SPM-based manipulation — •Joshua Scheidt[1,2,3], Kurt Driessens[4], F. Stefan Tautz[1,2], and Christian Wagner[1,2] — [1]1Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA Fundamentals of Future Information Technology, Jülich, Germany — [3]Institut für Softwaretechnik und Theoretische Informatik, Technische Universität Berlin, Germany — [4]Department of Data Science and Knowledge Engineering, Maastricht University, The Netherlands

Molecular nanorobotics with a scanning probe microscope (SPM) would place the construction of complex supramolecular structures that are not accessible by self-assembly within reach. A fundamental obstacle on the way towards this goal is the poor observability of the atomic-scale molecular conformation during manipulation. Here we present a solution to this problem which utilises the particle filter localisation (PF) technique: Force-gradient data along a manipulation trajectory as received from the SPM is compared to data from a molecular simulation stored using a finite state automaton[1]. The simulation contains all inequivalent tip-molecule-surface configurations on a high-symmetry surface. The PF uses a set of sampling points to identify simulated conformations which likely match the experimental data. The particles from the PF are subsequently clustered to allow for a single or small set of likely molecule conformations to be retrieved. We test the performance of the PF on synthetic as well as experimentally acquired data.

[1] A. Diener, Master's thesis, Maastricht University, 2018

O 25.2 Mon 18:15 P1A

Classification of grazing incidence x-ray diffraction patterns using neural networks — •Verena Eslbauer, Johannes J. Cartus, Roland Resel, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

Grazing incidence X-ray diffraction is a frequently used tool to investigate the crystalline properties of thin films. Hereby, indexing Bragg peaks is a fundamental procedure for phase analysis and detection of unknown polymorphs. The current solution is an iterative approach, which is both tedious and requires the knowledge of an experienced material scientist. We are currently developing a software based on convolutional neural networks that should enable automatic classification of crystal systems. We have created a large set of crystal structures with pre-determined symmetries and their diffraction patterns. These serve as a training dataset for our convolutional neural network. At the current status of our work we can differentiate between different crystal systems, independent of the preferred orientation of their crystallites.

The next steps of our research involve the assignment of Laue indices to Bragg peaks and finally the determination of the lattice constants of the crystallographic unit cell.

O 25.3 Mon 18:15 P1A

Neural Network Controlled Nanocar — •Bernhard Ramsauer and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

In 2021 at the nanocar race at Center for Materials Development and Structure Studies (CEMES-CNRS) in Toulouse, France we are planning to participate with the world*s first neural-network-controlled nanocar. At this race, participants have to direct a single molecule across a 'race-track' set on a metallic substrate, controlling their nanocars via an STM-tip without being in physical contact with it.

Although nanocars can be readily synthesized with different shapes and properties, the physics that govern the molecule's movement is complex and involves the interaction between the molecule and the tip as well as between the molecule and the substrate. Therefore, it is far from straightforward for humans to manoeuvre the nanocar and predict the result of a performed action.

To improve the performance, we implement Deep Neural Networks (DNNs), which are able to perform various actions even for subsequently changing environmental conditions. The DNN enables an 'autonomous' driving of nanocars by controlling the STM-tip position and the applied voltage based on the nanocars position and orientation on the surface. Moreover, the DNNs will yield direct physical insight into the interaction that governs the nanocar maneuvers.

O 26: Poster Session - Graphene: Growth, Structure and Substrate Interaction

Time: Monday 18:15–20:00 Location: P1A

O 26.1 Mon 18:15 P1A

Investigating the quality of CVD-grown graphene on germanium using in-situ surface science methods — •Andreas Becker, Jarek Dabrowski, Mindaugas Lukosius, and Christian Wenger — IHP, Frankfurt (Oder), Germany

Germanium epitaxially grown on silicon has emerged as a relevant substrate for graphene growth because it is possibly compatible with established CMOS processing. Besides optimizing wafer-scale graphene growth on germanium template and subsequent transfer, we are exploring ways to directly integrate graphene growth into technological processing. However, major challenges are the relatively low quality of graphene on the standard orientation Ge(001) and the high required synthesis temperature. These challenges motivated an investigation of the growth process using a high-pressure preparation chamber for chemical vapor deposition that is connected to a surface science cluster tool. As a prerequisite for reliable graphene growth, we present a detailed study of the germanium substrate pre-cleaning and describe how to avoid etch pit formation. Furthermore, we investigated the influence of growth temperature on quality of graphene on Ge(001), Ge(110) and Ge(111) using scanning tunneling microscopy, low-energy electron diffraction and Raman spectroscopy. We discuss graphene grain size and morphology, epitaxial alignment and intragranular defect density and conclude that the best graphene quality is obtained on Ge(110) at a growth temperature near the substrate melting point. Finally, we intend to bring up a discussion how enhancement of substrate-mediated catalytic etching might help improve the graphene quality.

O 26.2 Mon 18:15 P1A

Reducing the step bunching during the growth of epitaxial graphene on silicon carbide — •Robert Appel, Richard Hönig, Philipp Weinert, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Otto-Hahn-Strasse 4a, 44227 Dortmund, Germany

Epitaxial graphene (EG) has attracted significant interest in the recent years due to the simple preparation method by heating silicon carbide (0001). One drawback of this approach is step bunching (SB) that leads to large terraces and tall step heights. These tall steps result in anisotropic electronic and magnetic properties of EG. In order to restore the electronic and magnetic properties of graphene, samples with shallow steps are desirable. The $(6\sqrt{3} \times 6\sqrt{3})$R30°-reconstruction (so-called buffer layer (BL)) of the SiC(0001) that forms while heating constrains the SB. Therefore, a fast formation of the BL is of utmost importance.

We use the confinement controlled sublimation (CCS) method in argon atmosphere because it is known for reproducibility and tunability. Thus, it is a promising method to find the ideal parameters for fast BL formation. Kruskopf et al. demonstrated the preparation of EG with shallow steps and less SB by using a high heating rate, a short heating time and a high preparation temperature.

In this study, we explore the applicability of the CCS method in order to obtain similar results with shallow steps and less SB. For this purpose, we systematically modify the preparation parameters and characterize the obtained samples with atomic force microscopy.

O 26.3 Mon 18:15 P1A

LEED and LEEM Study of Hexagonal Boron Nitride Islands and 6x2 Boron Reconstruction on Ir(111) Grown via Thermal Catalytic Decomposition of Borazine ($B_3H_6N_3$) — •Marko Kriegel[1], Karim Omambac[1], Christian Brand[1], Pascal Dreher[1], David Janoschka[1], Ulrich Hagemann[2], Nils Hartmann[2], Frank Meyer zu Heringdorf[1,2], and Michael Horn-von Hoegen[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — [2]Interdisciplinary Center for Analytics on the Nanoscale (ICAN) Carl-Benz-Str. 199, 47057 Duisburg, Germany

High quality large area hexagonal boron nitride layers are grown on Ir(111) via thermal catalytic decomposition of borazine ($B_3H_6N_3$) using CVD technique. The preparation of large (6x2) reconstructed 2D boron islands [1] is initiated by the dissolution of boron into the bulk at high temperatures followed by subsequent segregation of boron atoms to the surface upon cooling [2]. The surface morphology and structure determination has been performed in-situ by high-resolution spot profile analyzing-LEED (SPA-LEED), real-time growth observation via low energy electron microscopy (LEEM) and ex-situ by atomic force microscopy (AFM). The chemical composition has been determined ex-situ by X-ray photoemission spectroscopy (XPS) and time-of-flight secondary ion mass spectroscopy (ToF-SIMS) measurements.

[1] Applied Surface Science 420, 504-510 (2017)

[2] ACS Nano 13, 3816-3822 (2019)

O 26.4 Mon 18:15 P1A

Twisted Graphene on Ir(111) and SiC(0001) Studied by SPA-LEED — •Christian Brand[1], Birk Finke[1], Karim M. Omambac[1], Laurenz Kremeyer[1], Frank-J. Meyer zu Heringdorf[1,2], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen and CENIDE, Germany — [2]ICAN, Duisburg, Germany

When graphene is placed on a crystalline surface, the periodic structures within the layers superimpose and moiré superlattices form. Small lattice rotations between the two materials in contact strongly modify the moiré superlattice, upon which many electronic, vibrational, and chemical properties depend. Here we report on the structural manipulation of epitaxial graphene grown on metallic Ir(111) and semiconducting SiC(0001) surfaces. The spontaneous reorientation in the degree- and sub-degree-range of graphene on Ir(111) depends on the substrate temperature during growth. This effect is described by a 2D coincidence network favored by strain reduction together with the dissimilar thermal expansion of the substrate and graphene. The resulting effective compressive biaxial pressure is more easily accommodated in graphene by small rotations rather than by compression [Nano Lett. **19**, 4594 (2019)]. For graphene on SiC(0001) only the oriented R0° phase is found due to the higher bonding strength to the substrate. Upon H and Sn intercalation this interaction can be reduced such that the graphene layer is lifted from the substrate. Finally, we present a detailed analysis of an unusually broad diffraction background found for graphene and hex-BN on both substrates [Phys. Rev. B **110**, 155307 (2019)].

O 27: Poster Session - Graphene: Electronic Structure, Excitations, etc.

Time: Monday 18:15–20:00 Location: P1A

O 27.1 Mon 18:15 P1A

Anisotropic Carrier Dynamics in HOPG — •Hauke Beyer, Tim Jacobsen, Gerald Rohde, Kai Rossnagel, and Michael Bauer — Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany

Time- and angle-resolved photoelectron spectroscopy is employed to study the decay of an anisotropic momentum distribution generated in the Dirac-cone of HOPG upon excitation with linearly polarized light. At the primary excitation energy the transient population within the probed momentum cut shows distinct delays of up to $\sim$ 10 fs for indirect excitations in comparison to the direct photoexcitation channel. The observed delay times are associated with momentum isotropization processes and show a good qualitative agreement with calculations based on a model introduced in Ref. [1]. As excited carriers are redistributed towards the Dirac-point via electron-electron and electron-phonon scattering we furthermore observe that the momentum anisotropy gets gradually weaker. In contrast to previous quasistatic studies [2, 3], our results allow also capturing the temporal evolution of momentum redistribution processes driven by fundamental interactions in graphitic materials.

[1] E. Malic *et al.*, Phys. Rev. B **84**, 205406 (2011).
[2] S. Aeschlimann *et al.*, Phys. Rev. B **96**, 020301(R) (2017).
[3] M. Mittendorff *et al.*, Nano Letters **12**, 1504 (2014).

O 27.2 Mon 18:15 P1A

Spatial Variations in the Electronic Structure of Twisted Bilayer Graphene on HOPG — •Birce Sena Tömekce[1], Dilek Yildiz[1,2], and Oguzhan Gürlü[1] — [1]Department of Physics, Istanbul Technical University, 34460, Istanbul, Turkey — [2]Department of Physics, Harvard University, Cambridge, MA 02138, USA

Twist of a bilayer graphene generates moiré superlattices with a periodicity that depends on the twist angle. Such periodic pattern arises due to modulation of local density of states (LDOS) along the surface which can be detected by scanning tunneling microscopy (STM). It is known that the electronic properties of twisted bilayer graphene vary with the twist angle. Cyclohexane dropcasting on highly oriented pyrolytic graphite (HOPG) induces twist between graphene layers. Hence, we used this method to form moiré zones on HOPG. In this study, we investigated the electronic properties of moiré patterns with various periodicities and their boundaries on HOPG surface by STM and scanning tunneling spectroscopy (STS) together with lock-in technique. We studied spatial distribution of charge density of the surface by differential conductance (dI/dV) mapping. For most of the observed moiré patterns, charge density modulation tends to decrease and becomes homogenous with increasing magnitude of bias voltage, while moiré boundaries might show arbitrary changes. In addition, we obtained dI/dV spectra on different positions on moiré regions, their boundaries and HOPG surface adjacent to the moiré regions. In this presentation, we will report on bias dependent dI/dV maps and discuss conducting behaviors of the encountered moiré zones.

O 28: Poster Session - Scanning Probe techniques: Method Development

Time: Monday 18:15–20:00 Location: P1A

O 28.1 Mon 18:15 P1A

Understanding lateral force microscopy data of organic molecules — •Elisabeth Riegel, Oliver Gretz, Alfred J. Weymouth, and Franz J. Giessibl — Universität Regensburg, Regensburg, Germany

Frequency-modulation lateral force microscopy (LFM) is a variant of the highly-successful frequency-modulation atomic force microscopy in which the direction of the tip oscillation is along the surface. In this geometry, the setup is not sensitive to long-range background forces in the direction of the surface normal, but only to the short-range interactions. To achieve high spatial resolution, we oscillate our tip at sub-Angstrom amplitudes. We applied this technique to study islands of PTCDA on Cu(111). On Cu(111), PTCDA forms roughly a herringbone pattern. In this contribution, we discuss the interpretation and understanding of the frequency shift and dissipation data with a model of the tip-sample interaction including CO bending.

O 28.2 Mon 18:15 P1A

Probing relaxations of atomic-scale junctions in the Pauli repulsion range — Jonathan Brand, •Nicolas Néel, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

Clean metal as well as C_{60}-terminated tips of an atomic force microscope probe the interaction with C_{60} molecules adsorbed on Cu(111) and Pb(111). The force measurements unveil a monotonic shift of the point of maximum attraction with the bias voltage. The conventional superposition of long-range van der Waals and electrostatic forces with short-range Pauli repulsion does not reproduce the shift. By phenomenologically including bias-dependent relaxations of the electrode geometry in the analytical expression for the short-range force the experimental data can qualitatively be described.

O 28.3 Mon 18:15 P1A

Fast low-noise transimpedance amplifier for scanning tunneling microscopy — Martin Štubian[1,2], Juraj Bobek[1,2], Martin Setvin[1], and •Michael Schmid[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Brno University of Technology, Brno, CZ

Scanning tunneling microscopy is one of the most versatile techniques in surface physics. One of the factors limiting its performance is the bandwidth and noise of the preamplifier. Higher bandwidth enables faster scanning, and also implies low phase shifts, which reduces the susceptibility to feedback loop oscillations. STM preamplifiers are current-voltage converters (transimpedance amplifiers, TIAs), usually with a high feedback resistor. Increasing its resistance leads to lower current noise (Johnson noise of the resistor), but at the same time usually results in lower bandwidth. Using a multi-stage amplifier design, we could achieve an input noise of $\approx 5\,\mathrm{fA}/\sqrt{\mathrm{Hz}}$ at room temperature and low frequencies, but nevertheless a large bandwidth of 50–200 kHz and large dynamic range (sub-pA to 50 nA). We also demonstrate that minimizing the input capacitance is of paramount importance for low noise. This means that connecting the STM tip to the preamplifier via a long coaxial cable is unfavorable, and the performance can be substantially improved by placing the first amplifier stage into vacuum. Additionally, for low-temperature STMs, the Johnson noise is reduced by placing the feedback resistor in thermal contact with the cryostat. We also discuss a source of noise in operational amplifiers usually not considered, but important for TIAs.

O 28.4 Mon 18:15 P1A

Simultaneous length extensional- and flexural operation of a qPlus sensor for biaxial force detection. — •Jinglan Qiu[1,2], Dominik Kirpal[1], and Franz J. Giessibl[1] — [1]University of Regensburg, Germany — [2]Hebei Normal University, Shijiazhuang, China

In dynamic atomic force microscopy, the tip of the cantilever usually is oscillating in the z-direction perpendicular to the surface. By adding a second oscillation in the x-direction, parallel to the surface, lateral forces can be directly investigated. In the case of a silicon cantilever this can be realized by using a torsional mode [1]. In the case of the qPlus sensor, the length extensional mode (LE-mode) can be used, analogous to a needle sensor. However, this requires an adjustment of the electrode configuration. We have prepared a qPlus sensor for the length extensional mode, characterized the properties of the mode and showed the capability of atomic resolution in both, the LE-mode and the lateral 1st flexural mode.

[1] O. Pfeiffer, R. Bennewitz, A. Baratoff, E. Meyer, P. Grütter, Phys. Rev. B, 65, 161403 (2002).

O 28.5 Mon 18:15 P1A

Setup of a THz-STM for pump-probe experiments using a commercial THz-source — •Philip Kapitza, Hüseyin Azazoglu, and Rolf Möller — Fakultät für Physik/Cenide, Universität Duisburg-Essen, Germany

To study the excitations of single atoms or molecules on their intrinsic timescales ultrafast temporal and atomic-scale spatial resolution is essential. This can be achieved by combining the very high spatial resolution of a scanning tunneling microscope (STM) with picosecond duration terahertz (THz) pulses. When coupled to the tip of a STM the THz pulses can modulate the bias voltage in the tunneling junction [1,2,3]. The setup presented on this poster consists of a homebuilt low-temperature STM (LT-STM) and a commercial THz-pulse source for time domain spectroscopy (THz-TDS). The THz-emitter of this THz-TDS system is a photoconducting antenna irradiated by a fs-IR laser. For pump-probe experiments using the THz-pulses two THz-emitters will be used with both terahertz beams focused onto the tip. The time delay between the pump and the probe pulse will be created by splitting the beam of the fs-IR laser with one part of the beam going through an optical delay line.

[1] Cocker, T. L. et al., Nat. Photon. 7, 620-625 (2013).

[2] Cocker, T. L. et al., Nature 539, 263-267 (2016).

[3] Yoshioka, K. et al., Nat. Photon. 10, 762-765 (2016).

O 28.6 Mon 18:15 P1A

Atom manipulation capabilities of MnNi Tips in STM — •Nicolaj Betz[1], Max Hanze[1,2], Luigi Malavolty[1,2], Fabian D. Natterer[3], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany. — [3]University of Zurich, CH-8057 Zurich, Switzerland.

Scanning tunneling microscopy (STM) with spin-polarized tips can combine the ability to manipulate individual atoms with the ability to gain fundamental insights into magnetic interactions via the spin-sensitivity in the current [1]. In this work, we investigate the performance and the manipulation capabilities of antiferromagnetic MnNi tips. Antiferromagnetic tips are promising candidates for spin-polarized STM because of their robust microscopic magnetization, that defines spin contrast, and their small stray field, which reduces perturbations on the probed magnetic structures. We etch our tips using a HCl solution [2] and characterize them with scanning electron microscopy. The tips require intense in-vacuum cleaning. We find that self-sputtering using field emission in an Ar atmosphere yields clean and sharp tips. We perform STM measurements at different magnetic fields on Cobalt islands evaporated on Au(111). And we investigate the atom manipulation capabilities by dropping individual atoms from the tip.

[1] Toskovic, R. et al., Nature Phys 12, 656-660 (2016)

[4] Forrester et al., Rev. Sci. Instrum. 89, 123706 (2018)

O 28.7 Mon 18:15 P1A

Design of low temperature ESR-STM — •Denis Krylov, Wonjun Jang, Yujeong Bae, and Andreas J. Heinrich — Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Republic of Korea

A combination of electron spin resonance (ESR) and scanning tunneling microscopy (STM) enables a time-domain control over electron and nuclear spins with atomic-scale resolution. This technique provides a great potential for chemical structure analysis, quantum coherent manipulation and quantum sensing. The critical points of the ESR-STM system design are low loss RF wiring with sufficient coupling to the cooling stage and a vibration free environment.

We report about the progress in developing of the home-built system with two-dimensional vector magnetic field and sub Kelvin temperatures.

O 28.8 Mon 18:15 P1A

How to Resolve Dynamic Surface Processes by High-Speed Scanning Tunneling Microscopy — •Zechao Yang, Leonard Gura, Jens Hartmann, Heinz Junkes, William Kirstädter, Patrik Marschalik, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Here we present the concept of a new high-speed scanning tunneling microscope (STM) for resolving dynamic processes in amorphous network structures at the atomic scale.

The design of the microscope body is compact, rigid, and highly symmetric to ensure vibrational stability and low drift characteristics. The scanner unit in this microscope consists of two independent tube piezos for slow and fast scanning, respectively. A commercial scanning probe microscopy (SPM) controller is used for the slow scanner unit, while a high-speed Versa Module Eurocard bus (VMEbus) system controls the fast scanning. The data acquisition of the tunneling signal, x-, y-, and z-position is realized by a high-speed digitizer. Scan control and data acquisition has been programmed in an EPICS framework.

Another important feature in our approach is the implementation of a spiral scan option for avoiding internal resonance frequencies of the microscope body. The tip scans in a quasi-constant height mode, where the logarithm of the tunneling current signal can be regarded as roughly proportional to the surface topography.

In first test measurements at room temperature, diffusion processes within an O(2x2) coverage on Ru(0001) have been atomically resolved with a time resolution of 25 milliseconds per frame.

O 28.9 Mon 18:15 P1A

Design of a high-stability miniaturized STM — •Felix Huber[1], Stephan Spieker[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany. — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany.

State-of-the-art low-temperature scanning tunneling microscopy setups are typically housed in large cryostats, require proportionally large vacuum chambers, as well as extensively shielded custom built laboratories to reach the signal-to-noise ratios (SNR) required for cutting-edge experiments. However, by miniaturizing the STM-head, the SNR can be significantly improved, due to the favorable scaling of resonant frequency [1], thermal characteristics, and measurement time. The STM design presented here is optimized to work in noisy environments, and due to its small volume and dimensions can be used in a standard bore cryogenic dewar [2]. The setup is designed for long hold times, as well as for a short turn-around, allowing for rapid sample preparation and characterization. This design could be used for extended averaging experiments, or it could be utilized as an easy upgrade to existing UHV setups.

[1] Ast, C. R., Assig, M., Ast, A. & Kern, K. Design criteria for scanning tunneling microscopes to reduce the response to external mechanical disturbances. Rev. Sci. Instrum. 79, 093704 (2008).

[2] Schlegel, R. et al. Design and properties of a cryogenic dip-stick scanning tunneling microscope with capacitive coarse approach control. Review of Scientific Instruments 85, 013706 (2014).

O 28.10 Mon 18:15 P1A

Single-atom electron paramagnetic resonance in a scanning tunneling microscope driven by a radiofrequency antenna at 4K
— •Stepan Kovarik, Tom S. Seifert, Corneliu Nistor, Luca Persichetti, Sebastian Stepanow, and Pietro Gambardella — Department of Materials, ETH Zurich, Switzerland

Combining electron paramagnetic resonance (EPR) with scanning tunneling microscopy (STM) enables detailed insight into the interactions and magnetic properties of single atoms on surfaces [1]. A requirement for EPR-STM is the efficient coupling of microwave excitations to the tunnel junction. Here, we present a coupling efficiency of the order of unity by using a radiofrequency antenna placed parallel to the STM tip, which we interpret using a simple capacitive-coupling model [2]. We further demonstrate the possibility to perform EPR-STM routinely above 4 K using amplitude as well as frequency modulation of the radiofrequency excitation. We directly compare different acquisition modes on hydrogenated Ti atoms on bilayer MgO on Ag and highlight the advantages of frequency and magnetic field sweeps as well as amplitude and frequency modulation in order to maximize the EPR signal. The possibility to tune the microwave-excitation scheme and to perform EPR-STM at relatively high temperature and high power opens this technique to a broad range of experiments.

[1] S. Baumann *et al.*, *Science* **350**, 417 (2015)

[2] T. S. Seifert *et al.*, arXiv:1908.03379 (2019)

O 28.11 Mon 18:15 P1A

Control of broadband THz near fields in an STM junction — •Natalia Martín Sabanés[1,2], Sarojini Mahajan[1], Martin Wolf[1], and Melanie Müller[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]Freie Universität Berlin, Berlin, Germany

In THz-gated Scanning Tunneling Microscopy (THz-STM),[1] the electric field of a single-cycle THz pulse acts as a transient bias modulating the STM-junction, enabling control of the tunneling current on femtosecond time scales. Optimal operation of a THz-STM requires exact knowledge and precise control of the THz near field waveform. In this regard, we demonstrate THz near field sampling via THz-induced modulation of ultrafast photocurrents in a metal-metal junction,[2] and characterize in detail the coupling of broadband (1-30 THz) single-cycle THz pulses generated from a spintronic emitter to the STM tip. Specifically, we show that employing NIR laser pulses with a curved wavefront for THz generation allows for precise control of the phase, amplitude and bandwidth of the THz near field. Depending on the excitation conditions, THz near fields with frequencies up to 10 THz and peak voltages of several volts (up to 4 V) can be achieved at 1 MHz repetition rate. We further discuss the influence of non-instantaneous effects such as THz-streaking, space charge dynamics and hot carriers in the metals on the bandwidth and shape of the measured near field waveforms, and define operation regimes for reliable near field characterization. References: [1] Cocker T., el at, Nature 539, 263-267 (2016); [2] Yoshida S., et al, ACS Phot. 6, 1356-1364 (2019)

O 29: Poster Session - Solid-liquid Interfaces: Structure, Spectroscopy

Time: Monday 18:15–20:00 Location: P1A

O 29.1 Mon 18:15 P1A

Enantioselective interactions of L- and D-alpha polyalanine molecules investigated by STM and STS — •Shuyuan Xue[1], Nguyen Thi Ngoc Ha[1], and Christoph Tegenkamp[1,2] — [1]TU Chemnitz, Germany — [2]Leibniz Universität Hannover, Germany

The chiral induced spin selectivity (CISS) effect has been intensively investigated towards applications in molecular spintronics and spinselective processes in biology. The adsorption of a chiral molecules with a specific handedness affects the direction of the spin-polarization as well as magnetization of a surface [1]. For L alpha-helical polyalanine (PA) films on HOPG and Au(111) we found recently densely packed self-assembled monolayers. Thereby, interdigitation in between adjacent molecules favors also rotational order [2]. In this study we co-adsorbed L- and D-alpha polyalanine molecules from the liquid phase on HOPG and investigated the structure by scanning tunneling microscopy under ambient conditions. In contrast to L-alpha polyalanine molecules, the enantiometric mixture revealed a (2 x 1) structure. Apparently, the interdigitation takes place only along one crystallographic direction with one kind of molecules leading to phase separation of the enantiomers. [1] R. Naaman et al., Chimia 72, 394 (2018). [2] T.N.H. Nguyen et al. J. Phys. Chem. C 123, 612 (2019)

O 29.2 Mon 18:15 P1A

Ion adsorption and interface potentials of electrolyte solutions in contact with Au(111) including polarizability effects — Victor G. Ruiz[1], Zhujie Li[2], Matej Kanduč[3], and •Joachim Dzubiella[1,2] — [1]Research Group for Simulations of Energy Materials, Helmholtz-Zentrum Berlin — [2]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany — [3]Department of Theoretical Physics, Jozef Stefan Institute, Ljublijana, Slovenia

Solid-liquid interfaces (SLI) are of growing interest to basic science and technology. SLI including gold (Au) have received much attention due to applications in catalysis and biotechnology. The need of including biomolecular and ionic species in the aqueous environment within atomistic simulations necessitates the accurate inclusion of charge and fluctuations effects of the liquids [Small 12, 2395 (2016)]. The formed interfaces are complex due to the interplay of van der Waals (vdW) interactions, covalent bonds, and image-charge effects induced by the highly polarizable Au surface. Using a polarizable Lennard-Jones potential [I. Geada, *et al*, Nat. Comm. 9, 716 (2018)], we present molecular dynamics simulations of ionic adsorbates on Au(111) which include image-charge effects induced in the metal surface in a classical approximation. We present studies on the adsorption structures and interface electrostatic potentials of sodium chloride, sodium nitrophenolate, and sodium hexacyanoferrate salts, showing the influence which image-charge effects have on the interfacial microstructures and electrostatic properties.

O 29.3 Mon 18:15 P1A

Determining redox-dependent Cu-ligand chelating behaviour in a single metallo-protein — •Giovanni Giuzio[1], Masoud Baghernejad[1,2], and Katrin F. Domke[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Hemholtz-Institute, Münster, Germany

The copper metallo-protein azurin is a widely studied system in which ET is performed under physiological conditions by switching the oxidation state of the Cu center between +1 and +2.

In the presented project, we study individual azurin proteins bound to a Au(111) surface combining scanning tunneling microscopy and TERS under electrochemical conditions. In-air TER spectra show that the electronic, optical and vibrational properties of the azurin Cu center are preserved upon molecule conjugation with the Au surface. STM images prove that we TERS-probe individual proteins at a time.

Under EC conditions, we control the Au(111) potential which in turn regulates the oxidation state of the Cu center. The results show a potential-dependent behavior of the TER spectra. Comparing the S/N of in-air and in-liquid EC-experiment, a drastic signal reduction is observed under operando conditions. To improve the EC-TERS sensitivity, we use a spatial light modulator to optimize the laser-tip coupling, using either the focus size or the TER signal as a feedback. TERS potentio-dynamic mapping of a single molecule switch and extracting structural information about the metallo-protein under switching conditions can be expected to provide unprecedented insights into ET transfer characteristics in biomolecular switches.

O 30: Poster Session - Surface Magnetism

Time: Monday 18:15–20:00 Location: P1A

O 30.1 Mon 18:15 P1A

Study of Magnetic Molecules on Superconductors by STM/AFM — •soroush arabi[1], yuqi wang[1], klaus kern[2], and markus ternes[3,4] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [3]RWTH Aachen University, Institute of Physics, D-52074 Aachen, Germany — [4]Peter-Grünberg-Institute (PGI-3), Forschungszentrum Jülich, D-52425 Jülich, Germany

We use a combined scanning tunneling microscope (STM) and atomic force microscope (AFM) to investigate the interplay of magnetism and superconductivity in single magnetic molecules adsorbed on s-wave superconductors. For this study, we use cobalt phthalocyanine (CoPc) adsorbed on $NbSe_2$ and Fe-porphin (FeP) adsorbed on Pb(111). Such proximity offers a rich spectrum of phenomena, due to the formation of Yu-Shiba-Rosinov (YSR) states inside the superconducting gap which at strong enough interaction can screen the magnetic moment by breaking off a cooper pair [1]. Taking advantage of the unique capabilities of the AFM, we can dynamically drive the ground state of FeP/Pb(111) towards or away from such a quantum phase transition by manipulating the exchange interaction between the molecule and substrate while tracking the interacting force. Moreover, we show that symmetry-reduced adsorption sites for CoPc molecules leads to a singlet ground state and a sharp molecular singlet-triplet transition at an energy outside the superconducting gap of the $NbSe_2$.

[1] Laetitia Farinacci, et al., Phys. Rev. Lett. **121**, 196803 (2018).

O 30.2 Mon 18:15 P1A

Yu-Shiba-Rusinov states of Manganese atoms on Vanadium — •Jennifer Hartfiel, Gaël Reecht, Martina Trahms, Rika Simon, and Katharina J. Franke — Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

The adsorption of a magnetic adatom on a superconducting substrate perturbes the Cooper pair condensate in close proximity to the surface. The unpaired magnetic moment induces localized bound states, so-called Yu-Shiba-Rusinov (YSR) states, inside the superconducting energy gap, which can be probed by scanning tunneling spectroscopy (STS). The coupling strength between the magnetic moment of the impurity and the Cooper pairs determines the energy needed for tunneling into the YSR state.

In this work, we perform STS measurements on Mn adatoms on a V(110) surface and find a variety of YSR state energies. Vanadium is very reactive and therefore oxygen atoms assemble on the surface, causing reconstructions in the upmost layer [1]. This makes it difficult to investigate a possible adsorption-site dependence of the YSR energies. To obtain a more homogeneous surface structure we grow Ag islands of a few monolayers on top of the Vanadium, before depositing the Mn atoms. We find that the islands exhibit a preferential growth direction with a specific angle to the V lattice. The Ag is proximitized by the superconducting substrate, and we also observe YSR states for Mn on Ag/V. In both cases we are able to manipulate the Mn atoms with the STM tip, causing a change in the YSR state energies.

[1] R. Koller et al., Surface Science 512 (2002).

O 30.3 Mon 18:15 P1A

Single-Co and two-site Kondo effect in atomic Cu wires on Cu(111) — •Nicolas Néel[1], Markus Bohn[1], Jörg Kröger[1], Malte Schüler[2], Bin Shao[2], Tim O. Wehling[2], Alexander Kowalski[3], and Giorgio Sangiovanni[3] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [2]Institute for Theoretical Physics, University Bremen, D-28359 Bremen, Germany — [3]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany

Linear atomic chains containing a single (two) Co and several non-magnetic Cu atoms were assembled on Cu(111) with the tip of a STM. For single Kondo atom chains the resulting Cu$_m$CoCu$_n$ clusters ($0 \leq m, n \leq 5$) exhibit a rich evolution of the Kondo effect with the variation of m and n, as inferred from changes in the line shape of the Abrikosov-Suhl-Kondo (ASK) resonance. The most striking result is the quenching of the resonance in CuCoCu$_2$ and Cu$_2$CoCu$_2$ clusters. State-of-the-art first-principles calculations were performed to unravel possible microscopic origins of the experimental observations.

For linear atomic chains containing two Kondo atoms, CoCu$_n$CoCu$_m$, the addition of a Cu atom to one edge Co atom of the chain ($m = 0 \to m = 1$) strongly reduces the amplitude and line width of the ASK resonance of that Co atom for all investigated chain lengths ($n = 2 - 4$). On the opposite edge Co atom the Kondo effect remains unaffected. Hybridization together with the linear geometry of the cluster are likely to drive the effect.

O 30.4 Mon 18:15 P1A

Demonstration of single atom ESR and pump-probe with a 30 mK STM setup — •Werner M.J. van Weerdenburg[1], Manuel Steinbrecher[1], Niels P.E. van Mullekom[1], Jan W. Gerritsen[1], Fabian D. Natterer[2], and Alexander A. Khajetoorians[1] — [1]IMM, Radboud University Nijmegen, the Netherlands — [2]Physik Institut, University of Zurich, Switzerland

The recent advances in electron spin resonance (ESR) with STM have allowed the detection of low-energy spin excitations with neV energy resolution on a single atom [1]. Combined with all-electrical pump-probe schemes, these methods have been used to probe spin relaxation times [2,3] and decoherence times [4] in the nanosecond regime.

Here, we demonstrate the implementation of ESR and all-electrical pump-probe on a 30 mK STM. By measuring the transmission of rf voltages and doing pulse shape analysis, we characterize the time-domain performance of our setup. We extract the magnetic moments of Fe on MgO/Ag(100) from the linear progression of the ESR resonance in field-sweep and frequency-sweep mode. With pump-probe schemes [5], we also reproduce comparable lifetimes for Fe on MgO/Ag(100) [3] and show how these are affected by an externally applied in-plane and out-of-plane magnetic field.

[1] S. Baumann et al., Science 350, 417-420 (2015)
[2] S. Loth et al., Science 329, 1628-1630 (2010)
[3] W. Paul et al., Nature Physics 13, 403-407 (2017)
[4] K. Yang et al., Science 366, 509-512 (2019)
[5] F. Natterer, ArXiv. 1902.05609 (2019)

O 30.5 Mon 18:15 P1A

Magnetic coupling between ferromagnetic semiconductors and organometallic phtalocyanines — •Carmen González-Orellana[1], Maxim Ilyn[1], Marco Gobbi[1,2,3], Paul Dreher[4], and Celia Rogero[1] — [1]Centro de Física de Materiales, San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [3]CIC nanoGUNE, San Sebastián, Spain — [4]DIPC, San Sebastián, Spain

The study of the interaction between organometallic phtalocyanines and magnetic metals has attracted interest due to its application in the field of spintronics. Most of the studies were focused on the magnetic properties of these metal-organic complexes coupled to ferromagnetic and antiferromagnetic metallic surfaces [1]. In the present work we study the interaction between the organic layer and ferromagnetic semiconducting/insulating substrates, in particular EuS and CrSiTe3. EuS is a 3D material where all the neighbours interact magnetically, whereas CrSiTe3 is a laminar material where magnetic interactions are confined in the plane and has been proposed as candidate single-layer ferromagnetic semiconductor.

Using a multi-technique surface science approach, combining XPS, LEED, XAS and XMCD, we analyze the coupling of the organic layer and its effect on the magnetic response of the system.

[1] A. Lodi et al., Surf. Sci., vol. 630, pp. 361-374, 2014.

O 30.6 Mon 18:15 P1A

The alloy Mn$_{88}$Ni$_{12}$: An Intrinsically Spin-Polarised Tip Material? — •J. Rika Simon, Martina Trahms, Jennifer Hartfiel, Gaël Reecht, and Katharina J. Franke — Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Spin-polarised tips are necessary for the realisation of electron-spin resonance (ESR) in a scanning tunnelling microscope (STM). These tips are typically obtained by transferring a few magnetic atoms to the tip apex and controlling their magnetisation by an external magnetic field [1]. Recently, Forrester et. al. have suggested Mn$_{88}$Ni$_{12}$ as an alternative tip material because of its intrinsic magnetic properties [2]. Moreover, it has been shown very recently by Willke et. al. that the magnetic field created by a spin-polarised tip is sufficient to perform single-atom ESR [3]. Combining both would allow for ESR-setups without the need for an external magnetic field.

We fabricate a Mn$_{88}$Ni$_{12}$ tip and investigate its properties using different model systems to study their spin-polarisation: Co nano-islands on Cu(111), and Fe(III)-octaethylporphyrin (FeOEP) on Au(111) and on Pb(111). Our experimental results do not yield unambiguous observation of spin-polarisation. The discrepancy of the results of our measurement techniques to those utilised by Forrester et. al. could be due to differences in preparation and treatment of the tip prior to the measurements, requiring a detailed analysis of the tip fabrication.

[1] M. Bode, Reports on Progress in Physics 66, 523–582 (2003)
[2] P. R. Forrester et al, Rev. Sci. Instrum. 89, 123706 (2018)
[3] P. Willke et al., arXiv: 1908.11061 [cond-mat.mes-hall] (2019)

O 30.7 Mon 18:15 P1A

Quantum Stochastic Resonance in a Single Atom — •Gregory McMurtrie[1], Max Hänze[1,2], Luigi Malavolti[1,2], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany. — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany.

The behavior of fluctuating spins is particularly relevant in nanoscale materials, where it determines the observable magnetic phases as well as giving rise to exciting phenomena such as quantum critical behavior.

Accessing these dynamic phenomena on their intrinsic atomic length and time scales is an important step towards an understanding of their underlying quantum behavior.

Scanning tunneling microscopy experiments with high frequency signals [1, 2] both give access to the spin dynamics of nanostructures as well as allowing them to be resolved in real space on the atomic scale.

In particular, by applying a small harmonic voltage signal, stochastic resonance [3] can be induced, leading to a synchronization of the spin state evolution.

This phenomenon has never been observed previously in atomic systems, and gives unprecedented access to the time domain behavior of spins, even allowing transduction of picosecond-speed dynamics.

References 1. S. Loth, Science 329 1628 (2010) 2. S. Baumann, Science 350 6259 (2015) 3. R. Benzi, J. Phys. A: Math. Gen 14, L453 (1981)

O 30.8 Mon 18:15 P1A

Spin dependent transmission of nickelocene-copper contacts

probed with shot noise — Michael Mohr[1], Manuel Gruber[1], Alexander Weismann[1], David Jacob[2], Paula Abufager[3], Nicolás Lorente[4], and •Richard Berndt[1] — [1]Christian-Albrechts-Universität zu Kiel, Kiel, Germany — [2]UPV/EHU, Donostia-San Sebastián, and IKERBASQUE, Bilbao, Spain — [3]CONICET and Universidad Nacional de Rosario, Rosario, Argentina — [4]CFM/MPC and DIPC, Donostia-Sebastián, Spain

The current I through nickelocene molecules and its noise are measured with a low temperature STM on a Cu(100) substrate. Density functional theory calculations and many-body modeling are used to analyze the data. During contact formation, two types of current evolution are observed, an abrupt jump to contact and a smooth transition. These data along with conductance spectra (dI/dV) recorded deep in the contact range are interpreted in terms of a transition from a spin-1 to a spin-1/2 state that is Kondo screened. Many-body calculations show that the smooth transition is also consistent with a renormalization of spin excitations of a spin-1 molecule by Kondo exchange coupling. The shot noise is significantly reduced compared to the Schottky value of $2eI$ but no influence of the Kondo effect or spin excitations are resolved. The noise can be described in the Landauer picture in terms of spin-polarized transmission of $\approx 35\,\%$ through two degenerate d_π-orbitals of the nickelocene molecule. Support via the European Union's Horizon 2020 research and innovation programme (766726) is acknowledged.

O 30.9 Mon 18:15 P1A

Measuring the exchange force field of a non-collinear magnetic structure on the atomic scale — Nadine Hauptmann[1], Soumyaiyoti Haldar[2], Tzu-Chao Hung[1], Wouter Jolie[1], •Lorena Niggli[1,3], Mara Gutzeit[2], Daniel Wegner[1], Stefan Heinze[2], and Alexander A. Khajetoorians[1] — [1]Scanning Probe Microscopy Department, IMM, Radboud University, Nijmegen, Netherlands — [2]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Germany — [3]Department of Physics, University of Zurich, CH-8057 Zurich, Switzerland

One route toward creating magnetic memory down to the level of individual atoms, relies on utilizing chiral magnetic structures, which are stabilized by a combination of various atomic-scale exchange interactions. Understanding these interactions is vital toward creating magnetic memory, necessitating methodology to quantify and manipulate exchange interactions on the atomic scale. Here, we present highresolution imaging of a chiral magnetic structure along with quantifying atomic-scale magnetic exchange interactions [1]. Using the combination of spin-polarized tunneling current and exchange force detection (SPEX), we quantify the exchange interaction between a ferromagnetic probe and the cycloidal spin spiral in 1ML Mn/W(110). We not only resolve the nearly antiferromagnetic atomic unit cell, but also the exchange force field along the spin spiral.

[1] N. Hauptmann et al., arXiv:1908.00959

O 30.10 Mon 18:15 P1A

Kondo Resonance of NO on Au(110)–(1×2) — •Hiroyuki Koshida, Hiroshi Okuyama, Shinichiro Hatta, and Tetsuya Aruga — Department of Chemistry, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan

Nitric oxide (NO) is a diatomic molecule that has a localized spin due to its unpaired electron in a $2\pi^*$ state. We studied the interaction of NO with Au(110)–(1×2) using STM/STS, and observed Kondo resonance states originated from the survived spin of NO.

We found three types of NO adsorbed states on the surface: two kinds of NO monomer (denoted as A and B), and a NO trimer. Monomer (B) could be produced from monomer (A) by applying a voltage pulse ($\sim \pm 300$ mV) onto the monomer (A). By conducting STS (dI/dV) measurements using a lock-in amplifier at 4.5 K, we observed dip and peak structures at 0 mV for monomer (B) and the trimer, respectively, whereas no structure was observed for monomer (A). From the temperature-dependent measurements, the dip and peak structures were attributed to Kondo resonance states. Besides, we observed sidebands at ±5 meV and ±36 meV for the trimer, which stemmed from the coupling of Kondo resonance with molecular vibrations. This study demonstrates the strong dependence of the Kondo resonance states of NO, i.e., the magnetic properties of the molecule, on the adsorbed states.

O 30.11 Mon 18:15 P1A

Setup for time-resolved photoemission electron microscopy of ferromagnetic surfaces and magnetization dynamics triggered by back-side illumination — •Maximilian Paleschke, Cheng-Tien Chiang, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Institute of Physics, Halle (Saale), Germany

Over the last 20 years, the growing interest in the field of ultrafast magnetism and spintronics sparked a demand for experimental techniques capable of detecting dynamical phenomena on the nanometer-femtosecond scale[1]. Our approach combines state-of-the-art time-resolved photoemission electron microscopy (tr-PEEM) with a back-side pumping geometry. A tunable laser system with MHz repetition rate and a wide selection of different wavelengths enhances the PEEM's capabilities by eliminating inadvertent effects like space charge broadening. The setup is optimized to image magnetic nanostructures using magnetic valence band dichroism in photoemission[2,3]. In this poster, we will present the experimental setup and the achieved temporal and spatial resolutions. First results for ultrathin films of Fe grown on MgO(001) will be discussed.

[1] A. Kirilyuk *et al.*, Rev. Mod. Phys. **82**, 2731 (2010)
[2] C. M. Schneider, G. Schönhense, Rep. Prog. Phys. **65**, 1785 (2002)
[3] W. Kuch, C. M. Schneider, Rep. Prog. Phys. **64**, 147 (2001)

O 31: Poster Session - Metal substrates: Structure, Epitaxy and Growth

Time: Monday 18:15–20:00 Location: P1C

O 31.1 Mon 18:15 P1C

Influence of strain on dendrite growth in battery materials — •Daniel Stottmeister and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

The growth of dendrites to this date represents a significant safety problem in the operation of high-performance batteries. Unraveling the underlying mechanics of dendritic growth has been the focus of many studies, and recent results strongly suggest that strain effects might influence the growth mechanism. Density functional theory (DFT) is a well-established method for the description of metal systems on an atomic level and can help to understand the underlying processes behind dendrite growth. In this contribution, ab initio calculations were performed in order to investigate the effects of strain on diffusion processes for a selection of promising battery materials such as lithium, sodium, and potassium. In order to address the possible influence of the electrochemical environment on the dendrite growth, first attempts to include the presence of electrolytes in the calculations will be presented.

O 31.2 Mon 18:15 P1C

Production and transfer of h-BN monolayers: Exploratory study — •Marco Thaler, Tobias Bonczyk, and Erminald Bertel — Physikalische Chemie, Universität Innsbruck, Österreich

Hexagonal Boron Nitride (h-BN) monolayers belong to the rapidly growing family of two-dimensional materials. h-BN is intensely studied, on the one hand as a template for graphene growth, on the other hand as a dielectric barrier in graphene-based electronic and spintronic devices. In electro-catalysis, h-BN can serve as support for active clusters, but is active also by itself[1,2]. Recently, h-BN monolayers were found to host defects acting as single-photon sources with excellent spectral properties[3]. In view of these diverse applications, an easy, clean, and reproducible procedure for h-BN synthesis and transfer is highly desirable. We present a simple, load-lock equipped UHV chamber allowing the preparation of Pt foils as recyclable templates and the deposition of h-BN monolayers. The morphology and cleanliness of Pt templates after various pretreatments is studied by AFM and XPS. h-BN deposition is monitored by XPS and different transfer protocols for the monolayers to metallic or dielectric substrates are evaluated.

[1] Elumalai, G. et al., Phys. Chem. Chem. Phys. **16**, 13755(2014).
[2] Lyalin, A. et al., The Chemical Record **16**, 2324(2016).
[3] Li, C. et al., Nanophotonics **8**, 2049 (2019).

O 31.3 Mon 18:15 P1C

Inverse melting of Ni on Re(0001) — Johannes Regel, •Torge Mashoff, and Hans-Joachim Elmers — Institut für Physik, Johannes Gutenberg-Universität, Mainz

Usually, cooling a metal sample down to cryogenic temperatures leads to an immobility of the surface atoms. In rare cases an opposite behavior has been observed under extreme conditions, where cooling leads to an increase in entropy and thus to a higher mobility of the surface atoms. This process is known as inverse melting. In our case a combination of a small force induced by the STM-tip and the weakened bonding between the Ni atoms results in mobile Ni atoms at island edges.

We prepare coverages between 0.1 ML and 10 ML of Ni on a Re(0001)-surface and investigate the mobility of the Ni atoms using scanning tunneling microscopy at temperatures between 4.8 K and room temperature. Sequences of STM-images show an increased mobility of Ni atoms at low temperatures.

O 31.4 Mon 18:15 P1C

$Al_2Cu(001)$ studied by photo electron spectroscopy — •Holger Schwarz[1], Niels Rösch[1], Stefan Püschel[2], Peter Gille[2], Marc Armbrüster[3], and Thomas Seyller[1] — [1]Institute of Physics, TU Chemnitz, Chemnitz, Germany — [2]Department of Earth and Environmental Sciences, LMU München, München, Germany — [3]Institute of Chemistry, TU Chemnitz, Chemnitz, Germany

Intermetallic compounds have received interest because of their performance as catalysts in, e.g., hydrogenation reactions. However, compared to the enormous number of surface studies on pure metals and on alloys, there are considerably fewer studies on the surface properties of intermetallic compounds. Recently, $Al_2Cu(001)$ showing a $(2\sqrt{2}\times\sqrt{2})R45^\circ$ reconstruction was studied using low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) in combination with ab initio calculations [1]. A structure model was derived which consists of a bulk termination with incomplete Al planes. The aim of our work is to further characterize the $Al_2Cu(001)$ surface by additional techniques, in particular X-ray photoelectron spectroscopy (XPS) and angle-resolved photoelectron spectroscopy (ARPES). The poster will present and discuss first results of our work, focusing on surface composition and structure as well as electronic structure.

[1] L. N. Serkovic Loli, et al., Phys. Rev. Lett. 108 (2019) 146101.

O 31.5 Mon 18:15 P1C

Structure analysis of ultrathin NaCl-layers on metallic substrates — •Kira Kolpatzeck, Ebru Ekici, Vijaya Begum, Markus Gruner, Rossitza Pentcheva, and Rolf Möller — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

To observe radiative transitions in molecules, single atoms or clusters it is necessary to decouple those from any metallic substrate. On the other hand, for surface science methods, such as scanning tunneling microscopy, a non-vanishing surface conductivity has to be ensured. Ultrathin insulating layers are the key to circumvent those two requirements. Therefore, we have studied the growth of ultrathin sodium chloride (NaCl) films with various layer thickness on different metallic substrates by low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) at low temperatures (8K and 80K). We could show that the evaporation of NaCl on Au(110) leads to the growth of NaCl islands of different height. The first two layers are showing a (1x4) superstructure rectangular to the missing-row reconstruction of the Au(110) surface. Incomplete growth structures like holes in the islands as well as the third sodium chloride layer show the well-known rectangular edge geometry. With the aid of DFT-calculations a first structure model could be found to explain the observed superstructure.

O 31.6 Mon 18:15 P1C

Surface structure and chemical composition of the Te covered $Au_{75}Ag_{25}(111)$ surface — •Tobias Kirschbaum, Tilman Kisslinger, Lutz Hammer, and M. Alexander Schneider — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

When depositing chalcogenides on clean transition metal surfaces the adsorbates coordinate substrate atoms to form a surface alloy or other surface structures [1,2]. The situation is unclear if a binary alloy functions as substrat. There, the chalcogenide has a variety of possibilities to bind within the surface and might be able to induce stoichiometries in the subsurface that differ from the bulk.

Here we present an investigation of the clean and Te covered $Au_{75}Ag_{25}(111)$ surface by means of room-temperature scanning tunneling microscopy (STM) and low-energy-electron diffraction (LEED). The clean $Au_{75}Ag_{25}(111)$ surface is that of a disordered substitutional alloy. Our LEED-IV analysis (R = 0.064) proves an enrichment in silver in the second layer to $\approx 50\%$, whereas the other layers stay nearly bulk-like within the errors. Upon deposition of 1/3 ML Te at 90 K and annealing to at least 473 K a $(\sqrt{3}\times\sqrt{3})R30^\circ$-structure forms. STM shows a honeycomb-like arrangement. A LEED-analysis confirms that this is a pure AgTe overlayer at hcp positions on a nearly bulk-like $Au_{75}Ag_{25}(111)$ crystal.

[1] Jiaqi et al., Surf. Sci., **669**, 198, 2018

[2] Liu et al., J. Phys. Chem. Lett., **10**, 1866, 2019

O 31.7 Mon 18:15 P1C

Scanning tunneling microscopy study of submonolayer growth of Mn_xAu_{1-x} on Cu(001) — •Ismet Gelen[1], Tauqir Shinwari[1], Yasser A. Shokr[1,2], Evangelos Golias[1], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Faculty of Science, Department of Physics, Helwan University, 17119 Cairo, Egypt

Mn_xAu_{1-x} exhibits many antiferromagnetic (AFM) phases. Mn_2Au is one of them that has a high Néel temperature ($\approx$ 1600 K) and, due to its noncentrosymmetric spin structure and metallic nature, is an interesting AFM material for spintronic applications. Here, we study the growth of Mn_xAu_{1-x} in the submonolayer (sub-ML) regime on Cu(001) by medium- and low-energy electron diffraction (MEED, LEED), Auger electron spectroscopy (AES), and scanning tunneling microscopy (STM). Different Mn concentrations ($x \approx 0.7-0.9$) and different thicknesses ($\approx 0.2-1.1$ ML) were studied, as monitored by AES. Mn and Au were coevaporated by electron bombardment on Cu(001) at room temperature (RT). The growth of thicker films showed MEED intensity oscillations up to around 9 ML. The LEED images display substrate patterns for thicknesses < 0.5 ML, while they display a $c(2\times2)$ structure for thicker sub-ML films. We observe Mn_xAu_{1-x} islands on Cu(001) for all sub-ML films with island sizes between $\approx 5\times5$ and 30×30 nm^2.

O 32: Poster Session - Organic Molecules on Inorganic Substrates: Adsorption and Growth

Time: Monday 18:15–20:00 Location: P1C

O 32.1 Mon 18:15 P1C

STM Investigations of Insulating Xenon Interfaces on Silver Surfaces as Low Interaction substrates for Advanced Carbene Studies — •Inga Langguth[1], Marvin Quack[1], Iris Trosien[2], Wolfram Sander[2], and Karina Morgenstern[1] — [1]Chair of Physical Chemistry I, Ruhr-University of Bochum, Germany — [2]Chair of Organic Chemistry II, Ruhr-University of Bochum, Germany

The outstanding high reactivity of carbene molecules is of central interest in catalysis and basic research. For the understanding of these reactive intermediates, scanning tunneling microscopy (STM) is a highly favorable technique to gain locally resolved insight into the electronic structure of carbenes and their precursors. For an unperturbed characterization of these molecules, advanced surface decoupling methods are needed, in order to exclude dominating surface influences. Hence, the strategy of this work is to mimic the low interaction conditions between carbenes and their chemical environment as present in rare gas matrices by preparation of an ultra-thin non-conducting rare gas interface. Thus, the consecutive adsorption of xenon (Xe) followed by fluorene based carbene precursors on silver single crystals is investigated by low-temperature STM in ultra-high vacuum. Kinetically restricted precursor molecules are found to dictate the rotational orientation of Xe domains.

O 32.2 Mon 18:15 P1C

Comparison of Donor-Acceptor Coupling Strength with

Chemisorption on Different Metal Substrates — •Qi Wang, Antoni Franco-Cañellas, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany

As crucial element in opto-electronic devices heterostructures are of pivotal importance. Here, we present a comprehensive study on the properties of a donor-acceptor (D-A) bilayer structure using X-ray photoelectron spectroscopy (XPS) and normal-incidence X-ray standing wave (NIXSW) measurements. Accordingly, an acceptor material-pentacene (PEN) and a donor material-perfluoropentacene (PFP) are chosen to build bilayer structures. PFP/PEN bilayers have been grown on Au(111) and Cu(111) substrates, i.e., coinage metal surfaces with different reactivity. By comparing the adsorption behavior of pentacene and its perfluorinated partner, we found that: i) on Au(111), the first layer (PEN) is physisorbed, whereas on Cu(111) the molecule-substrate interaction is much stronger, ii) the D-A bonding distances indicate that within the bilayer van-der-Waals interactions dominate.

O 32.3 Mon 18:15 P1C

The adsorption structure of acetophenone on Si(100) — •Paula L. Lalaguna[1,2], Paul T. P. Ryan[1,3], Procopi C. Constantinou[4], Matthias Muntwiler[5], Holly Hedgeland[6], Steven R. Schofield[4], and David A. Duncan[1] — [1]Diamond Light Source, Didcot, OX11 0QX, UK — [2]University of Glasgow, G12 8QQ, UK — [3]Imperial College London, SW7 2AZ, UK — [4]University College London, WC1H 0AH, UK — [5]Paul Scherrer Institute, 5232 Villigen, Switzerland — [6]The Open University, Milton Keynes, MK7 6AA, UK

Over the last decade, Moore's law has begun to slow as fundamental length scale limits are being reached in the utilization of Si for transistors ($\sim$14 nm)[1]. One potential method for delaying the end of Moore's law is to pattern Si surfaces with organic molecules, providing an accessible length scale in the order of a few ångstroms. However, in order to understand how these molecules interact and alter the Si substrate, high quality and high precision measurements are required. Here we will present one such study of Si(100) patterned with acetophenone by energy scanned photoelectron diffraction (PhD). Acetophenone is believed to anchor to the Si substrate via a strong covalent bond[2]. Utilizing PhD, we provide an insight into this anchoring, specifically measuring the Si-O bond length of the adsorbed molecule to a precision of a few hundredths of an ångstrom. [1] Nature 530, 144 (2016); [2] J. Phys. Condens. Matter 27, 054002 (2015).

O 32.4 Mon 18:15 P1C

Structure of tetracene films on hydrogen-passivated Si(111) and amorphous Si — •Hazem Aldahhak[1], Jens Niederhausen[2], Rowan W. MacQueen[2], Wolf Gero Schmidt[1], Klaus Lips[2], and Uwe Gerstmann[1] — [1]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany — [2]Institute for Nanospectroscopy, Helmholtz-Zentrum Berlin für Materialen und Energie GmbH, Berlin, Germany

The properties of the Tetracene (Tc)-Silicon (Si) interfaces are of particular interest when trying to augment the Si solar cells by singlet fission in Tc. Here, we combine Near-edge X-ray absorption fine structure (NEXAFS), x-ray photoelectron spectroscopy (XPS) as well as density functional theory (DFT) calculations to elucidate the structure of the first Tc monolayer on hydrogen-passivated Si(111) and amorphous Si (H:a-Si). Typically, the first monolayer is hampered by the significant dewetting tendency of Tc at room temperature. Here, we present a selective study using cooling to limit the thermal energy of the Tc molecules during growth and measurements. We find that the first Tc monolayer on cooled substrates exhibits a mixture of the bulk-like Tc (Tc I) and the surface-induced thin film (Tc II) phases. The DFT calculated total-energies and angle-dependent NEXAFS fingerprints support the measurements. Further heating of the cool Tc/H:Si(111) film to room temperature indicates structural changes towards lower Tc inclination, rendering the appearance of this phase to rely on sufficient amount of thermal energy being available.

O 32.5 Mon 18:15 P1C

Adsorption of miRNA molecules on metal surfaces studied by STM — •Miriam Meyer[1,2], Christophe Nacci[1], Grant J. Simpson[1], Oliver Werzer[2], Andreas Zimmer[2], and Leonhard Grill[1] — [1]Institute of Chemistry, University of Graz, Austria — [2]Institute of Pharmaceutical Sciences, University of Graz, Austria

In solution, microRNAs and protamine spontaneously form nanoparticles, which are auspicious candidates for the treatment of various diseases [1]. This self-assembly process is induced by strong electrostatic interactions. To deliberately modify this interplay, accurate knowledge of the molecular interactions at the single molecule level is desired. The deposition of microRNA molecules onto a metallic surface is done via electrospray ion beam deposition (ES-IBD). This method allows for the clean and intact transfer of large molecules onto a surface in ultrahigh vacuum (UHV) [2]. The adsorption geometry of microRNA is dependent on the kinetic energy with which it impinges on the surface. We have then investigated the adsorption of these molecules on metallic substrates by scanning tunneling microscopy (STM). The adsorption is compared for different preparation techniques, ES-IBD and drop-casting.

Acknowledgements: The financial support from the Doctoral Academy NanoGraz is highly acknowledged by the Grill and the Zimmer group.

[1] M. Junghans, J. Kreuter, and A. Zimmer, Nucleic Acids Res 28, 10 (2000). [2] Z. Deng, N. Thontasen, N. Malinowski, G. Rinke, L. Harnau, S. Rauschenbach, and K. Kern, Nano Lett 12, 5 (2012)

O 32.6 Mon 18:15 P1C

Investigation of the formation of densely packed caffeine monolayers on Au(111) — Malte G.H. Schulte[1,2], Andreas Jeindl[3], •Julian A. Hochhaus[1], Ismail Baltaci[1,2], Marie Schmitz[1,2], Ulf Berges[1,2], Oliver T. Hofmann[3], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1, TU Dortmund, Otto-Hahn-Str. 4, D-44221, Dortmund, Germany — [2]DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44221, Dortmund, Germany — [3]Institut für Festkörperphysik, NAWI Graz, Technische Universität Graz, Petersgasse 16, A-8010 Graz

In this study, we investigate caffeine monolayers on Au(111). Caffeine is well known for influencing the human central nervous system, therefore knowledge of the structural behaviour of caffeine is essential.

Low-energy electron diffraction (LEED), scanning tunneling microscopy (STM), and x-ray photoelectron spectroscopy (XPD) have been used to examine the formation of caffeine on Au(111). In addition, density functional theory (DFT) calculations were carried out which allow conclusive interpretation as well as a comparison with the measured data.

We observed the caffeine molecules to be adsorbed in a quasi-hexagonal formation similar to the high-temperature α-phase, comprising two domains. The DFT calculations suggested a unit cell containing three molecules, the theoretically calculated structure is in excellent agreement to the experimental measured LEED and STM pattern, as well as to the measured XP-spectra. Furthermore, within the XPS measurements, no strong adsorbate-surface interaction was found.

O 32.7 Mon 18:15 P1C

Atomistic Modeling of the Synthesis of New Carbon Structures by Surface-Assisted Cyclodehydrogenation — •Florian Wullschläger, Robert Maidl, Sebastian Gsänger, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

A new synthesis route for chirality-pure single-walled carbon nanotubes (SWCNTs) has been proposed, which relies on the surface-catalyzed cyclodehydrogenation (CDH) of appropriately designed precursor molecules on Au(111) [1] followed by a new roll-up synthesis technique. Using a hierarchy of methods, from atomistic force-fields to quantum-chemical density-functional theory (DFT) calculations and combining them in QM/MM approaches, we studied the SWCNT formation process in the gas phase and on the Au(111) surface. We were able to identify the crucial reaction step and we could show that structural hindrance leads to an interruption of the current CDH process. The same approach of on-surface cyclodehydrogenation can be used for the synthesis of new forms of carbon allotropes like nanocones, bowls or spoons. First insights into the formation process of nanocones with a porphyrin unit at the tip on Pt(111) surfaces will be shown.

[1] J.R. Sanchez-Valencia, T. Dienel, O. Gröning, I. Shorubalko, A. Mueller, M. Jansen, K. Amsharov, P. Ruffieux, R. Fasel, Nature **512** (2014) 61–64.

O 32.8 Mon 18:15 P1C

STM study of CuPC molecules codeposited with C60 on a Au(110) surface — •Hüseyin Azazoglu, Philip Kapitza, and Rolf Möller — Fakultät für Physik/Cenide, Universität Duisburg-Essen, Germany

Here, we show an STM study of CuPc molecules codeposited with C60 on a Au(110) surface at room temperature. It turns out that C60 molecules form close packed islands. In between the CuPc molecules form ordered rows along the rows of the Au(110) surface. The results are compared to previous for C60 on Au(110) [1], [2] and the codeposition of CuPc and C60 on Au(111) [3], [4].

[1] J. K. Gimzewski et al. J. Vac. Sci. Technol., B, 12, 2153 (1994).
[2] J. K. Gimzewski et al. Phys. Rev. Lett., 72, 1036 (1994).
[3] M. Stöhr et al. Adv. Funct. Mater., 11, 175 (2001).
[4] M. Fendrich et al. Phys. Rev. B, 73, 115433 (2006).

O 32.9 Mon 18:15 P1C

A highly ordered commensurate structure of merocyanine tetramers on Ag(100): STM- and SPA-LEED-investigations — •Anna J. Kny[1], Niklas Humberg[1], Dirk Hertel[2], Klaus Meerholz[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany — [2]Department Chemie, Universität zu Köln, Germany

Vacuum deposited films of the merocyanine molecule 2-[5-(5-dibutylamino-thiophen-2-yl-methylene)-4-*tert*-butyl-5*H*-thiazol-2-ylidene]-malononitrile (HB238) have been investigated in the context of organic solar cells [1]. Although the specific structural order in these films is important for photovoltaic properties, only very little is known about the adsorption, ordering and film growth of this molecule on surfaces. Therefore, we investigated monolayers of HB238 on a Ag(100) surface by SPA-LEED and STM.

When HB238 is deposited onto the Ag(100) at room temperature and then cooled down immediately to 34 K, the formation of two different phases can be observed. Directly after growth, a phase with chain-like aggregates and only short-range order prevails. Upon annealing at 68 K, it transforms into a second highly ordered phase with a commensurate superstructure. This phase is composed of homochiral tetramers of HB238 molecules. The thiophene and thiazole units are bonded to the Ag(100) surface yielding a flat lying molecular orientation. Upon further annealing dewetting and cluster formation occurs.

[1] JACS 137 (2015) 13524.

O 32.10 Mon 18:15 P1C

On-surface synthesis of BN-doped carbon nanostructures — •Tobias Weiss[1], Aleksandr Baklanov[1], Knud Seufert[1], Johannes Küchle[1], Marc Gonzalez Cuxart[1], Francesco Allegretti[1], Jacopo Dosso[3], Davide Bonifazi[3], Nicolas Bachellier[2], Matthias Muntwiler[2], and Willi Auwärter[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]Paul Scherrer Institute, Villigen, Switzerland — [3]School of Chemistry, Cardiff University, Cardiff, UK

Hybrid hexagonal boron nitride - carbon (BNC) layers provide promising properties for potential applications in electronics and gas adsorption [1]. Recently, BNC-based tectons were introduced to assemble covalent networks and supramolecular arrays on metal surfaces [1-3].

Here, we report the formation of BNC nanostructures on Ag(111) and Au(111) via bottom-up synthesis from borazine derivatives in UHV. We employed both a dehydrogenation approach using a BN-doped coronene derivative and an Ullmann-type coupling approach using a chlorine- and bromine-functionalized hexaphenylborazine. The resulting 2D structures, the sequential dehalogenation steps, and the Ullmann coupling are investigated with (fast) XPS and STM. Additionally, we probed the CO, CO_2, and borazine adsorption on the BNC structures, revealing the inertness of the borazine core.

[1] M. M. Lorenzo-García et al., Chimia, 2017 **71**, 9, 550-557.
[2] C. Sánchez-Sánchez et al., ACS Nano, 2015 **9**, 9, 922.
[3] M. Schwarz et al., Chem. Eur. J., 2018 **24**, 9565.

O 32.11 Mon 18:15 P1C

Influence of polarity on adsorption and growth of conjugated organic molecules on inorganic substrates — •Mila Miletic[1], Karol Palczynski[1,2], and Joachim Dzubiella[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universität, Freiburg, Germany

We present atomistically resolved computer simulations of the vapor-phase deposition and layer-by-layer growth of organic molecules on inorganic substrates. We study the effects of chemical tuning of the organic para-sexiphenyl (p-6P) molecule on the nucleation and growth on amorphous silicon dioxide: We characterize surface diffusion barriers and the growth of layers of upright standing molecules once a critical coverage is achieved.

Crystalline islands of standing molecules form as a result of a collective reorientation of clusters of flat-lying molecules. The growth proceeds by molecules attaching to the clusters and ascending over the terraces to integrate into the existing cluster units. We describe the crossing mechanisms and quantify the barriers for descending over the terraces. Our simulations reveal some of the interesting features of molecular surface kinetics and binding. The results shall be useful to control thin film growth in order to obtain desired structures and properties in experiments.

O 32.12 Mon 18:15 P1C

Explaining surface polymorphism of acenequinones on Ag(111) with SAMPLE — •Andreas Jeindl[1], Lukas Hörmann[1], Jari Domke[2], Alexander T. Egger[1], Falko Sojka[2], and Oliver T. Hofmann[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Understanding (and modifying) the formation of surface polymorphs is still not straightforward as it is hardly known why specific structures form. Normally, the exponential growth of possible polymorphs with system size prohibits rigorous computational studies, that could explore the full configurational and thermodynamic search space. The peculiar physics that govern the interface formation, however, allow to reduce the search space and make the problem tractable.

In this contribution we use SAMPLE, a program package developed to efficiently predict energies for commensurate surface layers. It employs machine learning to suitably fit a physical energy model which consists only of molecule-substrate and molecule-molecule interactions. We perform a comprehensive structure search for a homologous series of acenequinones on Ag(111) to explain the mechanisms driving the formation of surface polymorphs and compare some of our results to experimental observations. Our research shows that the structures differ fundamentally. Insights from our model suggest that this originates mostly from the van-der-Waals interaction of the substrate with the backbone as well as the fact that upon increasing the backbone length, vdW interactions between the molecules become more important.

O 32.13 Mon 18:15 P1C

The Effect of Plasma Treatment of Gold Electrodes on the Molecular Orientation of CuPc films — •Felix Widdascheck, Michael Kothe, Alrun A. Hauke, and Gregor Witte — Philipps Universität Marburg

Gold is a commonly used material for many organic electronic device electrodes due to its chemical stability and high work function, which is required for p-type semiconductors. The orientation and morphology of organic semiconductors deposited on such electrodes often depends crucially on the cleanliness of the Au surface. In this study, we examine the effect of a common cleaning method, namely oxygen plasma cleaning, on sputter-deposited polycrystalline Au electrodes and subsequently deposited copper-(II)-phthalocyanine (CuPc) films. Using X-ray diffraction (XRD), atomic force microscopy (AFM) and near-edge X-ray absorption fine structure (NEXAFS) measurements, we show that the metastable Au oxide typically formed during an oxygen plasma cleaning process significantly impacts the molecular orientation and morphology in CuPc thin films, forcing molecules to adopt an upright orientation. We further demonstrate that the typical recumbent orientation of CuPc adopted on clean polycrystalline Au can be achieved by an additional annealing step after oxygen plasma treatment of the Au electrode that causes a decomposition of the gold oxide.

O 33: Poster Session - Plasmonics and Nanooptics: Applications and other Aspects

Time: Monday 18:15–20:00 Location: P1C

O 33.1 Mon 18:15 P1C

Shape optimization of magneto-optic metasurfaces for enhanced Faraday rotation — •Thomas Kiel[1], Paris Varytis[1,2], Bettina Beverungen[1], Philip Kristensen[1], and Kurt Busch[1,2] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin — [2]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin

Magneto-optic nanostructures and the associated effects such as Faraday rotation enable nonreciprocal devices, i.e. miniaturized photonic isolators etc. Although a large Faraday rotation is reported for various nanophotonic geometries, a simultaneous high transmittance is hard to achieve due to material losses. To overcome this limitation, it has been suggested to use a Huygens' metasurface composed of periodically arranged Ce:BIG nanodiscs embedded in SiO_2 [1].

Building on this original idea, we present here how to further increase the Faraday rotation with shape-optimized nanodiscs. The optimization is based on numerical solutions of the Maxwell equations using the discontinuous Galerkin time-domain method [2] with an extension to anisotropic materials [3] in order to model the Ce:BIG. We show that even with a simple optimization strategy, a doubling of the possible Faraday rotation is achievable for nearly the same effective optical thickness of the metasurface.

[1] A. Christofi et al., Opt. letters **43**, 1838 (2018)
[2] K. Busch et al., Laser & Photonics Rev. **5**, 773 (2011)
[3] J. Alvarez et al., IEEE Ant. Wirel. Propag. Lett. **11**, 1182 (2012)

O 33.2 Mon 18:15 P1C

Formation of conducting polymer by plasmon-induced photopolymerization — •Marisa Hoffmann[1,2], Anja Maria Steiner[1], Charlene Ng[1], and Andreas Fery[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [2]Department of Physical Chemistry of Polymeric Materials, TU Dresden, Germany

Metal nanoparticles (NPs) exhibit localized surface plasmon resonances (LSPRs). LSPRs of NPs can be utilized to induce various kinds of reactions in the vicinity of the NP surface, e.g. plasmon-induced polymerizations. By this, metal-polymer nanostructures can be created which can combine conducting polymers like polypyrrole with plasmonic gold NPs. Despite the potential of those hybrid materials, the mechanisms behind the plasmon-induced polymerizations are not fully understood. How LSPRs contribute to these reactions is still at debate and requires further investigations.

In this work, we investigate the mechanism of the formation of polypyrrole at the interface between a single plasmonic gold NP and a planar TiO2 surface upon visible light illumination. The parameters for the plasmon-induced oxidative polymerization process are evaluated by UV-Vis-NIR-spectroscopy, Scanning Electron Microscopy (SEM), conductivity measurements and Kelvin Probe Force Microscopy (KPFM). The results thereof are subsequently used to transfer the plasmon-induced photopolymerization from single particle level to NP lines, leading to a scalable bottom-up method for the fabrication of functional electronic devices.

O 33.3 Mon 18:15 P1C

A tuneable photochromic lens for the visible — •Till Leuteritz and Stefan Linden — Universität Bonn, Deutschland

Tuneable metasurfaces have attracted considerable attention in recent time. In order to modify their optical properties, different approaches like dynamic carrier doping, phase change materials, mechanical deformation and electrical tuning by capacitances have been used and different tunable devices like microwave metalenses and light controllable reflections have been demonstrated [1]. In our work, we employ the photochromic material XDTE for optical switching. Under incident of uv or red light it undertakes a ring-closing or opening transition of a carbon ring, respectively. This leads to a change of refractive index, which is used to shift the plasmonic resonance of V-shaped nanoslot antennas. Thus the phase of the emitted light of each antenna can be tuned and hence the focal length of the lens.

XDTE has the advantages, that it can be easily spin coated on a sample during fabrication and that it can undergo a large number of cycling transitions without degradation.

[1] He, Qiong, et al., AAAS Research Volume 2019, Article ID 1849272

O 33.4 Mon 18:15 P1C

Surface roughness in finite element meshes — •Fabian Loth[1,2], Thomas Kiel[1], Kurt Busch[1,2], and Philip Kristensen[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin — [2]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin

Surface roughness at the nanoscale is of great importance in nanooptics since it can have a significant effect on the optical properties of photonic and plasmonic nanostructures. We present a practical approach for constructing meshes of general rough surfaces with given autocorrelation functions based on the unstructured meshes of the nominal smooth surfaces. The approach builds on a well-known method to construct correlated random numbers from white noise using a decomposition of the autocorrelation matrix [1]. The resulting mesh can be used in numerical methods, such as the discontinuous Galerkin time domain method [2], to compute the electromagnetic fields and derived physical observables such as scattering and absorption cross sections. Apart from nanooptics, the approach can be used in a broad range of numerical methods in various fields of science and engineering.

[1] H. Kaiser, K. Dickman, Psychometrika **27**(2), 179–182 (1962)
[2] K. Busch et al., Laser & Photonics Rev. **5**, 773 (2011)

O 33.5 Mon 18:15 P1C

THG imaging with nonlinear dielectric metalenses — •Christian Schlickriede[1], Sergey Kruk[2], Basudeb Sain[1], Yuri Kivshar[2], and Thomas Zentgraf[1] — [1]Universität Paderborn, Paderborn, Deutschland — [2]Australian National University, Canberra, Australien

In our approach we fabricate a new kind of nonlinear all-dielectric metalenses of sub-micrometre thickness, which are working in the nonlinear regime by third-harmonic frequency conversion for the incident near-infrared light. Therefore, we use wavefront control via the nonlinear Huygens principle emerging from the different nanopillar geometries. In the experiments, we determine the formation of the real and virtual focal planes for illumination with Gaussian beams and we demonstrate nonlinear imaging abilities that giving rise to real and virtual images of real objects at visible wavelengths. Most importantly, we found that the nonlinear image evolution is not governed by the conventional lens equation but by a modified version of it.

O 33.6 Mon 18:15 P1C

Investigating the coupling of plasmonic metasurfaces and WS_2 — •Florian Spreyer and Thomas Zentgraf — Paderborn University, Paderborn, Germany

Recent studies show great potential for transition metal dicholgenides (TMD) and their optical application. By downscaling TMD*s to a monolayer flake of atomical thickness, TMD*s become semiconductors with a direct band gap. These monolayer flakes can be used to fabricate hybrid metasurfaces combining plasmonic nanoantennas and a monolayer of TMD. Hybrid metasurfaces with TMD*s with a band gap in the visible regime show great potential for an enhanced light matter interaction for nonlinear applications. Here we, investigate the coupling between a metasurface made of plasmonic gold nanoantennas and a monolayer of tungsten disulfide (WS_2). By using photoluminescence and nonlinear measurements, we present recent results of the characterization of WS_2 flakes with plasmonic nanoantennas fabricated on top of monolayer WS_2 flakes.

O 33.7 Mon 18:15 P1C

Optical trapping by silicon based high numerical aperture metalenses — •Rene Geromel, Basudeb Sain, Christian Schlickriede, Michael Tiemann, and Thomas Zentgraf — Universität Paderborn, Paderborn, Deutschland

In this work, we present a high numerical aperture metalens that focuses near-infrared laser light to optically trap dissolved polystyrene microbeads with different diameters. To increase the numerical aperture of our metalenses, the silicon antennas are embedded in porous silicon dioxide. The porous coating also acts as a protective layer and allows us to place the metalens directly inside the particle solution. In order to achieve an appropriate numerical aperture, we use the concept of a geometric phase emerging from the configuration of rotated silicon meta-atoms. Depending on the incident circular polarization of light, the phase profile can be switched between convex and concave which makes this lens a suitable candidate for polarization dependent particle drag and drop. In the experiments, we investigate the trap stiffness and potential of the metalenses.

O 33.8 Mon 18:15 P1C

Large-scale optical programming of phase-change material metasurfaces — •Laric Bobzien, Andreas Hessler, Julian Hanss, Thomas Kalix, Matthias Wuttig, and Thomas Taubner — Institute of Physics (IA), RWTH Aachen

Metasurfaces have the ability to arbitrarily manipulate light with the help of subwavelength, periodically arranged, scatterers. Functionalities like beam steering, lensing and holography have been realized. However, once fabricated, metasurfaces remain passive, i.e. they have one fixed functionality. They can be rendered active and programmable by including active materials like phase-change materials (PCMs) [1] which have large optical contrast between their metastable crystalline and amorphous phases.

A home-built setup for optical switching of PCMs was prevously applied to great success for reversible switching of ultra-confined surface phonon polariton resonators [2], advanced optical programming of individual antennas in metallic metasurfaces [3] and all-dielectric Huygens' metasurfaces [4]. So far, this setup has however been limited to small-scale programming of 20x20 μm^2. Here, we present our work on re-designing the switching setup for larger-scale optical programming. In the future, we hope to apply the improved setup to realize advanced functionalities like switching between holographic images.

[1] M. Wuttig et al., *Nature Photonics* **11**, 465-476 (2017)
[2] P. Li et al., *Nature Materials* **15**, 870-875 (2016)
[3] A.-K. U. Michel et al., *Advanced Materials* **31**, 1901033 (2019)
[4] A. Leitis et al. *submitted to Advanced Functional Materials*

O 33.9 Mon 18:15 P1C

Revealing time resolved electron-electron interactions on the nanoscale with ultrafast electron microscopy — •Andreas Wöste[1], Germann Hergert[1], Jan Vogelsang[2], Dong Wang[3], Petra Gross[1], and Christoph Lienau[1] — [1]Universität Oldenburg — [2]Lund University — [3]TU Ilmenau

New spectroscopic methods providing high spatial and temporal resolution are needed to improve our understanding of the dynamics of electrons, nuclei and their spin excitations on the nanoscale. Recently ultrafast point-projection electron microscopy (UPEM) emerged as a promising approach. Here ultrashort electron wavepackets are photoemitted from a metal nanotaper by fs laser pulses. The time resolution of the laser pulses is preserved by an arbitrarily small emitter-sample distance that makes electron pulse broadening negligible. Measuring the complete electron momentum by spatially resolved time of flight detection allows mapping of the electron beam-sample interactions. Here we have employed UPEM for probing the photoemission of electrons from a gold nanoresonator with 30fs temporal and 25nm spatial resolution. We compare our experimental results with numerical simulations to reconstruct the trajectories and the contributing forces. We show how the Coulomb interactions between a single probe electron and photemitted electrons from the sample governs the time-dependent image contrast in UPEM. Our results suggest that UPEM can provide a direct measurement of the time-dependent local charge density, opening up highly interesting new perspectives for probing various types of light-induced charge-transfer processes in nanoystems.

O 33.10 Mon 18:15 P1C

Nonreciprical Polarization Encryption of Holographic Images by Plasmonic Metasurfaces — •Daniel Frese[1], Qunshuo Wei[2], Yongtian Wang[2], Lingling Huang[2], and Thomas Zentgraf[1] — [1]Paderborn University, Warburger Str. 100, 33098 Paderborn, Germany — [2]Beijing Institute of Technology, 100081, Beijing, China

Metasurfaces provide high flexibility in tailoring optical wavefronts within subwavelength dimensions. However, two-dimensional metasurfaces consisting of nanostructures exhibit only weak spatial asymmetry perpendicular to the surface. Hence, the transmission properties are the same if one illuminates the metasurface from the front or the backside. To realize asymmetric transmission properties, we designed and fabricated a metasurface hologram consisting of two stacked layers of plasmonic meta-atom arrays, which allows full spatial phase and amplitude control of the transmitted light. The pixel-by-pixel encoded Fourier-hologram appears in a particular linear cross-polarization channel and disappears if one flips the sample around, illuminating the metasurface from the backside. This concept opens up new possibilities in information processing, designing security features, as well as nonreciprocal polarization optics.

O 33.11 Mon 18:15 P1C

Switchable plasmonic metasurfaces using the polymer PEDOT — •Juliane Ratzsch, Tobias Pohl, Andy Steinmann, Florian Sterl, Jinglin Fu, Mario Hentschel, and Harald Giessen — 4th Physics Institute, University of Stuttgart, Germany

Metasurfaces offer a wide range of interesting applications, such as metalenses, beam steering, and holograms. We have realized an electrochemically switchable metasurface, using plasmonic gold nanoantennas covered with the polymer PEDOT.

PEDOT changes its refractive index upon oxidation and reduction, and thus shifts the resonance of the nanoantenna array. This is achieved by applying small voltages in the range of -1V to 1V, and is reversible over many cycles. This enables us to switch on and off the desired functionality of the metasurface, which is designed to perform at a specific wavelength.

We have achieved a resonance shift of 130 nm, at switching times in the order of 10 seconds. This will enable us to apply this concept to a beam-steering metasurface, designed with the geometric phase approach, and thus realize an electrically switchable microscale beam-steering device.

O 34: Poster Session - Topological Insulators

Time: Monday 18:15–20:00 Location: P1C

O 34.1 Mon 18:15 P1C

Dirac-like Electrons in a Two-Dimensional Indium Layer on SiC(0001) — •Maximilian Bauernfeind[1], Jonas Erhardt[1], Philipp Eck[2], Victor Rogalev[1], Jörg Schäfer[1], Domenico Di Sante[2], Giorgio Sangiovanni[2], and Ralph Claessen[1] — [1]Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany — [2]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany

Mono- and sub-monolayer of In deposited on semiconducting or insulating substrates show a wide range of different surface reconstructions with unique electronic configurations. So far, none of them has been demonstrating Dirac-like electrons. Here we report first experimental results of an In (1×1) phase on SiC(0001) which clearly exhibits a linear band dispersion with Dirac points at the K/K' points in the hexagonal Brillouin zone in angle-resolved photoelectron spectroscopy (ARPES). Density functional theory (DFT) gives a remarkably good agreement and predicts a topologically non-trivial gap of approximately 50 meV at the K points rendering it applicable for room temperature devices. A sensitive parameter in DFT is the bonding distance between the In layer and the substrate which determines the non-trivial topology of this system. Additionally, the stabilization of the In layer on SiC leads to the surface Rashba effect and causes a large splitting of the valence band at the K points with strong out-of-plane spin polarization as predicted by theory.

O 34.2 Mon 18:15 P1C

Domain walls as possible realization of edge state coupling in a quantum spin Hall insulator — •Raul Stühler[1], André Kowalewski[1], Felix Reis[1], Johannes Weis[1], Joerg Schaefer[1], Gang Li[2], Werner R. Hanke[1], Dimitri Jungblut[1], Benedikt Scharf[1], Fernando Dominguez Tijero[1], Ewelina M. Hankiewicz[1], and Ralph Claessen[1] — [1]Universität Würzburg, Germany — [2]ShanghaiTech University, China

The recently discovered monolayer system bismuthene/SiC(0001) is a promising candidate for the realization of a room temperature quantum spin Hall (QSH) effect. Previous experiments have established a large fundamental band gap (0.8 eV) and the existence of one-dimensional metallic edge states [1]. As expected for a QSH insulator, the electronic edge channels do not show any signs of backscattering from kinky edge sections that would manifest in interference phenomena. Notwithstanding, topological protection against defect scattering may become lifted when two helical edge channels are brought into direct proximity, resulting in quantum interference. By scanning tunneling microscopy we study phase-slip domain boundaries (DB) with limited longitudinal extent. By spectroscopic means we scrutinize quasiparticle interference along these one-dimensional topographic defects that points towards a linear electronic dispersion strongly reminiscent of a Fabry-Pérot resonator. We discuss our findings as possible quantum interference between coupled helical edge states formed in the vicinity of a DB.

[1] F. Reis et al., Science 357, 287 (2017)

O 34.3 Mon 18:15 P1C

Topographic and electronic surface characterization of Bi_2Te_3-derivatives with periodic Mn sub-lattices via STM/STS — CHRISTIAN SALAZAR[1], •VLADISLAV NAGORKIN[1], ALEXANDER ZEUGNER[3], ANNA ISAEVA[1,2,3], BERND BÜCHNER[1,2], and CHRISTIAN HESS[1] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Faculty of Physics, Technische Universität Dresden, Germany — [3]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Germany

Materials combining topological surface states and intrinsic magnetism have gained great attention due to the possibility to be a platform to host tunable topological matter. Here we characterized topographically and spectroscopically two possible candidates through scanning tunneling microscopy. The studied compounds are Bi_2Te_3-derivatives with periodic Mn sub-lattices, i.e. $MnBi_2Te_4$ and $MnBi_4Te_7$. The two sample-types are composed on the one hand by only septuple layers ($MnBi_2Te_4$), and on the other hand by alternation of Bi_2Te_3-quintuple and septuple layers ($MnBi_4Te_7$). Single crystals of the van der Waals layered materials have been cleaved in cryogenic vacuum at 5 K and subsequently measured. Different characteristic surfaces were identified and spectroscopic data for the different materials and surfaces will be discussed.

O 34.4 Mon 18:15 P1C

Macroscopic investigation of conducting Na_2IrO_3 surfaces prepared in UHV — •MÁTÉ STARK[1], THOMAS DZIUBA[1], INA PIETSCH[2], PHILIPP GEGENWART[2], and MARTIN WENDEROTH[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Lehrstuhl für Experimentalphysik VI, Zentrum für elektronische Korrelationen und Magnetismus, Universität Augsburg, Germany

Na_2IrO_3 is a prototypical material in the honeycomb iridate family, which has also been proposed theoretically to exhibit topological protected surface states [1]. Experimental evidences for such surface states are lacking, possibly because of the high reactivity of Na_2IrO_3 in air, leading to rapid degradation of its surface. To overcome this problem we evaporated gold contacts and cleaved the crystal in UHV. We studied the electrical conductivity of the uncleaved and cleaved surface as well as of the surface after degradation in air as function of temperature between 100 K and 300 K, and compared the results with the conductivity of the bulk. The freshly cleaved crystal showed in contrast to the previously reported semiconductor-like behaviour a saturation of the sheet resistance at about 2,9 kΩ at low temperatures [2]. After the degradation of the surface in air, the conductivity of the surface decreased at low temperatures, and we measured a general change in the temperature dependence compared with the freshly cleaved surface. Conclusively we report a conducting surface on the freshly cleaved Na_2IrO_3 surface. **References**: [1] Phys. Rev. **108**, 106401 (2012), [2] Phys. Rev. **B82**, 064412 (2010)

O 34.5 Mon 18:15 P1C

Combined AFM/STM investigation of the topological insulators Bi_2Se_3 and $TlBiSe_2$ — •ADRIAN WEINDL, FELIZITAS LUISA KOLB, ALEXANDER LIEBIG, and FRANZ J. GIESSIBL — Institute of Experimental and Applied Physics, University of Regensburg, Universitätsstraße 31, D-93053 Regensburg, Germany

Topological insulators (TIs) are a class of materials whose bulk system is insulating, whereas the surface houses topologically-protected metallic states. This enables investigation of the surface via scanning tunneling microscopy (STM). The observed structure of the conducting surface states depends on the atomic structure of the surface and can be influenced by introduction of magnetic perturbations as demonstrated on the materials Bi_2Se_3 and Bi_2Te_3 [1,2]. After cleaving in vacuum, the surface of the TI $TlBiSe_2$ is terminated by half a monolayer of Tl atoms [3], which leads to the absence of a trivial surface state that was predicted for a completely filled Tl layer on the surface [4]. Simultaneous STM and atomic force microscopy (AFM) measurements on $TlBiSe_2$ yielded very distinct results. While in the STM images, the conducting surface states had a worm-like structure, atomic resolution of the surface atoms was possible in AFM [3]. Here, we evaporate single iron atoms onto the surfaces of Bi_2Se_3 and $TlBiSe_2$ to study the connection between surface structure, magnetic perturbations and electronic properties of TIs by a combination of AFM and STM measurements. [1] J. Honolka et al., PRB 108, 256811 (2012) [2] T. Eelbo et al., PRB 89, 104424 (2014) [3] F. Pielmeier et al., New J. Phys. 17, 023067 (2015) [4] B. Singh et al., PRB 93, 085113 (2016)

O 34.6 Mon 18:15 P1C

Photoemission Study on the Three Dimensional Topological Insulator HgTe(001) — •JULIA ISSING[1], RAPHAEL CRESPO VIDAL[1], LUKAS LUNCZER[2], LENA FÜRST[2], SIMON MOSER[3], HARTMUT BUHMANN[2], LAURENS W. MOLENKAMP[2], HENDRIK BENTMANN[1], and FRIEDRICH REINERT[1] — [1]Experimental Physics VII, University of Würzburg — [2]Experimental Physics III, University of Würzburg — [3]Experimental Physics IV, University of Würzburg

Mercury Telluride (HgTe) is a paradigmatic topological material that plays a key role in the exploration of topological physics in solids. For example, it is known to behave as a topological insulator under tensile strain and as a Weyl semimetal under compressive strain. In this contribution, we present the chemical and structural characterization of the (001)-surface of HgTe films grown by molecular beam epitaxy. The films are grown along the (001)-direction on a CdTe(001)-substrate, which induces a tensile strain. By means of LEED, we studied the surface geometric structure indicating a (2x1) reconstruction. Furthermore, the chemical composition of HgTe films is examined with XPS. The topologically non-trivial electronic structure was investigated by studying the angle resolved valence-band photoemission spectra of HgTe(001) using excitation with HeI_α as well as synchrotron radiation.

O 34.7 Mon 18:15 P1C

Photoelectron spectroscopy on thin Fe(Se,Te) superconductor films on Bi-based topological insulators — •PHILIPP KAGERER, THIAGO R. F. PEIXOTO, SIMON MÜLLER, ALI ALJANABI, CELSO FORNARI, HENDRIK BENTMANN, and FRIEDRICH REINERT — Experimental Physics VII, Julius Maximilian University of Würzburg

It has been shown that the electronic properties of thin layers of Fe-based superconductors can be manipulated by the choice of the substrate material. This includes an enhancement of T_c, *e.g.* as reported on $SrTiO_3$, as well as possible novel topological phases [1,2]. Owing to its simple cubic structure and good growth properties, thin layers of Fe(Se,Te) on a Bi-based three-dimensional topological insulator (TI) pose a promising platform for the research on superconductor-TI interface systems. Here we report on the epitaxial growth and characterization of thin layers of Fe(Se,Te) on the nearly lattice matched quaternary $(Bi,Sb)_2(Se,Te)_3$ TI single-crystal. LEED and XPS experiments, as well as STM and STS measurements, confirm the formation of a few monolayers of Fe(Se,Te) on top of the TI substrate. Using ARPES, we show the arising of the FeSeTe valence bands near the Fermi level, along with the heavily n-doped band structure of the underlying TI. In addition, photon-energy-dependent and resonant measurements using synchrotron radiation allow a distinction between substrate and overlayer bands, and show indications for strong electron correlation and a Hubbard-gap in the material.

[1] Liu D.F., Nat comm 3, 931(2012)

[2]Beenakker, C.W.J., Annu. Rev. Condens. Matter. Phys., 4 (2013)

O 34.8 Mon 18:15 P1C

Scanning tunneling Microscopy on the Magnetic Topological Insulator $MnBi_2Te_4$ — •PHILIPP KÜPPERS[1], GUNTHER SPRINGHOLZ[2], OLIVER RADER[3], MARCUS LIEBMANN[1], and MARKUS MORGENSTERN[1] — [1]II. Inst. Phys. B and JARA-FIT, RWTH Aachen University — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz — [3]Abteilung Materialien für grüne Spintronik, Helmholtz Zentrum Berlin

Recent angle resolved photoemission spectroscopy studies show both gapped and ungapped Dirac cones in the magnetic topological insulator $MnBi_2Te_4$ both above and below the Neil temperature.

We present scanning tunneling microscopy data on samples grown by molecular beam epitaxy. The samples have been transfered into a homebuild ultra high vacuum STM operating at 4.3K with a vacuum shuttle operating at a pressure of $1 * 10^{-10}$mbar. We observe variations in topography beyond the atomic corrugation and present quasi particle interference patterns at the energies of the Dirac cone.

O 35: Poster Session - Tribology: Surfaces and Nanostructures

Time: Monday 18:15–20:00 Location: P1C

O 35.1 Mon 18:15 P1C

Temperature dependent friction measurements of manganite films — •Niklas Weber, Hendrik Schmidt, Richard Vink, and Cynthia A. Volkert — Institute of Materials Physics, University of Göttingen, Germany

In this project, we use lateral force microscopy to investigate how friction of manganite films can be controlled by the properties of the surrounding materials. Recently we reported [1,2] a four-fold increase in the friction coefficient of $La_{0.7}Sr_{0.3}MnO_3$ as it is heated through the metal-insulator transition (MIT) and a two-fold increase upon resistively switching a $La_{0.55}Ca_{0.45}MnO_3$-film. Possible contributions from electrostatic forces and electronic and phononic dissipation were considered, with the conclusion that only dissipation via phononic channels were of the necessary order of magnitude.

To investigate the role of depleted surface layers and test the idea of phononic dissipation channels, temperature-dependent friction measurements near the MIT of a $(La_{0.6}Pr_{0.4})_{0.67}Ca_{0.33}MnO_3$ film were performed. However, the friction shows no evidence of the MIT and instead decreases continuously with temperature in accordance with the well known thermal lubricity effect [3]. Measurements of the effect of applied voltage on adhesion and friction indicate an insulating surface layer on the metallic phase, which may obscure possible changes in the friction of the film at the phase transformation.

[1] H. Schmidt et al., arXiv:1611.02684; [2] H. Schmidt, Ph.D. thesis, University Göttingen, (2018); [3] Barel et al., Tribology Letters, 39(3), 311-319, (2010).

O 35.2 Mon 18:15 P1C

Theoretical study of rotational transmission and friction of solid-state gears — Huang-Hsiang Lin[1,2], •Jonathan Heinze[1], Alexander Croy[1], Rafael Gutiérrez[1], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01069 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany

Downsizing gears to the nanoscale has become an emergent technology for implementing microscopic mechanical system. Here, we theoretically investigate how rotational motion can be transmitted across many gears by using molecular dynamics simulations. In particular, the influence of the elastic properties and the shape of the gears is elucidated. Furthermore, we study the effect of friction coming from the substrate and we find that the dissipation is dependent on the gear size and also its initial angular velocity.

O 35.3 Mon 18:15 P1C

Temperature dependence of friction anisotropy on crystalline materials — •Jennifer Konrad, Dirk Dietzel, and Andre Schirmeisen — Institute of Applied Physics, Justus-Liebig University Giessen, 35392 Giessen, Germany

On the nanoscale, the dependence of the friction force on the sliding direction is a well-known phenomenon. This anisotropy occurs as a consequence of the surface structure and is related to different energy barrier heights along different directions of the sample surface. If the sample temperature is varied, the friction force as deduced from the thermally activated Prandtl Tomlinson Model is expected to change, which has a direct influence on the stability of the different sliding directions. In this work, the directional friction force is analyzed under UHV conditions as a function of temperature on different crystalline materials. Our results show that not only the absolute friction and the anisotropy are influenced by temperature, but also the wear depends on temperature on ionic crystals.

O 35.4 Mon 18:15 P1C

Non-linear friction and load-induced hybridization on epitaxial graphene/SiC — •Bartosz Szczefanowicz[1], Andreas Klemenz[2], Michael Moseler[2], and Roland Bennewitz[1] — [1]INM - Leibniz Insitute for New Materials, Saarbrücken, Germany — [2]IWM - Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany

Graphene as 2D material is tough in plane but exhibits weak interactions normal to the plane. These features result in excellent tribological properties such as ultralow friction, which was demonstrated by Atomic Force Microscopy (AFM) measurements on many different substrates. For epitaxial graphene grown on SiC(0001) [1], friction forces increase dramatically above a threshold in normal pressure [2]. We present experimental results recorded by AFM in ultrahigh vacuum for the velocity dependence of friction in the low and high pressure regime. Molecular dynamics simulations identify the pressure-induced local and intermittent hybridization of graphene with the underlying SiC(0001) substrate as origin of the friction increase. A similar rehybridization from sp2 to sp3 and creation of covalent bonds under the pressure of an AFM tip has been suggested to explain extraordinary stiffness results [3]. We discuss models to bridge the time gap between molecular dynamics simulations and AFM experiments, which lead to quantitative agreement.

[1] K.V. Emtsev et al., Nature Materials 8 (2009), 203 [2] T. Filleter and R. Bennewitz, Physical Review B, 81 (2010), 155412. [3] Y. Gao et al, Nature Nanotechnology, 13 (2018), 133.

O 35.5 Mon 18:15 P1C

Atomic Scale Mechanisms in Nanoindentation and Scratching of MoS_2 — Azad Kirsan, •Mattis Gossler, Florian Wullschläger, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Molybdinum disulfide (MoS_2) as a 2D layered material is a very efficient solid lubricant which can be also applied under extreme conditions, for example, in vacuum. To obtain first insights into deformation and degradation mechanisms at high loads, we performed atomistic simulations of nanoindentation and scratching of MoS_2 thin films. For the plastically deformed and ruptured MoS_2 layers we analyze the changes in the chemical bonding pattern of the Mo and S atoms. The results are compared to amorphous structures obtained by *ab initio* molecular dynamics simulations in order to evaluate the reliability of our applied atomistic potential.

O 36: 2D Materials and their Heterostructures I (joint session DS/O/HL)

Time: Tuesday 9:30–11:30 Location: CHE 89

O 36.1 Tue 9:30 CHE 89

Plasma-enhanced atomic layer deposition of AlN at 40°C for encapsulation and dielectric integration of 2D materials — •Michele Bissolo, Alex Henning, Theresa Grünleitner, and Ian D. Sharp — Walter Schottky Institute, 85748 Garching, Germany

To date, hexagonal boron nitride (h-BN) is the material of choice for the dielectric integration of 2D materials since it preserves the intrinsic photoluminescence yield, charge carrier mobility, and band gap of 2D semiconductors by reducing strain, effects of interfacial defects, and remote phonons. However, h-BN must be either mechanically transferred with a polymer stamp onto a bulk substrate, which introduces contamination, or grown by MBE at temperatures above 800°C, which is incompatible with BEOL, microlithography, and temperature-sensitive materials. Here, we demonstrate atomically flat aluminum nitride (AlN), grown by plasma-enhanced atomic layer deposition (PEALD) at 40°C, as a scalable alternative to h-BN. AlN has a similar band gap ($E_g = \sim 6$ eV) and a larger dielectric constant ($\epsilon = \sim 9$) in comparison to h-BN. Because ALD is conformal, it enables the full enclosure of the 2D material. In this work, we test PEALD AlN as a substrate and encapsulation layer for mono- and few-layer MoS$_2$. Raman spectroscopy suggests a strain-free integration of MoS$_2$ with AlN and photoluminescence shows a relatively stronger emission from the A and B excitons without emission from defects. We demonstrate the improved field-effect mobility with MoS$_2$ field-effect transistors enclosed by an AlN dielectric layer. This work provides a scalable route to the dielectric integration of 2D materials critical for future optoelectronics.

O 36.2 Tue 9:45 CHE 89

Spin-Sensitive Readout of Two-Dimensional Wigner Crystals in Transition-Metal Dichalcogenides — •Johannes Knörzer[1,2], Martin Schuetz[3], Geza Giedke[4,5], Dominik Wild[3], Kristiaan de Greve[3], Richard Schmidt[1,2], Mikhail Lukin[3], and Ignacio Cirac[1,2] — [1]Max-Planck-Institut für Quantenoptik, Garching, Germany — [2]Munich Center for Quantum Science and Technology, München, Germany — [3]Physics Department, Harvard University, Cambridge, USA — [4]Donostia International Physics Center, San Sebastián, Spain — [5]Ikerbasque Foundation for Science, Bilbao, Spain

Wigner crystals are prime candidates for the realization of regular electron lattices under minimal requirements on external control and electronics. However, technical challenges have prevented their detailed experimental investigation to date. Here we propose an implementation of two-dimensional electron lattices for quantum simulation based on self-assembled Wigner crystals in transition-metal dichalcogenides. We show that these semiconductors allow for minimally invasive all-optical detection schemes of charge ordering and total spin. For incident light with optimally chosen beam parameters and polarization, we predict a strong dependence of the transmitted and reflected signals on the underlying lattice periodicity, thus revealing the charge order inherent in Wigner crystals. At the same time, the selection rules in transition-metal dichalcogenides provide direct access to the spin degree of freedom via Faraday rotation measurements.

O 36.3 Tue 10:00 CHE 89

Growth of ultra-thin large sized 2D WS$_2$ flakes in at air-liquid interface — •Talha Nisar[1], Torsten Balster[1], Ali Haider[2], and Veit Wagner[1] — [1]Department of Physics and Earth Science, Jacobs University Bremen, Campus Ring 1, 28759, Bremen, Germany — [2]Department of Life Sciences and Chemistry, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

2D tungsten disulfide (WS$_2$) flakes were obtained at the air-liquid interface by a technique recently developed [1]. For this purpose, aqueous solution of ammonium tetrathiotungstate (ATTW) is used as precursor. The process exhibit a clear temperature dependence. At the room temperature, no flakes are observed. When the aqueous solution of ATTW is kept at 80°C, formation of flakes is observed. These flakes can be transferred from the air-liquid interface to a silicon substrate by a controlled dip-coating process. Large flakes with lateral size of up to 100μm were obtained. Thicknesses ranging from bilayer WS$_2$ to 5 MLs as measured by atomic force microscopy. Various spectroscopic techniques (FTIR, Raman, UV-Vis and XPS) are applied to investigate the chemical reaction mechanism for the formation of the flakes. These results show that the initial flakes are made of WO$_3$. The obtained flakes are converted to WS$_2$ by a post annealing step at 500-900 °C with an additional sulfur source in Ar/H$_2$ environment. The successful conversion to WS$_2$ after annealing is confirmed by Raman and XPS. This non-expensive growth technique can be used to produce large WS$_2$ flakes for various applications. [1] X. Zeng, et al, Nanoscale, 2017, 9, 6575-6580

O 36.4 Tue 10:15 CHE 89

Electrical Properties and Doping effects of Chemical Vapor Deposition Growth Layered MoS2 Transistor on Different Back gate oxide Substrates — •Ying-Chun Shen and Yu-Lun Chueh — Department of Materials Science and Engineering National Tsing-Hua University 101, Sec. 2, Kuang-Fu Road, Hsinchu 30013, Taiwan, R. O. C

Recently, there have been many research evolvements in the transition-metal dichalcogenides (TMDCs) materials, which are featured by exotic properties of single or a few layers derivative in terms of direct or indirect bandgap, mechanical or electrochemical behavior. In addition to the pristine properties, the chemical and physical features of TMDCs can be controllably tuned by either nano-structure or dopants. Due to the nature of the TMDCs, they have been the promising candidates of the next-generation semiconductor devices. In our study, we have demonstrated the chemical vapor deposition growth layered MoS2 transistors on different back gate oxide substrates, such as SiO2, HfO*2 and Al2O3. Among these three substrates, HfO2 based MoS2 transistor exhibits the best performance, e.g., higher drain current up to 10 mA, on-off ratio about 106, stable mobility around 20 cm2/ V* s. Furthermore, we performed the doping effect by adding metal ions, and investigate the ion influence on the MoS2 transistor. Moreover, we also compared the electrical performance of distinct metal ions and the number of ions. Here, we provide not only the properties of back gate oxide selection but also a roadmap of ion doping effect to boost the electrical characteristics of the MoS2 transistors.

O 36.5 Tue 10:30 CHE 89

Optical properties of TMDC monolayers interfaced with 2D metals — •Katharina Nisi[1], Shruti Subramanian[2,3], Florian Sigger[1], Margaux Lassaunière[4], David O. Tiede[4], Hendrik Lambers[4], Alexander Holleitner[1], Joshua Robinson[2,3], and Ursula Wurstbauer[4] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany — [2]Department of Materials Science and Engineering, The Pennsylvania State University, USA — [3]Center for 2-Dimensional and Layered Materials, The Pennsylvania State University, USA — [4]Institute of Physics, University of Münster, Münster, Germany

Two-dimensional metals such as 2D-Ga or 2D-In prepared by confinement epitaxy are an emerging class of materials with peculiar properties including superconductivity and strong plasmonic response [1]. The plasmon resonance of those 2D metals spectrally overlaps with the excitonic transition energies of semiconducting transition metal dichalcogenides. Hybrid structures of 2D metals with TMDCs are promising for enhancing the light matter interaction. We investigate the optical response of 2D metal-TMDC hybrid structure by a combination of spectroscopic imaging ellipsometry, photoluminescence and Raman spectroscopy.

[1] B. Bersch et al. arXiv:1905.09938 (2019).

O 36.6 Tue 10:45 CHE 89

Rigid Band Shifts in Two-Dimensional Semiconductors through External Dielectric Screening — •Malte Rösner[1], Lutz Waldecker[2,3], Archana Raja[4,5], Christina Steinke[6], Aaron Bostwick[4], Roland J. Koch[4], Chris Jozwiak[4], Takashi Taniguchi[7], Kenji Watanabe[7], Eli Rotenberg[4], Tim O. Wehling[6], and Tony F. Heinz[2,3] — [1]Institute for Molecules and Materials, Radboud University, Netherlands — [2]Department of Applied Physics, Stanford University, USA — [3]SLAC National Accelerator Laboratory, USA — [4]Lawrence Berkeley National Laboratory, USA — [5]Kavli Energy NanoScience Institute, University of California Berkeley, USA — [6]Institute for Theoretical Physics, University of Bremen, Germany — [7]National Institute for Materials Science, Japan

We investigate the effects of external dielectric screening on the electronic dispersion and the band gap in the atomically thin, quasi-two-dimensional (2D) semiconductor WS2 using angle-resolved photoemission and optical spectroscopies, along with first-principles calculations. We find the main effect of increased external dielectric screening to be a reduction of the quasiparticle band gap, with rigid shifts to the bands themselves. Specifically, the band gap of monolayer WS2 is decreased by about 140 meV on a graphite substrate as compared to a hexagonal boron nitride substrate, while the electronic dispersion of WS2 remains unchanged within our experimental precision of 17 meV. These essentially rigid shifts of the valence and conduction bands result from the special spatial structure of the changes in the Coulomb potential induced by the dielectric environment of the monolayer.

O 36.7 Tue 11:00 CHE 89

Unveiling valley lifetimes of free charge carriers in monolayer WSe$_2$ — •Manfred Ersfeld[1], Frank Volmer[1], Lars Rathmann[1], Luca Kotewitz[1], Maximilian Heithoff[1], Mark Lohmann[2], Bowen Yang[3], Kenji Watanabe[4], Takashi Taniguchi[4], Ludwig Bartels[3], Jing Shi[2], Christoph Stampfer[1,5], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany — [2]Department of Physics and Astronomy, University of California, Riverside, California 92521, USA — [3]Department of Chemistry and

Materials Science & Engineering Program, University of California, Riverside, California 92521, USA — [4]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan — [5]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

We report on nanosecond long, gate-dependent valley lifetimes of free charge carriers in WSe_2, unambiguously identified by the combination of time-resolved Kerr rotation (TRKR) and electrical transport measurements. While the valley polarization increases when tuning the Fermi level into the conduction or valence band, there is a strong decrease of the respective valley lifetime consistent with both electron-phonon and spin-orbit scattering. The longest lifetimes are seen for spin-polarized bound excitons in the band gap region. We explain our findings via two distinct, Fermi level-dependent scattering channels of optically excited, valley polarized bright trions either via dark or bound states.

O 36.8 Tue 11:15 CHE 89

Superconducting Properties of MXene Monolayers — •Cem Sevik[1], Jonas Bekaert[2], and Milorad Milosevic[2] — [1]Department of Mechanical Engineering, Eskisehir Technical University, Ankara, Turkey — [2]Department of Physics, University of Antwerp, Antwerpen, Belgium

MXenes are a new class of two-dimensional materials, consisting of a carbon or nitrogen layer sandwiched in between two transition metal layers. Various experimental studies have demonstrated that these crystals have broad and growing areas of application, such as Li-ion batteries, super-capacitors, fuel-cells, and hydrogen storage. Since most of the MXene monolayers are metals, they could also host superconductivity, depending on their electronic and vibrational properties. Therefore, we have systematically investigated the superconducting properties of monolayer MXenes of stoichiometry M2X (M being the transition metal and X either C or N), with a first-principles approach to Eliashberg theory. Due to the presence of the transition metal, we found the choice of the type of exchange-correlation and inclusion of spin-orbit interactions to be crucial to describe the vibrational and superconducting properties of these monolayers. Cautiously considering these, we have identified five new superconducting monolayer MXenes, out of which three carbides (Mo2C, W2C, and Sc2C) and two nitrides (Mo2N and Ta2N). The highest predicted critical temperature (Tc) of 17 K is found for Mo2N. Our first principle-based systematic analysis clearly has opened up a whole new class of superconductors with sizeable Tc in the monolayer limit.

O 37: Overview Talk: Bjørk Hammer

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

Topical Talk O 37.1 Tue 9:30 TRE Phy

Automating computational surface structure determination — •Bjørk Hammer — Aarhus University, Denmark

Accurate models of surface structure are required whether rationalising experimental observations or providing theoretical predictions. In recent years, density functional theory (DFT) investigations have matured to a level where thousands of computations may be conducted in a reasonable time frame. This has opened up for automating the search for structure of the outermost layers or nano-scale agglomerates at surfaces. For few-dimensional problems, such as the structure of molecular adlayers, grid searches provide a reliable means for finding the global minimum energy structure. For higher-dimensional problems, such as entire surface structures or surface supported nano-particles, a stochastic approach toward identifying the global minimum energy structures may be adopted. Here, evolutionary algorithms (EAs) have proven succesful. In the talk, various ways of enhancing the success of EAs with machine learning and big data methods will be demonstrated. As EAs methods remain stochastic in nature, there is no buildup of knowledge that can be transferred from one EA run to the next. The talk will outline how image recognition and reinforcement learning techniques [1] may remedy this and help building artificially intelligent learning system that may transfer knowledge from solving one surface structure problem to the next.

[1] See: https://asla.au.dk

O 38: Interfaces and Thin Films II (joint session CPP/O/DY)

Time: Tuesday 9:30–13:00 Location: ZEU 260

Invited Talk O 38.1 Tue 9:30 ZEU 260

Phospholipid membranes as model systems for fundamental soft matter research — •Sebastian Jaksch — Forschungszentrum Jülich GmbH Jülich Centre for Neutron Science, Garching, Germany

Phospholipid membranes play an important role as interfaces in virtually all biological systems. By their interplay between structure and dynamics they provide the basic functions necessary to support living organisms, such as stability for the cells and trans-membrane transport for nutrients and drugs. Using SoyPC as an example, this presentation will give an overview of grazing incidence neutron techniques for structure and dynamics measurements of phospholipid membranes.[1] We investigated the structure with grazing incidence small-angle neutron scattering (GISANS) at extremely low background conditions [2] and correlated that data with grazing incidence neutron spin-echo spectroscopy [3] (GINSES). These investigations revealed thermally excited modes in the plane of the membrane and its corresponding structures. This modes could be frozen in at temperatures below room temperature and reappeared after reheating to physiological temperatures.

[1] Jaksch, S., Gutberlet, T., Müller-Buschbaum, P. (2019). Grazing Incidence Scattering - Status and Perspectives in Soft Matter and Biophysics. Current Opinion in Colloid & Interface Science.

[2] Jaksch, S., et al. (2019). Long-range excitations in phospholipid membranes. Chemistry and physics of lipids, 225, 104788.

[3] Jaksch, S., et al. (2017). Nanoscale rheology at solid-complex fluid interfaces. Scientific reports, 7(1), 4417.

O 38.2 Tue 10:00 ZEU 260

Brownian motion in near-surface pressure driven flows with 3D-nanometric spatial resolution — •Joshua McGraw[1], Alexandre Vilquin[1,2], Pierre Soulard[1], Vincent Bertin[1], Gabriel Guyard[1,2], David Lacoste[1], Elie Raphael[1], Frederic Restagno[2], and Thomas Salez[3] — [1]ESPCI Paris — [2]Université Paris Sud — [3]Université de Bordeaux

In near-surface flows, interfaces play a major role by imposing (typically) no-slip boundary conditions, greatly reducing the fluid velocity compared to the central part of a channel. With total internal reflection fluorescence (TIRF), a flow is illuminated with an evanescent field decaying over a few hundred nanometers into the channel; this decay allowing a determination of nanoparticle altitudes. Combined with particle tracking, experimental determination of the velocity profile and local velocity distributions in three dimensions are possible. Here we present a detailed look at the statistics of near-surface particle motions in pressure-driven water for which diffusion is important compared to advection. The distribution of displacements in the invariant flow direction is Gaussian as for normal diffusion. Significant anomalies are however observed for both of the other spatial dimensions. Combining experiments and simulations, we disentangle contributions from so-called Taylor-Aris dispersion, nanoparticle polydispersity and the optical measurement system. This description of TIRF allows for the study of many Brownian motion problems, such as near-surface polymer solution dynamics or particle motion near soft boundaries.

O 38.3 Tue 10:15 ZEU 260

Relation between stability and interfacial structure of polyelectrolyte containing foam films — •Larissa Braun and Regine von Klitzing — TU Darmstadt, Darmstadt, Germany

For many industrial applications foams of oppositely charged polyelectrolyte/surfactant-mixtures are of high impact, as they form surface active complexes.

Extensive research on such mixtures was already performed[1,2] but the influence of the ionic strength is still unclear.

This work focuses on the influence of added LiBr on foam films of mixtures of the anionic polyelectrolyte sPSO$_2$-220 (similar to PSS but stiffer) with the cationic surfactant C$_{14}$TAB. Therefore, disjoining pressure isotherms were measured with a fixed C$_{14}$TAB concentration and a variable polyelectrolyte concentration.

Different stability regimes were identified. Already a low salt concentration of 10^{-4} M leads to a considerably less stable foam films regarding the maximum disjoining pressure. An unexpected formation of an unstable Newton Black Film was found at this low salt concentration. Higher salt concentrations will also be considered. These findings will be correlated with the surface excesses of both compounds which can be separated from each other by neutron reflectometry measurements.

[1] N. Kristen, A. Vüllings, A. Laschewsky, R. Miller, R. v. Klitzing, Langmuir, 2010, 12, 9321-9327. [2] M. Uhlig, R. Miller, R. v. Klitzing, Phys. Chem. Chem. Phys., 2016, 18, 18414-18423

O 38.4 Tue 10:30 ZEU 260

Near-surface dynamics of semidilute polymer solutions: diffusion, nonlinear rheology, and the hydrodynamic boundary condition — •Gabriel Guyard[1,2], Alexandre Vilquin[1,2], Frederic Restagno[2], and Joshua McGraw[1] — [1]ESPCI Paris — [2]Université Paris Sud

The near-surface dynamics of polymer solutions challenge both experimental and theoretical efforts – especially in the case of semi-dilute solutions for which chains overlap – yet evanescent wave microscopy allows for the characterization of such interfacial flows. Here we report molecular-size-resolution particle motions in microfluidic channels for pressure-driven flows of semidilute polymer solutions. The results using polymer-free water are in good agreement with Stokes-flow hydrodynamic and diffusive theory. Experiments using polyacrylamide at different volume fractions close to and above the overlap concentration are done in the same chips as for the water experiments. In contrast to Newtonian fluid behaviour, the shear-rate/pressure drop relation is non-linear for the polymer solution flows, suggesting nanometrically-resolved, shear-thinning effects, accompanied with a non-trivial hydrodynamic boundary condition. The diffusive motion of the tracer particles is also distinguished from that of the water experiments, and such motions detailed here. These results set the basis for a study of near-wall hydrodynamic flow and diffusion in complex fluids, notably including semidilute polymer solutions.

O 38.5 Tue 10:45 ZEU 260

AFM Force-Distance-Curves on Different Lubricants — •Sebastian Friedrich and Brunero Cappella — Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, D-12205 Berlin

AFM force-distance-curves have been recorded on thin films of nine different lubricant liquids. Those lubricants wet the AFM-tip, which causes a capillary force. This force depends on the tip shape, as well as on liquid properties like surface tension, contact angle, and viscosity. Those liquid properties have been measured independently with other methods, so their influence on the shape of the force-distance-curves can be discussed. This study provides a tool for the characterization of thin lubricant films and contributes to the understanding of tribology on the nanoscale.

O 38.6 Tue 11:00 ZEU 260

Revealing the formation of sputter deposited copper nanolayers on functional polymer thin films for lithium-ion batteries — •Simon J. Schaper[1], Franziska C. Löhrer[1], Senlin Xia[1], Matthias Schwartzkopf[2], Pallavi Pandit[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Stephan V. Roth[2,4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, Photon Science, 22607 Hamburg — [3]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, 24143 Kiel — [4]KTH, Department of Fibre and Polymer Technology, 100 44 Stockholm, Sweden

Understanding the interface between metals, commonly used as current collectors, and ion-conducting polymers used in polymer lithium-ion batteries (LIBs) is crucial to develop highly reproducible, low-cost and reliable devices. To address these issues, sputter deposition is the technique of choice to fabricate scalable, reproducible and controllable nanometer and sub-nanometer metal layers on polymer thin films. The sputter deposition process, being well understood and controlled, offers advantages over chemical methods to tailor metal thin-film morphologies on the nanoscale and offers a superior adhesion of the deposited material. We use in-situ grazing incidence small angle X-ray scattering (GISAXS) to investigate the formation, growth and, self-assembled structuring of copper on polymer thin films and composites used in LIBs. The growth of copper on polymer thin films is described based on a model approach.

15 min. break

O 38.7 Tue 11:30 ZEU 260

Insight into ion transport across polypyrrole-electrolyte interfaces by in situ X-ray reflectivity and electrochemistry — •Pirmin H. Lakner[1,2], Manuel Brinker[3], Christoph Seitz[1], Sergey Volkov[1], Patrick Huber[3], and Thomas F. Keller[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Physics Department, Universität Hamburg, Germany — [3]Institute of Materials Physics and Technology, Technische Universität Hamburg-Harburg, Germany

Polypyrrole (PPy) is a conducting polymer with actuatoric and pseudocapacitive properties due to potential-induced ion incorporation/expulsion. Electrical potentials were applied to a perchlorate-doped PPy thin film (~ 30 nm) in an aqueous perchloric acid electrolyte and the associated changes in thickness and electron density were recorded by X-ray reflectivity (XRR). Assuming a sole perchlorate anion transfer carrying 50 electrons, a ratio of 50:1 is expected between electrons crossing the PPy-substrate interface and electrons crossing the electrolyte-PPy interface. By correlating the XRR data and the electrochemical data, a ratio of 10:1 was obtained, which indicates that water movement takes place as an anion counter-flow. The recorded low strain-charge coefficient supports this assumption. One explanation is the high stability and the low porosity of the PPy film due to its fast potentiodynamic deposition method. The properties of the analyzed PPy film make it a suitable choice for supercapacitor applications.

O 38.8 Tue 11:45 ZEU 260

Revealing Lithium Transport Processes in Lithium-Ion Battery Anodes Using Neutron Depth Profiling — •Markus Trunk[1,2], Fabian Linsenmann[3], Philip Rapp[3], Jamie Weaver[4], Lukas Werner[1], Roman Gernhäuser[1], Ralph Gilles[2], Bastian Märkisch[1], Zsolt Revay[2], and Hubert Gasteiger[3] — [1]TUM, Physik-Department, Garching — [2]TUM, Heinz Maier-Leibnitz Zentrum, Garching — [3]TUM, Lehrstuhl für Technische Elektrochemie, Chemie Department, Garching — [4]Material Measurement Laboratory, NIST, Gaithersburg, Maryland

Neutron Depth Profiling (NDP) is a non-destructive, isotope-specific, high-resolution nuclear analytical technique, which is often used to probe lithium or boron concentration profiles in different thin substrates. NDP provides depth sensitivities up to a few ten nanometers and the maximum viewing depth is limited to tens of micrometers. The non-destructive nature of the measurement is of special interest for lithium-ion batteries, where the lithium transport processes can be studied during operation. However, due to the limited viewing depth a special battery cell design is required, which is transparent for the charged particles while ensuring an undisturbed battery performance even at low ambient pressures. We present NDP measurements on lithium-ion batteries performed using a newly developed cell design and discuss insights into the lithium transport processes occurring in the anode material during battery operation.

O 38.9 Tue 12:00 ZEU 260

Comparison of the effects of solvent additives on the morphology development of printed PPDT2FBT:PC71BM films — •Dan Yang[1], Sebastian Grott[1], Xinyu Jiang[1], Kerstin S. Wienhold[1], Matthias Schwartzkopf[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1,3] — [1]TU München,Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [3]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Lichtenbergstr. 1, 85748 Garching, Germany

The morphology and crystallinity of bulk heterojunction (BHJ) films have profound effects on the performance of organic photovoltaics. Currently, most morphological studies on BHJ films are based on spin-coating as deposition technique. However, to commercialize organic photovoltaic products, large-scale fabrication processes such as printing must be taken into consideration. In the present study, the effects of solvent additives on the morphology formation and polymer crystallinity growth of printed BHJ films are investigated by in-situ grazing incidence small/wide-angle X-ray scattering (GISAXS/GIWAXS). The results show that the solvent additives with different boiling points lead to different film drying behaviors, and the phase demixing is changing in the forming BHJ film along with solvent evaporation. These findings provide valuable insights into the film morphology and crystallinity developments of printed BHJ films, which determines the future design of BHJ film printing for large-scale fabrication.

O 38.10 Tue 12:15 ZEU 260

Functionalization of Metalloxid surfaces with Porphyrins — •Klaus Götz[1,2], Annemarie Prihoda[1,2], and Tobias Unruh[1,2] — [1]Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg, Staudtstr. 3, 91058 — [2]Interdisziplinäres Zentrum für Nanostrukturierte Filme, Cauerstr. 3, 91058 Erlangen

Porphyrins are widely studied for their use as catalysts and in dye sensitized solar cells. In these systems the porphyrins are bound to metal oxide surfaces as a functionalizing layer.

We study the binding mechanism in the porphyrin - metal oxide interface on TiO_2 and Co_3O_4. Special emphasis of our work is focused on the exchange process of organic stabilizing molecules with porphyrins. This process is studied using a variation of different scattering techniques. The talk will focus on the characterization of the exchange reaction on the surface of nanoparticles.

Therefore, the combination of small angle x-ray and neutron scattering (SAXS and SANS) experiments will be a key element. These measurements are well suited to study core/shell systems. X-rays interact mainly with electrons and therefore SAXS yields information about the inorganic core of the nanoparticles. Neutrons on the other hand are very sensitive to hydrogen and therefore SANS is well suited to get information about the organic stabilizer shell.

The talk will focus on SAXS/SANS measurements and give an overview over complimentary technique. Furthermore, their usage in the characterization of the morphology of the produced particles and the ligand exchange to porphyrins will be presented.

O 38.11 Tue 12:30 ZEU 260

Atomistic modelling of confined molecules between atomically flat surfaces — •Jose D. Cojal Gonzalez and Jürgen P. Rabe — Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

The contact interface created between an atomically flat cleavage plane of a layered crystal and a 2D material forms a flexible slit or nano pore which can be occupied by (macro)molecules. This arrangement offers a versatile platform for the study of structural, vibrational, elastic and electrical properties of those highly confined molecules. Using molecular dynamics simulations of a graphene-mica slit pore filled with small solvent molecules such as water and ethanol, we provide an instructive model to establish structure and dynamics, i.e. nature and interactions of the molecular layers, mica and graphene. Furthermore, it provides the first step towards the incorporation of larger molecules, such as Rhodamine 6G and dendronized polymers (denpols) in order to complement and better understand the results obtained from Raman spectroscopy and scanning force microscopy measurements.

O 38.12 Tue 12:45 ZEU 260

Exploring the Resistive Switching Properties of HfO2 Nanoparticle Assemblies — •Sonam Maiti[1], Chen Liu[1], Thorsten Ohlerth[2], Ulrich Simon[2], and Silvia Karthäuser[1] — [1]Peter Grünberg Institut (PGI-7), Forschungszentrum Jülich GmbH, Germany — [2]Institute of Inorganic Chemistry (IAC), RWTH Aachen University, Germany

Hafnium oxide nanocrystals (NCs) can be considered as possible candidates for further miniaturization of future resistive random access memories. The switching properties of NC assemblies remain under-explored due to difficulties in fabricating ordered structures. Here, we use a facile, low-cost method to prepare highly ordered assemblies of 6 nm HfO2 NCs capped with TOPO via evaporation based self-assembly. X-ray photoelectron spectroscopy is applied to investigate the oxidation state of near surface HfOx under various conditions. Electrical transport measurements were performed on devices with micrometer and nanometer sized gaps to determine the resistive switching character of NCs arrays. They enable the observation of cyclic voltammograms with redox reaction peaks when used with micrometer sized gaps. We discuss the electronic properties of these devices in the light of varying contributions of electronic vs ionic transport and highlight the effect on the device stability. We especially focus on the resistive switching behaviour of the NP assemblies which is dependent on the oxygen vacancy formation under the influence of the capping ligand.

O 39: 2D Materials III: Growth and Heterostructures (joint session O/HL)

Time: Tuesday 10:30–13:45 Location: GER 38

O 39.1 Tue 10:30 GER 38

High structural and optical quality of transition metal dichalcogenides grown by chemical vapor deposition — •Antony George[1], Shivangi Shree[2], Tibor Lehnert[3], Christof Neumann[1], Meryam Benelajla[2], Cedric Robert[2], Xavier Marie[2], Kenji Watanabe[4], Takashi Taniguchi[4], Ute Kaiser[3], Bernhard Urbaszek[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, 07743 Jena, Germany — [2]Université de Toulouse, INSA-CNRS-UPS, LPCNO, 135 Avenue Rangueil, 31077 Toulouse, France — [3]Ulm University, Central Facility of Materials Science Electron Microscopy, D-89081 Ulm, Germany — [4]National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan

We have achieved highly reproducible large area growth of high-quality monolayer transition metal dichalcogenides (TMDs) by our modified chemical vapor deposition (CVD) process. We correlate the structure of our CVD grown MoS2 monolayers studied by high-resolution transmission electron microscopy (HRTEM) with the optical quality revealed in temperature dependent optical spectroscopy. We determine a defect concentration of the order of 10^{13} cm^{-2} for our samples with HRTEM. We show optical transition linewidth of 5 meV at low temperature (T = 4 K) for the free excitons in emission and absorption after encapsulation in hBN. This is comparable to the best monolayer samples obtained by mechanical exfoliation of bulk material.

O 39.2 Tue 10:45 GER 38

Analysis of Airborne Contamination on Transition Metal Dichalcogenides with Atomic Force Microscopy Revealing That Sulfur Is the Preferred Chalcogen Atom for Devices Made in Ambient Conditions — Korbinian Pürckhauer, •Dominik Kirpal, Alfred J. Weymouth, and Franz J. Giessibl — University of Regensburg, Germany

The fabrication of devices incorporating transition metal dichalcogenides (TMDCs) is mostly done in ambient conditions, and thus the investigation of TMDCs cleanliness in air at the nanoscale is important. We imaged MoS_2, WS_2, $MoSe_2$, and WSe_2 using atomic force microscopy. Mechanical exfoliation of the TMDCs provided clean terraces on sulfides MoS_2 and WS_2. In contrast, the selenides appeared to be contaminated directly after cleavage in most cases. Long-term measurements on $MoSe_2$ revealed that these unwanted adsorbates are mobile on the surface. In situ cleavage and imaging of WSe_2 in ultra-high vacuum shows clean surfaces, proving the airborne character of the adsorbed particles.

[1] K. Pürckhauer et al., ACS Appl. Nano Mater. 2(5), 2593 (2019)

O 39.3 Tue 11:00 GER 38

Capturing the Carpet Growth of 2D-Silica Films — •Leonard Gura, Adrian Leandro Lewandowski, Zechao Yang, Heinz Junkes, Markus Heyde, Wolf-Dieter Schneider, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Silica films represent a new class of two dimensional (2D) network formers with interesting material properties. To understand the growth process of these van der Waals bound films, we need to understand their mesoscopic structure.

Exfoliation experiments and low energy electron microscopy

(LEEM) studies emphasize a smooth and continuous growth of the silica films across single metal crystals [1,2].

In this study, we use scanning tunneling microscopy (STM) to resolve the ring structure of an amorphous silica bilayer film across Ru(0001) step edges. The structural analysis verifies areas of the film with an intact and closed network structure over step edges. The ring sizes are determined with a program for semi-automated ring detection. In this program, we perform a segmentation of the STM image and build a region adjacency graph (RAG) based on the detected ring center coordinates.

We observed areas with carpet growth characteristics in the amorphous 2D-silica film. In future we hope to apply these tools for the detection of structural dynamics as a function of time and temperature.

[1] DOI: 10.1016/B978-0-12-409547-2.14171-X

[2] DOI: 10.1002/anie.201802000

O 39.4 Tue 11:15 GER 38

Where the MoS_2 bilayer grows: An *in situ* LEEM study — •Moritz Ewert[1,2], Lars Buss[1,2], Francesca Genuzio[3], Tevfik Onur Menteş[3], Andrea Locatelli[3], Jens Falta[2], and Jan Ingo Flege[1,2] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]Institute of Solid State Physics, University of Bremen, Germany — [3]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, Trieste 34012, Italy

Molybdenum disulfide (MoS_2) is well-known for changing from an indirect to a direct semiconductor when its thickness is reduced to a single layer, rendering a high degree of growth control a necessity for optoelectronic applications. An extensively investigated model system is MoS_2 on Au(111), which using molecular beam epitaxy typically grows as clusters. Here, we present an in-situ low-energy electron microscopy (LEEM) study of the extended growth of MoS_2 at 700°C and 750°C. These conditions lead to the formation of micron-sized single-layer MoS_2 islands. The single-domain character of these islands is demonstrated by employing dark-field imaging and micro-diffraction (LEED), which allow quantifying the relative coverage of the two mirror domains. Furthermore, selected area angle-resolved photoelectron spectroscopy of these domains directly confirms their threefold symmetric electronic bandstructure. Interestingly, under certain conditions subsequent structural characterization by I(V)-LEEM clearly identifies regions where a bilayer of MoS_2 has nucleated. Parameters influencing the bilayer growth as well as its electronic properties will be discussed.

O 39.5 Tue 11:30 GER 38

Growth of Hexagonal Boron Nitride and Borophene on Ir(111) via Thermal Catalytic Decomposition of Borazine (B3H6N3) — •Karim Omambac[1], Marko Kriegel[1], Christian Brand[1], Pascal Dreher[1], David Janoschka[1], Ulrich Hagemann[2], Nils Hartmann[2], Frank-Joachim Meyer zu Heringdor[1,2], and Michael Horn-von Hoegen[1] — [1]University of Duisburg-Essen, Germany — [2]Interdisciplinary Center for the Analytics on the Nanoscale (ICAN), Germany

Preparation of borophene has been performed by deposition from an e-beam heated high-purity boron rod via molecular beam epitaxy (MBE) [1]. However, the MBE technique is very expensive with low yield and most of all, epitaxially grown borophene islands are found small sized. Here we report on the first successful growth of large area borophene via the thermal catalytic decomposition of borazine (B3H6N3) on a Ir(111) substrate at high temperatures using conventional CVD technique. The observed growth mode is describe to be similar with boron dissolving into the bulk at high temperatures and segregating to the surface forming large borophene sheets as the sample is cooled [1]. The surface morphology and structure determination has been performed in-situ by real-time growth observation via low energy electron microscopy (LEEM) and high-resolution spot profile analyzing-LEED (SPA-LEED). The chemical composition has been determined ex-situ by X-ray photoemission spectroscopy (XPS) and time-of-flight secondary ion mass spectroscopy (ToF-SIMS) measurements. [1] ACS Nano 13, 3816-3822 (2019)

O 39.6 Tue 11:45 GER 38

Electronic properties of coherently attached nanocrystals measured by scanning tunneling spectroscopy — •Pierre Capiod[1], Maaike van der Sluijs[1], Jeroen de Boer[1], Christophe Delerue[2], Ingmar Swart[1], and Daniel Vanmaekelbergh[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, PO Box 80 000, 3508 TA Utrecht, the Netherlands — [2]Université Lille, CNRS, Centrale Lille, ISEN, Université Valenciennes, UMR 8520 - IEMN, F-59000 Lille, France

2D systems have attracted considerable interest in recent years. The first 2D material was graphene which displays a rich band structure. While it is not possible to create a 2D honeycomb structure with any element we want, artificial lattices emerge as new field to explore. It was shown that it is possible to create superlattices based on semiconductor nanocrystals (PbSe, CdSe) as building blocks in a square and honeycomb geometry. It is of high interest to combine the large scale self-assembly of such superlattices with the possibility of optical and electrical switching. Theoretical works have been initiated based on tight-binding calculations. Those calculations have shown that the atomic crystalline structure of the nanocrystals combined with the square or honeycomb geometry determine the band structure of the system where Dirac-cones and non-trivial flat bands appear. Until now, the density of states of those structures has not been resolved. In this presentation, I will describe the synthesis and the preparation of the samples and present the measurements of the density of states on PbSe square superlattices by scanning tunneling spectroscopy

O 39.7 Tue 12:00 GER 38

Deconfinement in van der Waals Stacks: Turning Mott Localized Electrons into Dirac Fermions — •Jose Pizarro[1,2], Severino Adler[3], Karim Zantout[4], Thomas Mertz[4], Paolo Barone[5], Roser Valentí[4], Giorgio Sangiovanni[3], and Tim Wehling[1,2] — [1]University of Bremen — [2]Bremen Center for Computational Material Sciences — [3]University of Würzburg — [4]Goethe University Frankfurt am Main — [5]CNR-SPIN, Italy

The interplay of topology and electronic correlations forms a rich ground for the realization of exotic states of quantum matter, with an increased importance in emergent flat bands systems in superlattices. Here, we show how strongly correlated spin-orbit coupled Dirac fermions emerge in bilayers of 1T-TaSe2 and related group V transition metal dichalcogenides. These materials realize the so-called Star-of-David (SoD) charge density wave (CDW) patterns in each layer, where the stacking of the CDW centers defines the symmetry of the resulting superlattice. When the CDW centers are arranged in a honeycomb pattern, the system realizes a generalized Kane-Mele model with a sizable on-site Hubbard interaction U. The isoelectronic series of 1T-TaSe2, TaS2, and NbSe2 traverses a region of the electronic phase diagram where weakly-to-strongly correlated Dirac semimetallic, Mott antiferromagnetic insulating and quantum spin Hall states compete. We show that stacking and relative rotations between the layers as well as perpendicular electric fields affect the emergent correlated Dirac fermions as effective gauge and mass fields, and control their creation, annihiliation and topology.

O 39.8 Tue 12:15 GER 38

Proximity-induced superconducting gap in the quantum spin Hall edge state of monolayer WTe_2 — •Felix Lüpke[1], Dacen Waters[1], Sergio C. de la Barrera[1], Michael Widom[1], David G. Mandrus[2,3,4], Jiaqiang Yan[2], Randall M. Feenstra[1], and Benjamin M. Hunt[1] — [1]Department of Physics, Carnegie Mellon University, Pittsburgh, PA 15213, USA — [2]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — [3]Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN 37996, USA — [4]Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA

Van der Waals (vdW) heterostructures allow the combination of different material properties, e.g. non-trivial topology and superconductivity in order to create a topological superconducting state. We demonstrate a novel dry-transfer flip technique which we use to place atomically-thin layers of WTe_2, a quantum spin Hall (QSH) system, on $NbSe_2$, a vdW superconductor, while maintaining atomically clean surfaces and interfaces. Using scanning tunneling microscopy and spectroscopy (STM/STS), we demonstrate the presence of a proximity-induced superconducting gap in the WTe_2 for thicknesses from a monolayer up to 7 crystalline layers. At the edge of the WTe_2 monolayer, we show that the superconducting gap coexists with the characteristic spectroscopic signature of the QSH edge state [1].

[1] F. Lüpke *et al.*, arXiv:1903.00493 (2019)

O 39.9 Tue 12:30 GER 38

MoSe2-WSe2 lateral heterostructures grown by chemical vapour deposition — •Emad Najafidehaghani[1], Antony George[1], Ziyang Gan[1], Tibor Lehnert[2], Christof Neumann[1], Xingcheng Li[1], Ute Kaiser[2], and Andrey Turchanin[1] —

[1]Friedrich Schiller University Jena, Institute of Physical Chemistry, D-07743 Jena, Germany — [2]Ulm University, Central Facility of Materials Science Electron Microscopy, D-89081 Ulm, Germany

Recently two-dimensional (2D) transition metal dichalcogenides (TMDs) such as MoS2, WS2, WSe2, MoSe2 etc. attracted great research interest due to their superior electronic and optical properties. They are identified as promising candidates for applications such as ultrathin, transparent and flexible electronics, optoelectronics and sensing. In order to realize advanced device architectures such as p-n junctions, complementary logic devices, ultrathin photovoltaics, etc. it is essential to develop efficient growth strategies for combining dissimilar monolayer TMDs to form lateral heterostructures. Here we show large area growth of monolayer MoSe2 -WSe2 lateral heterostructures by our modified chemical vapour deposition (CVD) technique which uses Knudsen type effusion cells for controlled delivery of precursors [1]. The grown monolayer MoSe2-WSe2 lateral heterostructures were characterized using complementary microscopic and spectroscopic techniques such as optical microscopy, Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), Kelvin probe microscopy and high-resolution transmission electron microscopy (HRTEM) to reveal their structural and chemical quality.

O 39.10 Tue 12:45 GER 38

Two-dimensional metal phases and non-stoichiometric phases of transition metal dichalcogenides — •Thomas Joseph, Mahdi Ghorbani-Asl, and Arkady Krasheninnikov — Helmholtz-Zentrum Dresden Rossendorf, Bautzner Landstraße 400, Dresden

Changing the stoichiometry of a material in a controllable manner is a powerful tool to tailor the structure and the properties of a compound solid. For example, new morphologies, such as inversion domains with the associated mirror twin boundaries [1] can be produced in 2D transition metal dichaclogenides by sputtering chalcogen atoms using electron beam [1]. Moreover, suspended monolayer Mo membranes were recently fabricated from monolayer MoSe$_2$ sheets via complete sputtering of Se atoms in a scanning transmission electron microscope [2]. Motivated by these results, we performed first-principles calculations to understand the energetics of 2D phases of binary compounds which can be referred to as strongly non-stoichiometric transition-metal dichalcogenides. We found that other intermediate metallic non-stoichiometric phases, which are energetically more favourable than pure 2D metals [3], can also exist.

[1] Komsa, H.-P. et al.; Native Defects in Bulk and Monolayer MoS 2 from First Principles. Phys. Rev. B 2015, 91 (12), 125304.

[2] X. Zhao et al.; Atom-by-Atom Fabrication of Monolayer Molybdenum Membranes. Advanced Materials 2018, 30 (23), 1707281.

[3] T. Joseph et al.; Nonstoichiometric Phases of Two-Dimensional Transition-Metal Dichalcogenides: From Chalcogen Vacancies to Pure Metal Membranes. J. Phys. Chem. Lett. 2019, 10 (21), 6492.

O 39.11 Tue 13:00 GER 38

Visualization of multifractal superconductivity in a two-dimensional transition metal dichalcogenide in the weak-disorder regime — Carmen Rubio-Verdú[1], Antonio M. García-García[2], Hyejin Ryu[3], Deung-Jang Choi[1], Javier Zaldívar[1], Shujie Tang[3], Bo Fan[2], Zhi-Xun Shen[4], Sung-Kwan Mo[3], José Ignacio Pascual[1], and •Miguel M. Ugeda[5] — [1]CIC nanoGUNE, 20018 Donostia-San Sebastián, Spain. — [2]Shanghai Center for Complex Physics, Department of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China. — [3]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA. — [4]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA. — [5]Donostia International Physics Center (DIPC), 20018 San Sebastián, Spain.

Here we investigate the impact of multifractality on the superconducting state of a weakly disordered single-layer of NbSe2 by LT-STM/STS. The SC gap (width, depth and coherence peaks amplitude) shows characteristic spatial single-wavelength modulation coincident with the periodicity of the QPI pattern observed at EF. Spatial inhomogeneity of the SC gap width, which is proportional to the order parameter in the weak-disorder regime, shows a characteristic log-normal statistical distribution as well as a power-law decay of the two-point correlation function, in agreement with our theoretical model. This novel state is universal and governs the properties of even weakly disordered 2D superconductors with SOC.

O 39.12 Tue 13:15 GER 38

Role of dark trions in the optical response of doped atomically thin semiconductors — •Ashish Arora[1], Nils Kolja Wessling[1], Thorsten Deilmann[1], Till Reichenauer[1], Paul Steeger[1], Piotr Kossacki[2], Marek Potemski[2,3], Steffen Michaelis de Vasconcellos[1], Michael Rohlfing[1], and Rudolf Bratschitsch[1] — [1]University of Münster, Germany — [2]University of Warsaw, Poland — [3]Laboratoire National des Champs Magnétiques Intenses, Grenoble, France

We perform absorption and photoluminescence spectroscopy of intravalley and intervalley trions in transition metal dichalcogenide (TMDC) monolayers encapsulated in hBN, depending on temperature [1]. We find that an interplay between the thermal distribution of bright and dark trions, and their oscillator strengths gives rise to the unique optical response of each monolayer material. The observed trends in our experiments are excellently reproduced using a model based on the Fermi-Dirac distribution of bright and dark trions. Our analysis yields that there is a dark trion 19 meV *below* the lowest energy bright trion in WSe$_2$ and WS$_2$. However, in MoSe$_2$, the dark trion lies 6 meV *above* the bright trion, while it almost coincides in energy with the bright trion in MoS$_2$. These results are in excellent agreement with our GW-BSE *ab-initio* calculations of trions for these materials. Our observations provide a quantitative understanding of the temperature-dependent optical response of TMDCs. [1] Preprint at https://arxiv.org/abs/1911.06252

O 39.13 Tue 13:30 GER 38

Excited-State Trions in Monolayer WS$_2$ — •Thorsten Deilmann[1], Ashish Arora[2], Till Reichenauer[2], Johannes Kern[2], Steffen Michaelis de Vasconcellos[2], Michael Rohlfing[1], and Rudolf Bratschitsch[2] — [1]Institute of Solid State Theory, University of Münster, Germany — [2]Institute of Physics and Center for Nanotechnology, University of Münster, Germany

We discover an excited bound three-particle state, the 2s trion, appearing energetically below the 2s exciton in monolayer WS$_2$, using absorption spectroscopy and ab initio GW and Bethe-Salpeter equation calculations [1]. The measured binding energy of the 2s trion (22 meV) is smaller compared to the 1s intravalley and intervalley trions (37 and 31 meV). Our discovery underlines the importance of trions for the entire excitation spectrum of two-dimensional semiconductors. [1] *Phys. Rev. Lett.* **123**, 167401 (2019)

O 40: Organic Molecules on Inorganic Substrates III: Electronic, Optical and other Properties

Time: Tuesday 10:30–13:00 Location: REC C 213

O 40.1 Tue 10:30 REC C 213

Reaction dynamics simulation of an interface between Trecresyl phosphate and Iron oxide by a hybrid quantum and classical method — •Naoki Uemura[1], Yosuke Harada[2,3], and Shuji Ogata[1] — [1]Nagoya Institute of Technology, Nagoya, Japan — [2]Idemitsu Kosan Co. Ltd., Chiba, Japan — [3]ADMAT, Ibaraki, Japan

The understanding of reaction mechanics at the heterogeneous interface, e.g. organic-inorganic interfaces, is of fundamental importance for physics and industries. Trecresyl phosphate molecule (TCP) has been widely used for various industrial applications such as anti-wear additives. However the detailed mechanism of decomposition of TCP on metal and metal oxide under high pressure and high temperature has still been discussed [1, 2]. Our large-scale molecular dynamics simulations by the hybrid quantum and classical method based on DFT [3] indicated breaking P-O bonds of TCP near the surface.

This work was funded by New Energy and Industrial Technology Development Organization of Japan (NEDO) Grant (P16010).

[1] E. Osei-Agyemang et al., Tribol. Lett. 66, 48 (2018).

[2] B. Guan et al., Lubr. Sci. 28, 257 (2016).

[3] N. Ohba et al., Comp. Phys. Comm. 183, 1664 (2012).

O 40.2 Tue 10:45 REC C 213

Energy levels and charge distribution within dipolar molecules on MoS_2/Au(111) — •Sergey Trishin[1], Daniela Rolf[1], Christian Lotze[1], Johanna Richter[1], Philipp Rietsch[2], Siegfried Eigler[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin — [2]Institut für Chemie und Biochemie, Freie Universität Berlin

Molecules consisting of a donor and an acceptor moiety can exhibit large intrinsic dipole moments. Upon deposition on a metal surface, the dipole may be effectively screened and the charge distribution altered due to hybridization with substrate electronic states. Therefore, the inclusion of a thin band-gapped material can help to preserve gas-phase-like electronic properties. We study Ethyl-Diaminodicyanoquinone molecules on a Au(111) surface and on single-layer molybdenum disulfide (MoS_2) on Au(111) with scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM). By mapping the local contact potential difference (LCPD) over the molecules we show that the intrinsic dipole moment of the molecules is partially preserved upon adsorption on both the bare Au(111) surface and MoS_2. On Au(111), the molecular resonances show an apparent shift in energy within individual molecules. The high energy resolution on molecules adsorbed on MoS_2 allows us to conclude that the apparent shift is due to several resonances of varying intensity, arising from vibronic states. DFT calculations of the molecule in gas phase help to identify certain vibrations of the molecule from their signature in the tunneling spectra.

O 40.3 Tue 11:00 REC C 213

Electronic structure of a donor-acceptor molecule adsorbed on a Pt substrate — •Narendra P. Arasu and Hector Vazquez — Institute of Physics of the Czech Academy of Sciences, Cukrovarnicka 10, Prague 6, Czech Republic

Donor-bridge-acceptor molecules exhibit excellent intramolecular charge transfer properties and have a vast potential in optoelectronic applications. In this work, a Donor-bridge-acceptor molecule composed of carbazol and phenalenon derivatives is studied on a platinum substrate using Density Functional Theory (DFT) calculations and low-temperature Scanning Tunneling Microscopy (STM) experiments. Simulations include van der Waals interactions between the molecule and the substrate. After a screening of many interface geometries, two stable adsorption configurations can be identified, and a comparison of these structures is made with experimental STM Images. The donor-acceptor character and its changes upon adsorption are analyzed through the effect of binding and structural changes on the electronic properties. Calculations disentangle the different contributions from the donor, acceptor and bridge units of the molecule. Simulations of the molecular interface thus rationalize the STM experiments and provide an understanding of the role of the platinum-molecule interaction.

O 40.4 Tue 11:15 REC C 213

Hybridization of the NTCDA/Ag(111) interface state with molecular orbitals — •Lukas Eschmann, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische-Wilhelms Universität Münster, 48151 Münster, Germany

At the internal interfaces between adsorbed π-conjugated organic molecules and metallic substrates, two-dimensional, highly dispersive interface states (IS) appear. These states are mainly attributed to the Shockley surface state of the metal that is shifted up in energy and is scattered by an adsorbate induced scattering potential.

We employ density-functional theory (DFT) to analyze the dispersion of the IS between a monolayer of 1,4,5,8-naphthalene-tetracarboxylic acid dianhydride (NTCDA) and the Ag(111) surface. Complemented with a projection technique which maps the interface electronic structure onto the original Ag(111) Shockley state, the DFT calculations enable us to analyze the dispersion of the NTCDA/Ag(111) IS and its interactions with the molecular orbitals. We transfer the ab-initio data into a model Hamiltonian which allows us a deeper understanding of the interaction with the molecular orbitals.

Our analysis shows that interaction with molecular orbitals causes crucial changes in the dispersion of the IS and our model explains the recently both experimentally and theoretically observed pronounced anisotropy of the IS at NTCDA/Ag(111) [1].

[1]L. Eschmann, et al. , Phys. Rev. B 100, 125155 (2019).

O 40.5 Tue 11:30 REC C 213

Corrections to DFT energy level alignment of single molecule junctions using projected orbitals — •Enrique Montes and Hector Vazquez — Institute of Physics, Czech Academy of Sciences, Cukrovarnicka 10, Prague 16200, Czech Republic

The calculation of the electronic and transport properties of metal/molecule junctions is of paramount importance in many fields of molecular nanoscience. DFT struggles to accurately predict the energy level alignment between the frontier molecular orbitals and the Fermi level of the metal. Several approaches have been proposed to calculate the energy level alignment of metal/molecule interfaces beyond DFT, among them the DFT+Σ method [1] stands out as it reduces computational cost while maintaining good accuracy. Here, we develop a new method to correct the DFT-based energy level alignment of molecular junctions. We start by projecting the orbitals of the molecular subspace onto the full junction space. The projection coefficients are used to average parameters from DFT+Σ framework (gas phase and polarization). At variance with previous approaches we introduce the correction in the total junction Hamiltonian, i.e., operator is defined in junction space. Using this methodology we are able to correct the complete electronic structure. We have implemented this method in the DFT SIESTA code [2] because it describes electrons in a localized basis set, allowing for an unambiguous clustering of the system. We will show results for typical metal/molecule/metal junctions. [1] S. Quek, et al. Nano Lett. 7, 3477 (2007). [2] J. M. Soler, et al. J. Phys. Cond. Matt. 14, 2745 (2002).

O 40.6 Tue 11:45 REC C 213

Supramolecular networks assembled on superconducting Pb surfaces — •Carl Drechsel[1], Philipp D'Astolfo[1], Xunshan Liu[2], Shi-Xia Liu[2], Silvio Decurtins[2], Rémy Pawlak[1], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [2]Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, 3012 Bern, Switzerland

Due to their vast potential for functionalities, molecular assemblies at surfaces have attracted a certain interest in surface Physics. Recent experiments have shown the feasibility to create metal-organic nanochains with special catalytic properties [1], or to activate selected molecules for the use as molecular quantum cellular automata [2]. On superconductors, these molecules create ground states, formed by a balance between Kondo screening and superconducting pair-breaking interactions [3].

Here, we investigate the structural and electronic properties of self-assembled layers of 3-TBQP (3,6,14,17-tetrabromodibenzo[a,c]-dibenzo[5,6:7,8]-quinoxalino-[2,3-i]phenazine) on the superconducting Pb(111) surface. The layers are characterized at 4 K by scanning tunneling microscopy (STM) and atomic force microscopy (AFM) with CO-terminated tips. Our results show a fundamental step in developing functional supramolecular networks at supra-conductors [4].

[1] Krull, C. et al.; Nat Commun 9, 3211 (2018) - [2] Kocic, N. et al.; Nano Lett. 19, 5, 2750-2757 (2019) - [3] Franke, K.J. et al.; Science 332, 940 (2011) - [4] Drechsel, C. et al.; submitted

O 40.7 Tue 12:00 REC C 213

Organic alkali salt layer formation as surface decoupling strategy in metal organic thin films: K and TCNQ on Ag(111) — •Billal Sohail[1], Luke Rochford[1], Phil Blowey[1,3], Phil Woodruff[2], Giovanni Costantini[1], and Reinhard J. Maurer[1] — [1]Department of Chemistry, University of Warwick, UK — [2]Department of Physics, University of Warwick, UK — [3]Department of Chemistry, University of Leeds, UK

A detailed characterisation of structure and electronic properties at metal-organic interfaces is crucial for the design of novel molecular electronics devices such as organic photovoltaics (OPVs) and organic field effect transistors (OFETs). In these devices, strong donors such as alkaliatoms and acceptor molecules, such as TCNQ (7,7,8,8-tetracyanoquinodimethane), are often added to organic electronics devices to tune the charge injection properties at the metal-organic interface. We present a joint computational and experimental study to examine the intricate coupling of geometry and electronic structure for TCNQ coadsorbed with potassium atoms on a Ag(111) surface. By combining dispersion-inclusive Density-Functional Theory calculations, x-ray standing wave (XSW), LEED, and STM measurements, we find that K and TCNQ form a strongly interacting organic salt. This stands in contrast to TCNQ on Ag(111), which forms strongly surface-bound adlayers containing silver adatoms. We identify the energetic driving force for organic salt formation and discuss the intricate competition between donor, acceptor, and metal surface.

O 40.8 Tue 12:15 REC C 213

Kekulene synthesised on copper surfaces: Orientation and electronic properties — •Anja Haags[1,2], Qitang Fan[5], Xiaosheng Yang[1,2], Larissa Egger[3], Hans Kirschner[4], Tim Naumann[5], Simon Werner[5], Jörg Sundermeyer[5], François C. Bocquet[1,2], Georg Koller[3], Alexander Gottwald[4], Mathias Richter[4], Michael G. Ramsey[3], Peter Puschnig[3], Serguei Soubatch[1,2], F. Stefan Tautz[1,2], and Michael Gottfried[5] — [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]Institute of Physics, University of Graz, NAWI Graz, 8010 Graz, Austria — [4]Physikalisch-Technische Bundesanstalt (PTB), 10587 Berlin, Germany — [5]Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Straße 4, 35032 Marburg, Germany

The polycyclic aromatic molecule kekulene was synthesised on the copper (111) and (110) surfaces from a molecular precursor using a surface-assisted reaction. Scanning tunneling microscopy showed compact well-ordered monolayers of kekulene proving a high reaction yield. To address electronic properties of kekulene, we carried out momentum-space imaging photoelectron spectroscopy experiments. The photoemission intensity distributions of particular molecular states are compared to density functional theory calculations of free kekulene using the plane wave final state approximation. It allows us to prove the chemical nature of the reaction product and to elucidate its orientation and electronic structure on both copper surfaces.

O 40.9 Tue 12:30 REC C 213

Molecular Topology and Surface Chemical Bond of Aromatic Ring Systems — •Lukas Ruppenthal, Benedikt P. Klein, Jan Herritsch, Stefan R. Kachel, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

Metal/organic interfaces formed at the contacts between metal electrodes and organic semiconductors have a large impact on the performance of organic-electronic devices. The detailed understanding of their chemical, electronic and geometric structure is therefore important for the further technological development. Many common organic semiconductors contain π-electron systems with alternant topologies, whereas non-alternant alternatives have only recently found increasing attention due to their unusual electronic properties. Here, we compare naphthalene as an alternant aromatic molecule with azulene as its non-alternant isomer, both on Cu(111), using PES, NEXAFS, TPD, STM, and LEED. With the same approach, we compare the larger aromatic compounds pyrene and its isomer dicyclopenta[*ef,kl*]heptalene (azupyrene), which is also important as a model for the Stone-Wales defects in graphene. In both cases, we find that the non-alternant isomer forms a stronger bond to the metal surface than its alternant counterpart.The increased interaction of the non-alternant isomers is related to their reduced HOMO-LUMO gap, which brings the LUMO energetically close to the Fermi energy of the metal, causing stronger hybridization with electronic states of the metal surfaces. The resulting effects on the electronic and geometric structure will be discussed on the basis of DFT calculations.

O 40.10 Tue 12:45 REC C 213

Adsorption and Electronic Properties of Azaacenes on Au (111) — •Mohsen Ajdari[1], Friedrich Maass[1], Matthias Müller[2], Hilmar Reiss[2], Marvin Hoffmann[3], Uwe H. F. Bunz[2], Andreas Dreuw[3], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut — [2]Organisch-Chemisches Institut — [3]Interdisziplinäres Zentrum für Wissenschaftliches Rechnen, Ruprecht-Karls-Universität Heidelberg

Azaacenes are organic electron-transporting semiconductors that belong to N-heteropolycyclic aromatic compounds, which are promising candidates for a variety of (opto) electronic applications such as field effect transistors. In these molecules, introduction of nitrogen in their aromatic backbone in its pyridine form decreases the energy of both HOMO and LUMO, resulting in an improved stability due to an increased ionization potential and electron affinity of organic semiconductor.

In this study, we investigated the adsorption and electronic properties of azaacenes as a function of coverage on Au (111) by employing temperature-programmed desorption (TPD), vibrational and electronic high-resolution electron energy loss spectroscopy (HREELS) in combination with quantum-chemical theory to gain detailed insights into their adsorption geometry and electronic structure on Au(111) which is of great importance for optimizing and improving a device performance.

O 41: Focus Session: Functional Molecules at Surfaces II

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

O 41.1 Tue 10:30 TRE Ma

Tip-induced inversion of the chirality of a molecule's adsorption potential probed by the switching directionality — Anja Bauer[1], Markus Maier[2], Werner Schosser[1,3], Josefine Diegel[1], Fabian Paschke[1], Yuriy Dedkov[4], Fabian Pauly[3,1], Rainer F. Winter[2], and •Mikhail Fonin[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Department of Chemistry, University of Konstanz, 78457 Konstanz, Germany — [3]Okinawa Institute of Science and Technology Graduate University, Onna-son, Okinawa 904-0495, Japan — [4]Department of Physics, Shanghai University, 99 Shangda Road, 200444 Shanghai, China

The switching behaviour of surface-supported molecular units is determined by the shape of the adsorption potential. Here, by means of scanning tunneling microscopy, we study a triazatruxene (TAT) molecule on Ag(111), which shows a switching behavior characterized by transitions of the molecule between three states, and which we attribute to three energetically degenerate bonding configurations. Upon tunneling current injection the system can be excited, showing a pronounced switching directionality. Two surface enantiomers of TAT show opposite switching directions pointing at the chirality of the energy landscape of the adsorption potential as a key indigent for directional switching. Further we show that by modifying the tunneling parameters, the symmetry of the adsorption potential can be controlled, leading to a suppression of the directionality or an inversion of the switching direction.

Invited Talk O 41.2 Tue 10:45 TRE Ma

Molecular switches at surfaces — •Petra Rudolf — Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

Molecular motors and switches form the basis of many important biological processes. In contrast to these solutions chosen by Nature for achieving complex tasks, mankind's present day technologies function exclusively through their static or equilibrium properties. On can therefore easily anticipate that the controlled movement of molecules or parts of molecules offers unprecedented technological possibilities for the future. In this presentation I shall show how to build molecular engines that allow movements at the molecular level to be coupled to the macroscopic world, e.g. to transport macroscopic objects like drops of liquid over a surface. I shall also discuss self-assembled monolayers of switches that can be addressed with light and charge transfer and demonstrate how such systems can be employed for *read and write* functions.

O 41.3 Tue 11:15 TRE Ma

The role of double bond isomerization in the design of functioning metal-adsorbed molecular switches — •Martin Lea[1], Vasilios G. Stavros[1], David A. Duncan[2], and Reinhard J. Maurer[1] — [1]Department of Chemistry, University of Warwick, Coventry, United Kingdom, CV4 7AL — [2]Diamond Light Source, Didcot, United Kingdom, OX11 0DE.

Photoswitches are a class of organic molecules which have the ability to reversibly interconvert between two geometric states as a response to light absorption. Integration of such organic molecules in electronic devices requires adsorption upon a metal surface, which most often leads to the loss of switching function. In the case of the well-studied photoswitch Azobenzene, this loss of function upon surface adsorption has been previously identified computationally as a loss of bistability in the ground state, which is caused by strong coupling of the central nitrogen double bond with the metal substrate. [Angew. Chem. Int. Ed. 51, 12009 (2012)] However, it is unclear if this effect is common to all switches based on double bond isomerization or unique to the case of Azobenzene. In this study, we perform dispersion-inclusive Density Functional Theory calculations on a set of similar metal-adsorbed molecular switches which differ in the chemical composition of the photochromic moiety. By comparing the structure, stability, and electronic properties of metal-adsorbed molecular conformers, we establish mechanistic trends, which will potentially guide the design and synthesis of molecular switches in the future.

O 41.4 Tue 11:30 TRE Ma

STM-induced tautomerization of phthalocyanines on BiAg$_2$/Ag(111) — •Markus Böhme[1], Markus Leisegang[1], David Maiberger[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

Organic molecules such as deprotonated phthalocyanines can show a tautomerization process in which the inner hydrogen atom changes its position. This electron-induced process cannot only be be triggered when the STM tip is positioned directly above the molecule, but also by injecting charge carriers into the substrate a few nm away from the molecules [1,2]. Whereas experiments have mostly been performed on noble metals with a relatively simple electronic structure, such as Ag(111) with its electron-like quasi-free surface state, we will focus in this talk on a surface with a more complex band structure, i.e., the BiAg$_2$ surface alloy on Ag(111) which exhibits a giant Rashba effect [3]. We will present voltage- and current-dependent data of the tautomerization rate of HPc on BiAg$_2$ /Ag(111) and discuss the angular dependency of the switching rate of the molecule.
[1] P. Liljeroth *et. al.*, Science **317**, 1203-1206 (2007).
[2] M. Leisegang *et. al.*, Nano. Lett. **18**, 2165 (2018).
[3] C. Ast *et. al.*, Phys. Rev. Lett. **98**, 186807 (2007).

Invited Talk O 41.5 Tue 11:45 TRE Ma

Molecular Nanoprobe - utilizing a single molecule as detector — •Markus Leisegang — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The transport properties of electrically conducting materials are determined by charge carriers scattering at electrons, phonons, and defects. A fundamental understanding of the underlying processes will require experiments on the level of single defects, bringing along the necessity of resolving transport properties down to the nanometer or even atomic scale. One approach towards this goal has been the development of multi-probe STMs, but their minimal tip–tip distance is usually limited to $> 30\,\mathrm{nm}$ [1]. To circumvent this limitation, we invented the molecular nanoprobe (MONA) technique [2]. In MONA we utilize a charge-induced switching between discrete states of a single surface-adsorbed molecule, e.g. a tautomerization process, to detect the current injected remotely by the STM tip. Due to the local, near-field charge injection mechanism and the small size of the detector molecule, MONA allows for transport measurements in atomically controlled environments and over distances of a few nanometers. Our investigations on Ag(111) with its electron-like surface state show how scattering and interference processes affect the atomic-scale transport. Furthermore, we reveal the influence of the atomic lattice on transport properties in anisotropic surfaces.
[1] S. Yoshimoto *et al.*, Nano Lett. **7**, 956-959 (2007).
[2] M. Leisegang *et al.*, Nano Lett. **18**, 2165-2171 (2018).

O 41.6 Tue 12:15 TRE Ma

Quantum Tunneling in Intramolecular Hydrogen Transfer: The Case of Porphycene on Metal Surfaces — •Yair Litman[1] and Mariana Rossi[1,2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany. — [2]MPI for Structure and Dynamics of Matter, Hamburg, Germany

The intramolecular hydrogen transfer (IHT) of porphycene represents a paradigmatic process where nuclear quantum effects and anharmonicity result in unconventional hydrogen dynamics[1]. Here, we study the IHT of porphycene adsorbed on Cu and Ag surfaces at different temperatures. We couple density functional theory calculations including dispersion corrections with the ring-polymer instanton method[2]. This combination gives us access to unprecedented full-dimensional quantum mechanical reaction rates for porphycene on Cu(110) and Ag(110) in the deep tunneling regime. We predict rates in excellent agreement with experiments [3,4] and show the importance of heavy-atom tunneling in the reaction. We address the thus-far unexplained temperature dependence of the IHT and reveal that the observed activation energy is related to the energy difference between reactant and product, rather than reactant and transition state. Finally, we unequivocally identify the IHT mechanism as stepwise for Cu(110) and show the existence of a sharp transition between concerted and stepwise mechanisms on Ag(110) surface. [1] Y. Litman, et al., J. Am. Chem. Soc. 141, 2526 (2019); [2] J. O. Richardson and S. Althorpe, J. Chem. Phys. 131, 214106 (2009); [3] T. Kumagai, et al., Phys. Rev. Lett. 111, 246101 (2013); [4] M. Koch, et al., J. Am. Chem. Soc. 139, 12681 (2017).

O 41.7 Tue 12:30 TRE Ma

Controlled switching of a single CuPc molecule on Cu(111) — •Thilo Glatzel[1], Sweetlana Fremy-Koch[1], Ali Sadeghi[2], Rémy Pawlak[1], Shigeki Kawai[3], Alexis Baratoff[1], Stefan Goedecker[1], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [2]Department of Physics, Shahid Beheshti University, G.C., Evin, 19839-63113 Tehran, Iran — [3]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki Tsukuba, Ibaraki 305-0044, Japan

Low temperature measurements of the tunneling current as a function of the applied bias voltage have been performed above individual copper phthalocyanine molecules adsorbed on Cu(111). By tuning of the applied bias, the molecule can be reversibly switched between two configurations. The underlying conformations are revealed by density functional calculations including van der Waals interactions, a C2v symmetric ground state and two energetically equivalent states, in which the molecule is twisted and rotated around its center by +/- 7°. For tip biases above 200mV position-dependent current switching is observed, as in previous measurements of telegraph noise [Schaffert et al., Nat. Mater. 12, 223 (2013)]. In a small voltage interval around zero the measured current becomes bistable. Switching to a particular state can be initiated by sweeping the voltage past well-defined positive and negative thresholds at certain positions above the molecule or by scanning at constant current and a reduced reverse bias.

O 41.8 Tue 12:45 TRE Ma

Electronic Structure of a prototypical organic-inorganic interface: CuPc on In$_2$O$_3$(111) — •Matthias A. Blatnik[1], Peter Jacobson[2], Michael Schmid[1], Jan Čechal[3], Ulrike Diebold[1], and Margareta Wagner[1,3] — [1]Institute of Applied Physics, TU Wien, Wien, Austria — [2]School of Mathematics and Physics, University of Queensland, St. Lucia, Australia — [3]CEITEC, Brno University of Technology, Brno, Czech Republic

Indium oxide (In$_2$O$_3$) is a ubiquitous material in OLEDs and photovoltaics due to an ideally matched optical transmission window and metallic conduction at room temperature. When In$_2$O$_3$ is paired with organic materials, a nearly universal fabrication step is the introduction of a thin organic buffer layer to improve the charge injection efficiency from In$_2$O$_3$ to the organic active layers. Using a combination of STM, AFM and local spectroscopy (STS), we probe the adsorption structure and density of states at the prototypical copper phthalocyanine (CuPc) - In$_2$O$_3$ interface. Two surface terminations were examined, the 1×1 oxidized surface and the 1×1 hydroxylated surface. Differential conductance (dI/dV) measurements reveal the energetic positions of the HOMO and LUMO states which are critical for improving charge injection. STM/AFM imaging reveals single molecules adsorb in a flat, slightly tilted geometry in three symmetry-equivalent orientations. Increasing the coverage leads to a (densely packed) 1D chains oriented along the $<1\bar{1}0>$ directions. Finally, a (2×2) superstructure with a building block consisting of three CuPc molecules is formed.

O 42: Focus Session: Innovation in Machine learning PRocEsses for Surface Science (IMPRESS)

Self-learning and -improving algorithms, more-commonly referred to known as *machine learning*, are being increasingly used for various applications in surface science, both in theory and experiment. On the experimental side, they hold great promise to automate tedious, repetitive tasks (for example in image recognition) or allow to determine automated procedures to manipulate interfaces with STM tips. Computationally, machine learning algorithms provide the means to significantly speed up calculations without (significant) loss of accuracy or even to extract the physics determining specific processes (such as structure formations) from comparatively small data sets. The aim of this session is to provide a focussed overview over the recent applications and development of machine learning algorithms for surface science applications.

Organizers: Oliver Hoffmann (TU Graz), Patrick Rinke (Aalto University), Milica Todorović (Aaalto University)

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

Invited Talk O 42.1 Tue 10:30 TRE Phy

Exploring the Design Space of Organic Semiconductors with Machine Learning — •Harald Oberhofer — Chair for Theoretical Chemistry, Technical University Munich

Organic electronics—in the form of field effect transistors, light emitting diodes, or solar cells—are slowly finding their use in everyday consumer devices. So far though, one of the main challenges holding back their wide-scale adoption are their low intrinsic charge carrier mobilities. Improving these is usually attempted by structural tuning of a promising compound family, thereby relying on intuition, experience, or simply trial and error. While sometimes quite successful, such incremental changes only lead to a local exploration of the vast chemical space of possible molecules, potentially overlooking many interesting materials.

In contrast, modern data mining strategies allow the extraction of general design rules through the systematic evaluation of large compound databases. Starting from an analysis of such a database consisting of >64.000 molecular crystals we evaluate the impact of molecular scaffolds and side groups on the charge transport properties of each crystal contained in our database to reveal statistically reliable, general design criteria. A visualization of the chemical space contained in our dataset highlights large gaps in the experimentally covered range of synthesized organic materials. Adopting an active learning strategy we venture to fill these gaps to uncover promising new organic semiconductor materials.

Invited Talk O 42.2 Tue 11:00 TRE Phy

Machine learning for molecular nanorobotics — •Christian Wagner — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — JARA Fundamentals of Future Information Technology, Jülich, Germany

The ability to handle single molecules as effectively as macroscopic building-blocks would enable the construction of complex supramolecular structures that are not accessible by self-assembly. A central difficulty on the way towards this technology is the uncontrolled variability and poor observability of atomic-scale conformations, especially during the manipulation process. We present a generic strategy to overcome both obstacles, and demonstrate autonomous nanorobotics with single molecules using reinforcement learning (RL). Quite generally, RL is able to learn strategies even in the face of large uncertainty and with sparse feedback. Indeed, RL based prediction models recently exceeded human performance in several games. However, to be useful for nanorobotics, standard RL algorithms must be adapted to also cope with the limited training opportunities that are available there. We demonstrate our correspondingly enhanced RL approach by applying it to an exemplary task of subtractive manufacturing with a scanning probe microscope (SPM). Complementary to that we outline how machine learning and control theory methods in combination with molecular simulations can be utilized to recover atomic-scale conformations from the sparse experimental SPM data available during manipulation.

O 42.3 Tue 11:30 TRE Phy

The search of new catalysts for an OCM reaction based on CO_2 adsorption properties using data mining technique — •Aliaksei Mazheika[1], Frank Rosowski[1,2], and Ralph Kraehnert[1] — [1]BasCat, Technische Universitaet Berlin, Berlin, DE — [2]BASF SE, Ludwigshafen, DE

The interest in oxidative coupling of methane (OCM) reaction is caused by the fact that this is a relatively simple way for conversion of C_1 hydrocarbons (methane) to C_2 products (ethane, ethylene). Despite quite many years spent for the search of an efficient catalyst, still the catalyst which would be commercially viable has not been found. Recently Kraehnert et al. have shown that formation of surface carbonates and their decomposition energies play significant role in catalytic performance of materials in OCM reaction [1]. In this study we find the correlation between CO_2 adsorption energies on oxide surfaces and formation energies of carbonates. The adsorption energies of carbon dioxide are predicted based on properties of bulk materials, free gasphase atoms and relaxed surfaces of oxides as proposed by Mazheika et al. [2]. This observation allows us to reformulate experimentally observed volcano plots as the dependence of C_2-yield on CO_2 adsorption energies. Based on this observation we use a data mining technique subgroup discovery [3] and identify a subgroup of materials with high catalytic activity, and find a way for the search of new materials.
[1] R. Schmack *et al.*, Nat. Comm. **10**, 441 (2019).
[2] A. Mazheika *et al.*, manuscript in preparation.
[3] M. Boley *et al.*, Data Min. Knowl. Disc. **31**, 1391 (2017).

O 42.4 Tue 11:45 TRE Phy

Symmetry-adapted neural network representations of electronic friction to simulate nonadiabatic dynamics at metal surfaces — •Reinhard J Maurer[1], Yaolong Zhang[2], and Bin Jiang[2] — [1]Department of Chemistry, University of Warwick, United Kingdom — [2]Hefei National Laboratory for Physical Science at the Microscale & Department of Chemical Physics, USTC, Hefei, China

In catalytic reactions or molecular scattering, molecules impinging on metal surfaces excite electronic excitations. This leads to nonadiabatic energy transfer between the adsorbate and the metal that can measurably affect reaction outcomes. We study these effects with abinitio molecular dynamics simulations using Density Functional Theory (DFT), where electron-phonon coupling is modelled as system-bath coupling, so-called electronic friction, in a Generalised Langevin equation framework. [1] To enable statistical averaging over many reaction events, we employ neural-network-based representations of the electronic friction tensor (EFT) calculated with time-dependent perturbation theory and DFT. [2] A particular challenge hereby is to capture the symmetry equivariance properties of the electronic friction tensor as a function of all atom positions by constructing a neural network with a tensor output layer. Our approach achieves an efficient and continuous representation of EFT, which we apply to metal surface scattering of diatomic molecules. [3]

[1] PRL 116, 217601 (2016); [2] Chem. Sci. 10, 1089-1097 (2019); [3] arXiv:1910.09774

O 42.5 Tue 12:00 TRE Phy

SAMPLE: Surface structure search enabled by coarse graining and statistical learning — •Lukas Hörmann, Andreas Jeindl, Alexander T. Egger, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, TU Graz, Petersgasse 16, 8010 Graz, Austria

The structure is the key information of an organic monolayer on an inorganic substrate. Virtually all properties depend on the polymorph.

On top of that, monolayers often display diverse molecular arrangements in different unit cells. Determining these polymorphs from first principles poses a considerable challenge due to the large number of possible molecular arrangements.

To meet this challenge, SAMPLE[1] employs coarse-grained modeling and machine learning to efficiently map the minima of the potential energy surface of commensurate organic adlayers. Requiring only a few hundred DFT calculations of possible polymorphs, we use Bayesian linear regression to determine the parameters of a physically motivated energy model. These parameters yield meaningful physical insight and allow predicting adsorption energies for millions of possible polymorphs with high accuracy.

We demonstrate SAMPLE's capabilities on the systems of naphthalene[1] and TCNE[2,3] on coinage metals where we predict the energetically most favorable polymorphs and compare them to experiment.

[1] Hörmann et al., Computer Physics Communications 244, 143-155, 2019 [2] Scherbela et al., Phys. Rev. Materials 2, 043803, 2018 [3] Obersteiner et al., Nano Lett. 17, 4453-4460, 2017

O 42.6 Tue 12:15 TRE Phy

(Re)interpreting TCNE adsorption on Cu(111) with machine learning — Alexander Egger[1], Lukas Hörmann[1], Andreas Jeindl[1], Milica Todorovic[2], Patrick Rinke[2], and •Oliver T. Hofmann[1] — [1]TU Graz, Austria — [2]Aalto University, Helsinki, Finland

Tetracyanoethylene (TCNE) layers on Cu(111) surfaces are a prototypical organic/inorganic interface. Measured vibrational spectra [1] of this interface evoke charge transfer between the substrate and molecules in the second layer and beyond. However, such "long-range" charge transfer defies our current understanding of organic/inorganic interfaces and is at variance with results from conventional density-functional theory (DFT) calculations.

In this work, we employ two new structure search methods, SAMPLE [2] and BOSS [3], that combine DFT with machine-learning algorithms, to computationally determine the geometric structure of TCNE mono- and bilayers on Cu 111. We then calculate vibrational spectra to compare to experiment. Our results show that the first TCNE layer re-orients with respect to the surface before molecules in the second layer are adsorbed. This reorientation changes the interaction with the surface qualitatively and brings the computed vibrational spectra into agreement with the measured ones. This structural phase change explains the observed spectral features without having to evoke long-range charge transfer. [1] Erley and Ibach, J. Phys. Chem. 91 2947 (1987) [2] Hörmann *et al.*, CPC 244, 143 (2019) [3] Todorović *et al.*, njp Comp. Mater. 5, 35 (2019)

O 42.7 Tue 12:30 TRE Phy

Chemicaly reasonable models for automatic interpretation of AFM images — •Prokop Hapala[1], Niko Oinonen[2], Fedor Urtev[2], Benjamin Alldritt[2], Ondrej Krejci[2], Filippo F. Canova[2], Fabian Schulz[2], Juho Kannala[2], Peter Liljeroth[2], and Adam S. Foster[2] — [1]Dep. Condensed Matter Theory, FZÚ AV ČR — [2]Dep. Applied Physics, Aalto University

During the last year we pioneered machine-learning methods for reconstruction of molecular structure from high-resolution AFM images of non-planar organic molecules [1], which opens the way to broader application of this experimental technique for single-molecule analysis [2] e.g. in the pharmaceutical industry. Nevertheless, a scheme relying purely on general-purpose image recognition tools (such as convolutional neural networks) is sub-optimal as it discards physical insight. Incorporation of physical models and chemical intuition (e.g. bonding topology of carbon) into the scheme could considerably regularize the model, thus making it more reliable in situations when input information is limited. This is especially important, since the AFM provides rather limited information about deeper molecular structure which does not come into direct contact with the tip. The challenge is to formulate a model which encode relevant rules of organic chemistry, including both atomic and electronic structure (such as *electron force-field* [3]), while it is simple enough to be conveniently embedded into machine learning framework,[1]B.Alldritt,et.al.,Science Advances,(2019)accepted,[2]B.Schuler,et.al.,JACS,137(31),9870-9876,(2015),[3]H.Xiao,et.al.,Mechanics of Materials,90,243-252,(2015)

Invited Talk O 42.8 Tue 12:45 TRE Phy

Theory-informed Machine Learning for Interface Structure Reconstruction from Experimental Data — Eric Schwenker[1,2], Chaitanya Kolluru[1], Spencer Hills[1], Arun Mannodi Kanakkithodi[1], Fatih Sen[1], Michael Sternberg[1], and •Maria Chan[1] — [1]Center for Nanoscale Materials, Argonne National Laboratory, Lemont IL, USA — [2]Materials Science and Engineering, Northwestern University, Evanston IL, USA

Determining atomistic structure at interfaces is challenging because metastable interfaces are likely accessible under realistic conditions, rendering energy-only searches insufficient, and experimental data often give incomplete information. Therefore, neither theory nor experimental data alone is sufficient to determine these structures. In this talk, we will discuss how we use machine learning to combine experimental and theory-based data to determine interfacial structures.

O 43: Plasmonics and Nanooptics III: Periodic Structures and Theory

Time: Tuesday 10:30–13:45 Location: WIL A317

O 43.1 Tue 10:30 WIL A317

Mie Theory in terms of Axion-Plasmonics — •Johannes Schultz[1], Axel Lubk[1,2], Flavio S. Nogueira[3], and Bernd Büchner[1,2] — [1]IFF, IFW Dresden, Helmholtzstr. 20, 01069 Dresden — [2]IFMP, TU Dresden, Haeckelstr. 3, 01069 Dresden — [3]ITF, IFW Dresden, Helmholtzstr. 20, 01069 Dresden

Calculations of the scattering of electromagnetic (e.m.) waves is a usefull and important tool to investigate the dielectric response of nanoparticles (NPs) theoretically. Of particular interest are NPs with negativ dieletric function and low damping in a certain frequency regime at the same time. This leads to standing waves of oscillating electrons at the surface of the NP, so called localized surface plasmons. Solving the problem using Maxwells equations leads to determin the so called scattering coefficients from the boundary conditions at the interface. For arbitrary geometries it is hard to obtain the boundary conditions and consequently to get a complete analytic solution. However, exploiting the symmetry of spherical NPs we can determin a full analytic solution. This approach is known as Mie-Thoery and can be applied on many scattering problems including scattering at plasmonic NPs. In our study we generalized the common Mie-Theory to spheres consisting of Topological Insulators (TIs). The exceptional so called Axion-coupling of the e.m. fields in TIs leads to modified boundary conditions and resultant scattered fields. In summary we found uncommon magnetic field contributions for the scattering on TIs which vanish for trivial materials. This exceptional field contributions can maybe measured in the transmission electron microscope.

O 43.2 Tue 10:45 WIL A317

Broadband plasmonic spectroscopy of vectorial near-field coupling — •Martin Esmann[1,2], Simon F. Becker[2], Julia Witt[2], Jinxin Zhan[2], Abbas Chimeh[2], Anke Korte[2], Jinhui Zhong[2], Ralf Vogelgesang[2], Gunther Wittstock[2], and Christoph Lienau[2] — [1]CNRS Centre for Nanoscience and Nanotechnology (C2N), Palaiseau, France — [2]Carl von Ossietzky University, Oldenburg, Germany

The coherent coupling of optical near fields between dipole momenta determines the function and optical properties of many nanostructures[1]. These interactions extend over a few nanometers only and depend sensitively on the vectorial properties of the coupled near fields, i.e., on relative dipole orientation, spectral detuning and dephasing. This makes it challenging to analyze and control them experimentally.

Here, we introduce plasmonic nanofocusing [2] spectroscopy [3] as a tool to record coherent light scattering spectra with 5-nm spatial resolution from a small dipole antenna, excited solely by evanescent fields. We couple the antenna to plasmon resonances in single gold nanorods and resolve mode couplings, resonance energy shifts and Purcell effects as a function of dipole distance and relative orientation. We show how they arise from different vectorial components of the interacting near-fields. Our results pave the way to using dipolar alignment for the in-situ control of optical properties and function in nanoscale systems.

[1] Zhang, Y. et al., Nature 531, 623 (2016).
[2] Stockman, M.I., PRL 93, 137404 (2004).
[3] Esmann, M. et al., Nature Nanotech. 14, 698 (2019).

O 43.3 Tue 11:00 WIL A317

Solution of electrodynamics on plasmonic nanohelices by boundary element method — •Daniel Nürenberg[1], Peer Fischer[2], and Helmut Zacharias[1] — [1]Uni Münster Center for Soft Nanoscience, Münster — [2]MPI für intelligente Systeme, Stuttgart

We present electrodynamical simulations of the absorption, scattering and near-fields of plasmonic Ag, Cu and Ag:Cu alloy nanohelices from the UV to the near infrared of the optical spectrum. The helix models were designed to reproduce helices, which were fabricated by nano glancing angle vapor deposition [1]. The calculations were carried out with a boundary element approach using the MNPBEM toolbox [2]. The inherent chirality of the nanohelices leads to a strong circular dichroism (CD), which was calculated for all directions of incidence. The CD is found to be very sensitive to the direction of the impinging light. Infact, even changes in sign of the CD are common for most wavelengths, if the incidence is changed from parallel to the helical axis to a perpendicular orientation.

[1] A.G. Mark, J.G. Gibbs, T.-C. Lee, and P. Fischer, Nat. Mater. 12, 802 (2013).
[2] J. Waxenegger, A. Trügler, and U. Hohenester, Comput. Phys. Commun. 193, 138 (2015).

O 43.4 Tue 11:15 WIL A317

Perturbation theory as an efficient tool for modelling chiral and achiral plasmonic sensors — •Steffen Both, Harald Giessen, and Thomas Weiss — 4th Physics Institute and Research Center SCoPE, University of Stuttgart

Plasmonic nanostructures comprise optical resonances with strong electromagnetic near-fields. If we place chemical substances in these near-fields, even tiny amounts of the substance can have dramatic effects on the resulting spectral responses. This effect is the key to various kinds of sensing applications. Conventionally, the theoretical modelling of such interactions utilizes extensive numerical simulations. As we have recently shown [1,2], an alternative approach consists in the use of perturbation theories, which provide the benefit of drastically reduced computational times and allow to gain deep insights into the underlying physical mechanisms. Here, we discuss this approach especially with regard to applications in chiral sensing [3].

[1] T. Weiss, et al., Phys. Rev. Lett. **116**, 237401 (2016).
[2] S. Both and T. Weiss, Opt. Lett., *accepted* (2019).
[3] M. Nesterov et al., ACS Photonics **3**, 578 (2016).

O 43.5 Tue 11:30 WIL A317

Generalized 1D description of light coupling to arbitrarily curved plasmonic wires — •Thorsten Feichtner[1], Katja Höflich[2], Jer-Shing Huang[3], and Bert Hecht[1] — [1]Nano-Optics & Biophotonics Group, Wilhelm-Conrad-Röntgen-Center for Complex Material Systems (RCCM), Experimental physics 5 - Universität Würzburg, Germany — [2]Max Planck Institute for the Science of Light, Erlangen, Germany — [3]Leibniz Institute of Photonic Technology, Albert-Einstein Strasse 9, Jena D-07745, Germany

Plasmons propagating on metallic nano wires (MNWs) with spherical cross sections are fully understood and analytical solutions for the decomposition of the fields in Mie modes exist. We have already shown that for helically curved wires, so-called plasmonic helices, also an analytical one-dimensional model can be used to calculate their coupling to circular polarized planar wave far-field excitation [1].

Here we first extend this model to also describe coupling of helices to point dipoles. This is done to explain the results from [2] which shows strongly directed emission. We also extend the model to more arbitrary curved wires to explain the near-field behavior of 3D Archimedian spirals as introduced in [3]. This powerful tool will allow the fast development of plasmonic wire geometries for tailored near-fields or far-field scattering.

[1] Hoeflich, Katja, et al., *Optica* 6.9 (2019): 1098-1105.
[2] Wang, Mengjia, et al., *Light: Science & Applications* 8.1 (2019): 1-8.
[3] Tseng, Ming Lun, et al., *Adv. Opt. Mat.* (2019): 1900617.

O 43.6 Tue 11:45 WIL A317

Polar semiconductor heterostructures as hyperbolic metamaterials — •Christopher J. Winta[1], Daniel C. Ratchford[2], Martin Wolf[1], Joshua D. Caldwell[3], and Alexander Paarmann[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin (Germany) — [2]U.S. Naval Research Laboratory, Washington, D.C. (USA) — [3]Vanderbilt University, Nashville, TN (USA)

We present a novel approach towards engineering the infrared dielectric response of polaritonic materials by means of atomic-scale superlattices of polar semiconductors. [1] With layer thicknesses on the order of just a few atomic monolayers, new optic phonon modes arise at the many interfaces, resulting in a unique and strongly anisotropic dielectric response of the heterostructure.

We show experimentally that these crystalline hybrids exhibit multiple spectral regions where the principal dielectric components have opposite signs. These so-called hyperbolic bands support hyperbolic phonon polariton (h-PhP) modes, i.e., large-momentum states with rigid directionality, facilitating, e.g., subdiffractional imaging by means of hyperlens designs. [2] We employ transfer-matrix calculations [3], simulating the h-PhP dispersion, showing that these modes are highly dispersive, as well as finite elements calculations, revealing their rigid directionality. The crystalline hybrid approach presents itself as a versatile platform for user-designed hyperbolic metamaterials.

[1] Ratchford, Winta et al., *ACS Nano* **13**, 6730-6741 (2019)
[2] Liu et al., *Science* **23**, 1686 (2007)
[3] Passler, Paarmann, *JOSA B* **34**, 2128-2139 (2017)

O 43.7 Tue 12:00 WIL A317

Optical Nano-Imaging of Electronic Shear Modes — Jun Yong Khoo[1], Po-Yao Chang[2,1], Inti Sodemann[1], and •Falko Pientka[1] — [1]Max-Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany — [2]Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan

Plasmons are collective excitations of metals that consist of modulations of the electron density similar to compressional waves in classical liquids, which allows for an efficient coupling to light. In addition, moderately interacting two-dimensional metals can feature a second type of collective mode, involving electron motion transverse to the propagation direction. Such shear modes are akin to transverse sound waves in a crystal and have no counterpart in classical liquids. Experimental evidence of such shear modes has remained elusive so far, as a lack density fluctuations strongly suppresses the coupling to light. Here, we show that shear modes can nevertheless be probed by optical techniques in the presence of a static magnetic field. Specifically, we predict signatures in scanning near-field optical microscopy, where spatial oscillations of the near-field signal at the wavelength of the shear mode emerge as the field strength is increased. Our proposals is largely based on existing experimental technology operating at frequencies in the far infrared to terahertz regime.

O 43.8 Tue 12:15 WIL A317

Chiral Scatterometry on Chemically Synthesized Single Plasmonic Nanoparticles — •Julian Karst[1], Nam Heon Cho[2], Hyeohn Kim[2], Hye-Eun Lee[2], Ki Tae Nam[2], Harald Giessen[1], and Mario Hentschel[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Department of Materials Science and Engineering, Seoul National University, Korea

Being intrinsically scalable, bottom-up nanoparticle synthesis shows an ever-growing control over particle morphology, enabling even chirally selective shapes. So far, imaging technologies such as electron microscopy are mostly used to investigate the quality of the synthesis. We show that single particle chiral scatterometry holds great potential as a feedback to characterize the (chir-)optical quality of chemically synthesized nanoparticles. The spectra of single helicoid nanoparticles reveal a diverse set of chiroptical responses with hugely varying absolute chiral asymmetry in spite of the well-controlled morphology of the particles. Averaging over the single nanoparticles reproduces the solution ensemble measurement remarkably well. This demonstrates that the single particles, despite their morphological and consequently chiroptical differences, exhibit a clearly pronounced chiral spectral and structural feature. We find that the g-factor of single nanoparticles can be up to four times larger than the ensemble g-factor. This proves that chiral scatterometry can be a highly important optical feedback for bottom-up nanoparticle synthesis as it reveals that the asymmetry of the ensemble solution can be further increased and maximized by appropriate refinement methods or by post-fabrication purification.

O 43.9 Tue 12:30 WIL A317

Reconfigurable high-quality surface phonon polariton resonators — Andreas Hessler[1], •Konstantin G. Wirth[1], Yvonne Bente[1], Laric Bobzien[1], Joshua Caldwell[2], Matthias

Wuttig[1], Dimitry N. Chigrin[1], and Thomas Taubner[1] — [1]Institute of Physics (IA), RWTH Aachen — [2]Department of Mechanical Engineering, Vanderbilt University, United States

The recent discovery of highly confined mid-infrared surface phonon polaritons (SPhPs) on SPhP-resonant substrates covered by a thin dielectric layer and the reversible switching of laser written circular resonators in a thin film of the phase change material $Ge_3Sb_2Te_6$ (GST) offer new exciting potential for tailoring light-matter interactions [1]. Planar circular cavities in a gold film on GST and SiC have been shown to yield high Q-factors of 150 [2]. Using the low loss polar crystal SiC as substrate should result in an increased resonance quality compared to SiO_2 in [1]. Here we will present the optical writing of arbitrary infrared-resonant structures into an amorphous GST film on top of an SiC substrate. The resonances have a high Q factor, despite the absence of any metal boundary like in a metallic cavity. The laser written structures are characterized and spatially resolved with an FPA detector and near-field optical microscopy (s-SNOM). The resulting resonances will be verified by an analytical model, which can be used to predict the characteristic features of such a resonance.
[1] Li et al., Nat. Mater. 15, 870-875 (2016)
[2] Sumikura et al., Nano Lett. 19, 2549-2554 (2019)

O 43.10 Tue 12:45 WIL A317

Photonic wheels and magnetic field induced directional emission of excitons — •Lars Klompmaker[1], Felix Spitzer[1], Alexander N. Poddubny[2], Ilya A. Akimov[1,2], Leonid V. Litvin[3], Ralf Jede[3], Grzegorz Karczewski[4], Maciej Wiater[4], Tomasz Wojtowicz[5], Dmitri R. Yakovlev[1,2], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Ioffe Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Raith GmbH, 44263 Dortmund, Germany — [4]Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland — [5]International Research Centre MagTop, Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland

Photonic wheels carry transverse spin, which is locked to the propagation direction of the electromagnetic wave. Therefore, photonic wheels are attractive for spin manipulation and read-out in magnetic media. Emission effects are of particular interest. In this work emission phenomena are discussed where directionality is established perpendicular to an externally applied magnetic field for light sources (excitons) located near a surface, breaking the mirror symmetry. In hybrid plasmonic semiconductor structures, we observe a significantly enhanced directionality of up to 60%. The directional emission is studied regarding period dependence of the plasmonic grating and different emission geometries are considered.

O 43.11 Tue 13:00 WIL A317

Tuning the coupling of plasmonic structures with photonic crystals — •Rahim Benrali, Constance Schmidt, Teresa I. Madeira, and Dietrich R. T. Zahn — Semiconductor Physics, Chemnitz University of Technology, D-09107 , Germany

One-dimensional photonic crystals (PCs) are multilayered stacks with alternating refractive index (RI) and layer thicknesses (LT). PCs show a high reflectivity in a broad spectral range known as photonic bandgap (PBG). It was already shown that coupling of PCs with metallic nanoparticles (MNPs) in a photonic crystal plasmonic hybrid system (PCPHS) provides new ways of controlling and enhancing the optical response of plasmonic resonances [1]. Here we investigate the coupling of PCs with MNPs and the effect of tuning the PBG over the visible spectral range. PCs were prepared by electrochemical etching of p-doped silicon with hydrofluoric acid (HF), resulting in porous silicon (PS). MNPs show a plasmonic behaviour, known as localized surface plasmonic resonance (LSPR). The LSPR depends mainly on the metal and the geometry of the MNPs. Here triangular MNPs were obtained by nanosphere lithography (NSL). We used spectroscopic ellipsometry to investigate the effects of etching time and current density on PS. Furthermore, different parameters to influence the PBG (LT, RI, interface roughness) were investigated. Raman spectroscopy was used to test the performance of the PCPHS. The impact on the intensity of the Raman signal due to the PCPHS is demonstrated using organic molecules as Raman probes. [1] M. Fränzl, S. Moras, O. D. Gordan, D. R. T. Zahn, J. Phys. Chem. C 2018, 122, 18, 10153-10158

O 43.12 Tue 13:15 WIL A317

Influence of number of grooves on spectral shape of grating-coupled surface plasmon polaritons — •Sven Stephan, Christoph Bennenhei, Christoph Lienau, and Martin Silies — Institute of Physics, Carl von Ossietzky Universität, Oldenburg

Surface plasmon polaritons (SPP) are evanescent waves that can propagate along metal-dielectric interfaces over mesoscopic distances. Since they can be used to confine light beyond the diffraction-limit of free-space light, SPPs can combine the high bandwidth of optics with the small feature size of electronics and are believed to enable all-optical circuitry [1]. A common way of converting light to SPPs is to use focused-ion beam written grating couplers in metal films. However, most models that investigate grating-coupling assume an infinitely extended grating, i.e. an infinite number of grooves and do not take into account a finite number of grooves [2, 3]. Here, we present a systematic study of the influence of the number of illuminated grooves, both for in- as well as outcoupling, on the spectrum of the generated SPP waves. Our experimental results enable for tailoring the spectral response of the grating coupler for ideal spectral selection of wavelengths and spectral bandwidth of the SPP, to suit experimental demands where specific spectral shapes are required.

[1] Surface-plasmon circuitry, T.W. Ebbesen et al., Physics Today, 61(5), 2008 [2] Physical origin of photonic energy gaps in the propagation of surface plasmons on gratings, W. L. Barnes et al., Phys. Rev. B, 54(9), 1996 [3] S. A. Maier, Plasmonics: Fundamentals and applications, Springer, 2007

O 43.13 Tue 13:30 WIL A317

Laser-induced periodic surface structures formation on various materials — •Pavel N. Terekhin, Pascal D. Ndione, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

The use of ultrashort laser pulses for surface nanostructuring is of great importance in technological and medical applications. Thus, understanding of the basic governing mechanisms of energy deposition to the irradiated material is very important. On a rough material surface, grating structures or at a step edge ultrashort laser pulses can excite surface plasmon polaritons (SPP), i.e. surface plasmons coupled to a laser electromagnetic wave. One of the possible scenarios for the description of laser-induced periodic surface structures (LIPSS) is based on the SPP excitation and their interference with the incident beam.

The spatial and temporal evolution of the periodically modulated absorbed laser energy is studied after irradiation of various metals in the framework of the two-temperature model (TTM). We present a new analytical source term in the TTM, which takes into account the excited plasmon subsystem and therefore spatial periodicity. The developed method can be used to study the mechanisms of laser energy absorption under controlled conditions and for investigation of the properties of the excited SPP.

O 44: Ultrafast Electron Dynamics II (joint session O/MA)

Time: Tuesday 10:30–13:30 Location: WIL B321

Invited Talk O 44.1 Tue 10:30 WIL B321

Attosecond coherent manipulation of electrons in tunneling microscopy — •Manish Garg[1] and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

We demonstrate coherent manipulation of electrons in a tunnel junction of a scanning tunneling microscope, by tuning the carrier-envelope-phase (CEP) of two-cycle long (< 6 fs) optical pulses. We explore two different tunneling regimes at the tunnel junction, photon and field-driven tunneling and demonstrate transition from one to the other regime. Spatially localized and atomically strong electric fields of strength ~ 1V/Å substantially modulate the tunneling barrier on attosecond timescales, hence allowing taming of flow of electrons to either side of the tunnel junction. Capability to tune CEP with precision of less than 0.1π enables manipulation of electron tunneling at timescales of ~ 200 as. The strong atomic confinement of tunneling current induced by laser pulses enables optical-field driven tunneling microscopy. Real-time tracing of decay dynamics of oscillations of quasiparticles (localized-surface plasmon) in a gold nanorod is studied with a nanoscale probe in tunneling contact; enabling concurrently angstrom-scale and sub-fs resolution. We expect our results to enable inducing, tracking, and controlling electronic current at atomic scales and pave the way to petahertz coherent nanoelectronics and microscopy.

O 44.2 Tue 11:00 WIL B321

Atomically resolved femtosecond pump probe measurements on Ta2NiSe5 — •Lukas Arnhold[1], Gregory McMurtrie[1], Shaoxiang Sheng[1], Mohamad Abdo[1,2], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

The investigation of new and interesting phases in solids is one of the major goals of condensed matter physics. Ta2NiSe5, a putative excitonic insulator, is a material in which the exciton binding energy can exceed the band gap energy, leading to spontaneous condensation of excitons [1] following Bose-Einstein-statistics.

In such a material, it would be particularly interesting to locally break individual excitons and observe the re-condensation into the ground state.

To this end, we combine scanning tunneling microscopy (STM) with ultrafast THz light pulses. This boosts the STM's time resolution to the femtosecond range [2] making it possible to observe the fast electronic dynamics of correlated ground states in real space.

In static measurements, as we decrease the tunnel resistance, we observe a closing of the excitonic band gap. This closing coincides with an unusual increase of THz current in pump probe measurements. We study the dynamic response with atomic spatial resolution in particular around atomic defects in the surface layer.

[1] Lu, Y. et al., Nat Commun 8, 14408 (2017) [2] Cocker, T. et al., Nature Photon 7, 620*625 (2013)

O 44.3 Tue 11:15 WIL B321

Ultrafast nano-imaging of the order parameter in a structural phase transition — •Thomas Danz, Till Domröse, and Claus Ropers — 4th Physical Institute – Solids and Nanostructures, University of Göttingen, Germany

Over the past decades, ultrafast optical techniques have considerably shaped our understanding of homogeneous materials, while transmission electron microscopy has greatly contributed to elucidating atomic structures and compositions on the sub-nanometer scale. Combining these concepts, ultrafast transmission electron microscopy allows for resolving femtosecond dynamics in heterogeneous materials using imaging, diffraction, and spectroscopy [1].

Here, we employ the Göttingen Ultrafast Transmission Electron Microscope (UTEM) [2] to demonstrate the ultrafast real-space mapping of the order parameter for a charge-density wave phase transition in the correlated material 1T-TaS$_2$. Specifically, we track the evolution of domain patterns on femtosecond to picosecond time and nanometer length scales, extracting characteristic observables not accessible by ultrafast electron or x-ray diffraction.

Additionally, we show that prominent features in the spatio-temporal domain evolution can be modeled in a time-dependent Ginzburg-Landau approach, allowing us to distinguish different regimes of the observed dynamics.

[1] A. H. Zewail, Science **328**, 187 (2010).

[2] A. Feist, Th. Danz *et al.*, Ultramicroscopy **176**, 63 (2017).

O 44.4 Tue 11:30 WIL B321

Visualisation of coherent phonons in Bi$_2$Se$_3$ by time-resolved photoelectron diffraction — •Klara Volckaert[1], Davide Curcio[1], Dmytro Kutnyakhov[2], Steinn Agustsson[3], Kevin Bühlmann[4], Federico Pressacco[2], Michael Heber[2], Siarhei Dziarzhytski[2], Harald Redin[2], Yves Acremann[4], Jure Demsar[3], Wilfried Wurth[2], Charlotte E. Sanders[5], and Philip Hofmann[1] — [1]Aarhus University, Aarhus, Denmark — [2]DESY, Hamburg, Germany — [3]Johannes Gutenberg-University, Mainz, Germany — [4]ETH Zürich, Zürich, Switzerland — [5]Rutherford Appleton Laboratories, Harwell, United Kingdom

We have developed X-ray photoelectron diffraction (XPD) as a pump-probe technique allowing for the visualisation of structural changes on femtosecond timescales. We use this new technique to observe the structural dynamics of Bi$_2$Se$_3$ when excited by a 800 nm optical pump pulse. Terahertz oscillations of the fine structure within the resulting XPD pattern were observed, which could originate from the excited A$_1g$ coherent phonons. These experiments were carried out at the FLASH free electron laser using a time-of-flight momentum microscope, which allows for simultaneous mapping of the emission angles in addition to kinetic energy of the electrons during a photoemission experiment (see D. Kutnyakhov et al. arXiv:1906.12155 (2019)).

O 44.5 Tue 11:45 WIL B321

Radio frequency controlled electron pulses for time-resolved LEED — •Dennis Epp, Marcel Möller, Gero Storeck, and Claus Ropers — IV. Physical Institute, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Solid state surface systems display complex structural and electronic phases, with properties that may drastically differ from the bulk [1]. The coupling between electronic, lattice and spin degrees of freedom can be studied by ultrafast techniques. The recently developed method of Ultrafast Low-Energy Electron Diffraction (ULEED) is suitable for studying such structural dynamics on surfaces [2,3,4]. In this stroboscopic method, miniaturised laser-driven photoelectron sources generate ultrashort low-energy electron pulses to probe pump-induced changes to the surface structure [2,3], with a temporal resolution down to 1 ps. This contribution will focus on the characterization and control of low-energy electron beams by radio-frequency fields. First measurements of the beam properties resolved by a streaking field and further strategies for pulse compression will be discussed. [1] J. M. Kosterlitz. & D. J. Thouless, J. Phys. C 6, 1181*1203 (1973). [2] G. Storeck et al., Structural Dynamics 4, 044024 (2017). [3] S. Vogelgesang, et al., Nature Physics 14,184-190 (2018). [4] G. Horstmann et al., in preparation.

O 44.6 Tue 12:00 WIL B321

VUV user station for femtosecond transmission, reflectivity and ellipsometry experiments — •Shirly Espinoza — ELI Beamlines. Institute of Physics. Czech Academy of Science. Czech Republic

Here, we present a versatile experimental platform, located in ELI Beamlines facility in the Czech Republic, dedicated to ultrafast pump-probe VUV absorption, transmission and ellipsometry with time resolution about 100 fs [1]. The whole system is based on a 30 mJ, 15 fs, 1 kHz in-house-developed laser with central wavelength 830 nm [2]. Its pulses are subsequently transformed into the desired pump and probe beams.

The platform is enclosed in an ultrahigh vacuum chamber equipped with reflective polarizing optics. This setup is equipped with a cryostat for measurements at temperatures from 20 K to 350 K. The upcoming upgrade with switchable Helmholtz coils will enable the experiments in magnetic field up to 1.5 T at 1 kHz. We present the experimental details of this cutting edge platform and discuss the possibilities that external scientists have to carry on their measurements on it.

Supported by the projects Structural dynamics of biomolecular systems (CZ.02.1.01/0.0/0.0/15-003/0000447) and Advanced research using high intensity laser produced photons and particles (CZ.02.1.01/0.0/0.0/16-019/0000789) from the European Regional Development Fund.

[1] S. Espinoza et al., Appl. Surf. Sci. 421, 378-382 (2017)

[2] F. Batysta et al., Opt. Express 24, 17843-17848 (2016)

Invited Talk O 44.7 Tue 12:15 WIL B321

Ultrafast dynamics of charge transfer and Frenkel excitons in molecular thin films — •Benjamin Stadtmüller — University of Kaiserslautern and Research Center OPTIMAS, Erwin-Schroedinger-Str. 46, 67663 Kaiserslautern, Germany

Molecular complexes are highly flexible materials with intriguing opportunities for future photovoltaic and spintronic applications. The crucial device-relevant processes in molecular materials are the excited state dynamics and the carrier transport. Despite their common origin - the molecular band structure - their interplay is far from being understood. In this work, we focus on the link between the excited state dynamics of excitons in fullerene thin films and the resulting ensemble dynamics of the transport states of the entire film using time- and momentum resolved photoemission with fs-XUV radiation. Upon the optical excitation of excitons in C_{60} films, we reveal a transient modification of the energy level alignment of the molecular valence states, which can be identified as the signature of charge transfer (CT) excitons in molecular materials [1]. Taking advantage of this observation, we are able to disentangle the dynamics of CT and Frenkel excitons in (endohedral) fullerene films. We find different decay dynamics depending on the sample temperature or the charge doping concentration of the molecular film. Finally, we will provide a first view onto the momentum-space signature of CT and Frenkel excitons as a first step towards imaging the orbital character of both types of excitons in molecular films. [1] Nat. Commun. 10, 1470 (2019)

O 44.8 Tue 12:45 WIL B321

Momentum resolved ultrafast organic molecular exciton dynamics — •Ralf Hemm, Martin Mitkov, Florian Haag, Sebastian Emmerich, Sebastian Hedwig, Martin Aeschlimann, and Benjamin Stadtmüller — University of Kaiserslautern (TUK) and research center OPTIMAS, Erwin-Schroedinger-Str.46, 67663 Kaiserslautern, Germany

Mapping the lowest unoccupied molecular orbitals (LUMOs) of an organic semiconducting thin film in momentum space is one of the great challenges of ultrafast surface science. Especially on the femto- to picosecond timescale, resolving the transient molecular orbital structure can help to disentangle excitonic decay mechanisms.

Here, we apply bichromatic time-resolved two-photon momentum microscopy [1] to image the excited state dynamics of excitons in molecular materials in momentum space. Our model system is a multilayer of ordered C60 on Cu(111), for which the energy dependent exciton dynamics was already reported in literature [2]. In this talk, we will therefore focus on the momentum space signatures of the excited states. We will identify the characteristic momentum space signatures of the excited states and follow their evolution above and below the critical temperature for the structural phase transition of C60. This will allow us to correlate the exciton dynamics in momentum space to the dominant energy and momentum dissipation process in molecular materials.

[1] F. Haag et al., Rev. Sci. Instr. 90, 103104 (2019)

[2] A. Rosenfeldt et al., J. Chem. Phys. 133, 23 (2010)

O 44.9 Tue 13:00 WIL B321

Ultrafast excited state dynamics and transient band structure renormalizations in endohedral metallofullerenes — •Sebastian Hedwig, Sebastian Emmerich, Benito Arnoldi, Johannes Stöckl, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany

Fullerenes have been object to intense research in the past decades, with promising potential for their implementation in optoelectronic devices. Embedding metal atoms or clusters into the fullerene by chemical synthesis can alter the cage symmetry, which strongly influences the molecular transport properties as well as the available relaxation channels of excited electronic states. Of special interest in this field is the cluster-cage electron transfer. Here, we present a time resolved photoemission study carried out on thin films of the prototypical endohedral metallofullerene $Sc_3N@C_{80}$ in a fs UV-pump XUV-probe experiment. We observe a transient broadening of all (polaronic) molecular valence states which follows the timescale of the exciton formation and decay in the molecular films, in analogy to our recent findings for the fullerene C_{60} [1]. Moreover, we show that the exciton and polaron dynamics are strongly altered upon K intercalation of the pristine film. This enables us to draw conclusions regarding cluster-cage charge transfer on ultrafast timescales. [1] B. Stadtmüller et al., Nat Commun 10, 1470 (2019)

O 44.10 Tue 13:15 WIL B321

Temperature effects on the electron dynamics of metal-organic interface states — •Klaus Stallberg[1], Masahiro Shibuta[1,2], and Ulrich Höfer[1] — [1]Fachbereich Physik, Philipps Universität Marburg, Germany — [2]Keio Institute of Pure and Applied Sciences, Keio University, Yokohama, Japan

The presence of electronic interface states (IS) can strongly affect the electron dynamics at organic/metal interfaces. In particular, IS mediated charge transfer has been observed for model systems comprising few layers of π-conjugated organic molecules on single-crystalline metal surfaces. The formation of Shockley derived IS is well understood in the meantime and experimentally observed properties, such as the free-electron-like momentum dispersion as well as the energy onset, are well reproduced by *ab initio* calculations. In contrast, the IS electron dynamics eludes a consistent theoretical description so far, and systematic experimental studies are still missing.

Here, we systematically investigate temperature effects on the formation and the relaxation dynamics of the IS for the organic/metal systems NTCDA/Ag(111) and PTCDA/Ag(111). Using two-photon photoemission (2PPE), we observe a pronounced decrease of the IS energy for increasing temperatures, which we attribute to an extended molecule-metal binding distance due to phonons in the molecular layer. Moreover, a drastic increase of the IS lifetime with temperature is found. While it can qualitatively be explained with a reduced phase space for electron scattering with metal bulk states, this temperature effect is much stronger than expected from a simple physical model.

O 45: Solid-Liquid Interfaces II: Reactions and Electrochemistry

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

O 45.1 Tue 10:30 WIL C107

Photo-sensitive 2D-arrangement of -OH/H_2O on brookite TiO_2 (210) — •Lei Yang[1], Eero Holmstrom[2], Takeshi Fukuma[3], and Adam Foster[2] — [1]WPI Nano Life Science Institute, Kanazawa University, Kanazawa 920-1192, Japan — [2]COMP, School of Science, Aalto University, P.O. Box 11100, FI-00076 Aalto, Finland — [3]Division of Electrical Engineering and Computer Science, Kanazawa University, Kanazawa 920-1192, Japan

The brookite phase of TiO_2 is much less explored than the other two polymorphs (rutile and anatase), despite its potential applications in photocatalytic CO_2 reduction and water splitting. The first hydration layer and surface hydroxyl groups on brookite (210) surface and their structural changes under photo-irradiation have been considered to play significant roles in the process of such applications, thus will be elucidated at the atomic scale in this study by means of combining high-resolution liquid-environment atomic force microscopy (AFM) imaging using a custom-built equipment and ab initio molecular dynamics simulations. An interesting structural feature of the hydration layer of brookite TiO_2 (210) was observed by AFM imaging, which later disappeared under ultraviolet irradiation in preliminary results. The origins of the feature and its photo-switching behavior will be clarified.

O 45.2 Tue 10:45 WIL C107

CPMD Performance Optimization for Large-Scale Simulations of Vibrational Spectra at Solid-Liquid Interfaces — •Tobias Klöffel[1,2], Paul Schwarz[1], Gerald Mathias[3], and Bernd Meyer[1] — [1]ICMM and CCC, FAU Erlangen-Nürnberg — [2]HPC Group at RRZE, FAU Erlangen-Nürnberg — [3]LRZ, Garching

We present our recent optimizations of the ultra-soft pseudo-potential (USPP) code path of the *ab initio* Car-Parrinello molecular dynamics program CPMD (www.cpmd.org). All relevant USPP routines have been revised to fully support hybrid MPI+OpenMP parallelization. For two time-critical routines, namely the multiple distributed 3d FFTs of the electronic states and a key distributed matrix–matrix multiplication, we have implemented hybrid parallel algorithms with overlapping computation and communication. Our latest improvements include autotuning of overlapping computation and communication, communication avoiding, and node level MPI+MPI shared memory parallelization to fully exploit the powerful compute capabilities of SuperMUC-NG 48 core nodes. The achievements in performance and scalability are demonstrated on simulations of liquid water with 256 and up to 2048 molecules. With the improved CPMD code we were able to study the structural evolution of water on ZnO for increasing water coverage from the monolayer to thick water films by providing fingerprints of anharmonic vibrational spectra. Altogether, we performed 1 ns of *ab initio* simulations for systems with up to 368 atoms.

[1] X. Yu, P. Schwarz, A. Nefedov, B. Meyer, Y. Wang, Ch. Wöll,

Angew. Chem. Int. Ed. **58** (2019) 17751.

Invited Talk O 45.3 Tue 11:00 WIL C107

In-situ identification of catalytically active surface sites using electrochemical STM — •Aliaksandr Bandarenka — Technical University of Munich, James-Franck-Str. 1, 85748 Garching, Germany

In the presentation, it will be demonstrated that common electrochemical STMs can be used to map the catalytic activity of the electrode surfaces with high spatial resolution. By monitoring relative changes in the tunnelling current noise, active sites can be distinguished in an almost quantitative fashion. Several important for energy provision reactions are used as model systems: the hydrogen evolution, oxygen reduction and oxygen evolution reactions. The above mentioned approach allowed to evaluate directly the nature of active sites at Pt(111), Pt3Ni(111), Pt and Pd monolayers on Au(111), HOPG, MoS2, MoSe2 and IrO2 electrodes in acidic and alkaline media.

References

- E. Mitterreiter, Y. Liang, M. Golibrzuch, D. McLaughlin, C. Csoklich, J.D. Bartl, A. Holleitner, U. Wurstbauer, A.S. Bandarenka. NPJ 2D Materials and Applications 3 (2019) 25 - Y. Liang, C. Csoklich, D. McLaughlin, O. Schneider, A.S. Bandarenka. ACS Applied Materials and Interfaces 11 (2019) 12476*12480 - Y. Liang, D. Mclaughlin, C. Csoklich, O. Schneider, A.S. Bandarenka. Energy & Environmental Science 12 (2019) 351-357 - J.H.K. Pfisterer, Y. Liang, O. Schneider, A.S. Bandarenka. Nature 549 (2017) 74*77

O 45.4 Tue 11:30 WIL C107

In-situ STM imaging of self-activated CO oxidation on Cu(111) electrocatalysts — Andrea Auer[1], Eva-Maria Wernig[1], Xing Ding[2], Aliaksandr Bandarenka[2], Nicolas Hörmann[3], Karsten Reuter[3], and •Julia Kunze-Liebhäuser[1] — [1]Institute of Physical Chemistry, University of Innsbruck, Innsbruck, Austria — [2]Physics of Energy Conversion and Storage, Technische Universität München, Garching, Germany — [3]Theoretical Chemistry, Technische Universität München, Garching, Germany

Carbon monoxide (CO) is a key intermediate in the electro-oxidation of energy carrying fuels. In this work, the ability of Cu(111) single crystals to electrochemically oxidize CO at low overpotentials is reported. In-situ infrared spectroscopy confirms weak adsorption of CO on Cu(111) as well as its oxidation to CO_2. Electrochemical scanning tunneling microscopy (EC-STM) reveals that during CO oxidation the Cu(111) surface reconstructs and concomitantly adsorbs OH, while forming low-dimensional Cu nanostructures that are effectively stabilized through the presence of CO. Therefore, CO itself activates the (111) surface of Cu and enhances its own oxidation. The potential of maximum entropy which is closely associated with the potential of zero charge (pzc) has been determined for Cu(111) and correlated with the corresponding surface structures through EC-STM studies. In combination with DFT calculations that include the effects of applied potential and the solvent environment, this helps to achieve a true atomistic understanding of the interfacial structures and the electrocatalytic activity.

O 45.5 Tue 11:45 WIL C107

Electrically triggered reactions at interfaces — •Florian Deissenbeck[1], Lei Yang[1], Marc Pander[1], Fang Niu[2], Andreas Erbe[1], Christoph Freysoldt[1], Mira Todorova[1], Jörg Neugebauer[1], and Stefan Wippermann[1] — [1]Max-Planck-Institut für Eisenforschung, Germany — [2]NTNU Trondheim, Norway

Presently, few experimental techniques are able to directly probe the microscopic structure of solid-liquid interfaces. In order to develop robust strategies to interpret experiments and validate theory, we carried out ab initio molecular dynamics (AIMD) calculations for interfaces between liquid water and well-controlled prototypical semiconductor substrates, supplemented by attenuated total internal reflection (ATR-IR) spectroelectrochemical measurements. We introduce a potentiostat scheme, allowing us to perform MD simulations either at constant electric field or constant dielectric displacement. We discuss interactions between commonly used thermostats and the potentiostat, and suggest to introduce temperature-induced dipole fluctuations directly into the potentiostat scheme. This new approach has been validated by extensive benchmarks and is shown to not affect the vibrational spectra at the solid-liquid interface. Support from BMBF NanoMatFutur grant No. 13N12972 is gratefully acknowledged.

O 45.6 Tue 12:00 WIL C107

Dependence of Electron and Ion Transport on the Intermolecular Coupling in Fluorinated Phthalocyanine Thin Films as Electrochromic Materials — •Thi Hai Quyen Nguyen[1], Marius Pelmus[2], Sergiu M. Gorun[2], and Derck Schlettwein[1] — [1]Justus Liebig University Gießen, Institute of Applied Physics — [2]Seton Hall University, Department of Chemistry and Biochemistry

Phthalocyanines as organic ionic and electronic conductors are of great interest for the application in electrochromic devices. An influence of the degree of fluorination in copper phthalocyanines on the intermolecular coupling of the molecules in the solid state and, thus, on the rate of electron and ion transport was observed: For $F_{16}PcCu$ the transport of electrons was faster than the diffusion of ions as opposed to $F_{64}PcCu$. In this work, thin films of a new type of fluorinated phthalocyanine ($F_{40}PcCu$) were prepared by physical vapor deposition. The dependence of the intermolecular coupling on the film thickness was analyzed by in situ UV/Vis spectroscopy. The transport of electrons and ions in these films as well as their electrochromic behaviour were investigated by electrochemical and spectroelectrochemical measurements with an aqueous solution of KCl as electrolyte. The films provided a well-balanced, equally fast transport of electrons and ions. The optical absorption spectra revealed reversible changes of the films upon reduction with intercalation of the K^+ counter ions and re-oxidation with extraction of the counter ions. Fast and stable electrochromic switching of the films was achieved over at least 200 cycles.

O 45.7 Tue 12:15 WIL C107

***Ab initio* thermodynamics study of two-dimensional Ir and Ru oxide nanosheets as active oxygen evolution reaction catalyst in acidic media** — •Po-Yuan Huang, Yonghyuk Lee, Christoph Scheurer, and Karsten Reuter — Technical University of Munich, Germany

Iridium and ruthenium oxides are among the most active oxygen evolution reaction (OER) catalysts in acidic media, with iridium oxide exhibiting somewhat lower activity, but higher durability. As one promising strand to maximize precious atom efficiency, highly active two-dimensional hexagonal nanosheets of both oxides have recently been reported [1,2]. Here, we use density-functional theory based *ab initio* thermodynamics to systematically compare the stable surface terminations of the isostructural Ir and Ru nanosheets as a function of the applied potential. Extending our investigation over both the sheet surface and the sheet edge, we find the Ir nanosheet to deprotonate already at much lower potentials. Thermodynamic Gibbs free energy barriers along the generally accepted OER reaction pathway are investigated to gain insight into the overpotentials and assess whether the earlier deprotonation can rationalize the different Tafel slopes measured for the two oxide nanosheets.

[1] D. Weber *et al.*, J. Mater. Chem. A **6**, 21558 (2018).

[2] S. Laha *et al.*, Adv. Energy Mater. **9**, 1803795 (2019).

O 45.8 Tue 12:30 WIL C107

Chemistry and phase transition of pyridine derivatives on gold electrode probed by vibrational sum frequency generation — Xin Gong, Martin Wolf, R. Kramer Campen, and •Yujin Tong — Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany

Pyridine and its derivatives are of both practical and fundamental importance in electrochemistry. While the flat to vertical phase transition has been extensively studied and well understood, knowledge on the deprotonation and protonation chemistry at the electrode/solution interface in aqueous solution is still very limited. In the current study, we employed vibrational sum frequency generation (VSFG) to monitor both the structral and chemical evolution of 4-(dimethylamino)pyridine (DMAP) adsorbed on a gold electrode as a function of external bias. Significant spectral changes are observed as a function of the applied bias voltage in the cyclic voltammetry. These features can be unambiguously assigned to the protonation/deprotonation and orientational changes respectively. The information revealed by this study is essential for the application of pyridine derivatives in nanoparticle manipulation, enhancement of CO_2 reduction, formic acid electro-oxidation, etc.

O 45.9 Tue 12:45 WIL C107

Influence of surface coating on electrochemical performance of Ni-rich NCM cathodes for Lithium ion batteries — •Rajendra Singh Negi and Matthias T. Elm — Center for Materials Research, Justus-Liebig-University Gießen, Germany, HeinrichBuff-Ring 16, 35392 Gießen

The Ni-rich NCM based cathode material has allured great research interest owing to its high energy density, high capacity and low costs. Nonetheless, the rapid capacity fading still hinders its wide range application. Surface modification became a feasible approach to handel this issue. However, achieving a homogenous coating using a simple approach is still challenging. In this work, a surface-active -OH group assisted homogenous Al2O3 coating on the NCM have been achieved. The Al2O3 coated cells show improved capacity retention (89.5% after 130 cycles) during long-term cycling test compared to pristine cells (i.e. 38.3% after 130 cycles). In addition, Electrochemical Impedance Analysis (EIS) showed the tremendous increase in cell resistance of uncoated electrodes compared to coated electrodes after long-term cycling.

O 45.10 Tue 13:00 WIL C107

Influence of Porosity on the Protonic Surface Conductivity of Yttria-Stabilized Zirconia Thin Films — •Erdogan Celik[1], Torsten Brezesinski[2], and Matthias T. Elm[1] — [1]Center for Materials Research, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Institute of Nanotechnology; Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

Yttria-stabilized zirconia (YSZ) is among the best-performing solid-state electrolytes for applications in fuel cells or heterogeneous catalysis because of its outstanding ionic conductivity at high temperatures. In addition, nanostructured oxides exhibit an even enhanced protonic conductivity at low temperatures. Nevertheless, the influence of material morphology on the protonic transport is still controversially discussed. To study the effect of surface and porosity on the protonic conductivity, porous YSZ thin films were prepared pulsed laser deposition. Such films represent an ideal model system because of their high surface-to-volume ratio. Electrochemical impedance spectroscopy was carried out as a function of temperature, oxygen activity and humidity of the surrounding atmosphere. The total conductivity is found to increase under humidified atmosphere conditions at all temperatures due to protonic surface conduction, especially below 100 °C. When coating a nanometer-thick layer of titania (TiO2) on the porous YSZ network using atomic layer deposition (ALD), the proton transport is suppressed, thus indicating the significant influence of surface properties on the protonic transport.

O 45.11 Tue 13:15 WIL C107

A DFT study of early steps of Au island nucleation on $c(2 \times 2)$-Cl Au(001) surface — •Alexandra C. Dávila and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, CAU Kiel, Germany

Electrodeposition experiments of Au on a Au(001) electrode in a Cl^- containing electrolyte have shown a dependence of the growth mode on sample potential and Au deposition rate [1]. While island nucleation is essential for layer-by-layer growth, a detailed atomic-scale description of the early steps leading to the formation of Au ad-structures on the $c(2 \times 2)$-Cl covered Au(001) electrode surface is still lacking (for Au adsorption structures at low Cl coverage see [2]). We present DFT calculations, carried out with PWscf [3], of Au_n adatom structures for $n \leq 4$ on the $c(2 \times 2)$-Cl Au(001) surface without as well as in the presence of a small number of Cl vacancies, and investigate the stability as a function of Cl chemical potential. The electrolyte has not been included in the simulations. In the absence of Cl vacancies $Au_{ad}Cl_2$ chains form on the surface. In the range of Cl chemical potential where Cl vacancies become part of the equilibrium atomic adsorption structure, we find Cl vacancies to modify and to bind to the Au ad-structures. In this case, the energy gain due to the addition of a Au_{ad} monomer increases from about 0.06 eV to about 0.23 eV. I.e, the presence of Cl vacancies tends to promote Au ad-structure formation.

[1] K. Krug *et* al., Phys. Rev. Lett. **96**, 246101 (2006).
[2] Mesgar *et* al., ChemPhysChem **11**, 1395 (2010).
[3] P. Giannozzi *et* al., J. Phys. Condens. Matter **21**, 395502 (2009).

O 46: 2D semiconductors and van der Waals heterostructures IV (joint session HL/DS/O)

Time: Tuesday 14:00–16:00 Location: POT 81

O 46.1 Tue 14:00 POT 81

Resolving the interlayer charge transfer in van der Waals heterostructures by ultrafast THz emission nanoscopy — •Markus Plankl[1], Martin Zizlsperger[1], Fabian Mooshammer[1], Felix Schiegl[1], Fabian Sandner[1], Markus A. Huber[1], Tom Siday[1], Jessica L. Boland[2], Tyler L. Cocker[3], and Rupert Huber[1] — [1]Department of Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Photon Science Institute, University of Manchester, Manchester M13 9PL, UK — [3]Department of Physics and Astronomy, Michigan State University, 48824 Michigan, USA

In van der Waals heterostructures composed of two transition metal dichalcogenide monolayers, photogenerated electron-hole pairs are spatially separated on ultrafast timescales, giving rise to the formation of interlayer excitons. Yet, the underlying interlayer charge transfer has only been investigated in a spatially averaged manner. Consequently, probing nanoscale transfer efficiencies and tunneling rates has so far remained elusive. Since the tunneling of photoexcited charge carriers between adjacent layers represents an ultrafast current along the out-of-plane direction, a concomitant electromagnetic pulse in the terahertz spectral range is emitted. By combining electro-optic time-domain spectroscopy with near-field microscopy, we resolve this characteristic fingerprint of the interlayer carrier dynamics on the nanoscale with sub-cycle temporal resolution. Thereby, we infer tunneling characteristics, which we relate with the nanoscale conductivity of the heterostructure.

O 46.2 Tue 14:15 POT 81

Influence of dark states on excitonic spin relaxation in transition metal dichalcogenides — •Malte Selig, Dominik Christiansen, and Florian Katsch — Technische Universität Berlin, Berlin, Germany

Energetically low lying dark exciton states with momenta well above the radiative cone manifest a significant relaxation channel for optically pumped excitons in transition metal dichalcogenides (TMDCs). While they have been demonstrated to influence the optical linewidth [1], lineshape [2], relaxation and luminescence properties [3], they can also be expected to play a crucial role for the spin relaxation of excitons.

Here we present a Heisenberg equation of motion theory for the intervalley exchange coupling, mediating the spin relaxation, and exciton phonon coupling. We demonstrate that the interplay of both mechanisms leads to unintuitive signatures in pump probe experiments where the A transition is pumped and either A or B transition are probed [4]. Additionally we reveal that the presence of energetically low lying dark excitons significantly quenches the efficiency of intervalley exchange coupling [5]. Our theoretical results shine new light on existing experimental data.

[1] M. Selig et al.,Nature Commun. 7,13279 (2016)
[2] D. Christiansen et al., Phys. Rev. Lett. 119, 187402 (2017)
[3] M. Selig et al., 2D Mat. 5, 035017 (2018)
[4] M. Selig et al., Phys. Rev. Research 1, 022007(R) (2019)
[5] M. Selig et al., arXiv:1908.11178 (2019)

O 46.3 Tue 14:30 POT 81

Kelvin probe force microscopy-based direct measurements of contact resistance in 2D semiconductor thin film transistors — •Aleksandar Matkovic[1], Andreas Petritz[2], Gerburg Schider[2], Markus Krammer[4], Markus Kratzer[1], Michael Gärtner[3], Andreas Terfort[3], Christian Teichert[1], Egbert Zojer[4], Karin Zojer[4], and Barbara Stadlober[2] — [1]Institute of Physics, Montanuniversität Leoben, Leoben, Austria. — [2]Joanneum Research MATERIALS, Institute for Surface Technologies and Photonics, Weiz, Austria. — [3]Institute of Solid State Physics, Graz University of Technology, Graz, Austria. — [4]Institut für Anorganische und Analytische Chemie, Goethe-University Frankfurt, Frankfurt am Main, Germany.

This study aims at direct determination of the contact resistance in MoS_2-based thin film transistors (TFTs). Exfoliated single-crystal flakes of MoS_2 have been used in a bottom-contact TFT configuration. Pyrimidine-containing self-assembled monolayers (SAMs) were employed to tune the work function of gold electrodes. Kelvin probe force microscopy measurements were carried out during operation of the devices in order to directly image potential drops across the channel and to study the influence of different SAM treatments on the contact resistance. By independently imaging potential drops at both, carrier injection and extraction points, we demonstrate the asymmetry of contact resistances in MoS_2-based TFTs, as well as their non-linear and bias-dependent behavior.

O 46.4 Tue 14:45 POT 81

MOVPE of large-scale 2D-2D heterostructures for optoelectronic applications — Annika Grundmann[1], Clifford McAleese[2], Ben Richard Conran[2], Andrew Pakes[2], Dominik Andrzejewski[3], Tilmar Kümmel[3], Gerd Bacher[3], Kenneth Bo Khin Teo[2], •Michael Heuken[1,4], Holger Kalisch[1], and Andrei Vescan[1] — [1]Compound Semiconductor Technology, RWTH Aachen University, Aachen, Germany — [2]AIXTRON Ltd., Cambridge, United Kingdom — [3]Werkstoffe der Elektrotechnik and CENIDE, University Duisburg-Essen, Duisburg, Germany — [4]AIXTRON SE, Herzogenrath, Germany

Vertical heterostructures of two (or more) different 2D layer provide many fascinating opportunities by combining the unique intrinsic chemical, physical and (opto)electronic properties of 2D materials. Without the need of consideration of lattice matching, a nearly infinite number of potential combinations of 2D layers are possible. Transition metal dichalcogenide (TMDC) monolayers are the most widely studied 2D semiconductors beyond graphene and thus provide a strong basis for understanding the properties of 2D heterostructures. Unlike mechanical exfoliation, direct successive growth of 2D-2D heterostructures requires a controlled synthesis of the respective monolayers with pristine interlayer interfaces and no intermixing of disparate layers. Here, we report on direct successive MOCVD of vertical MoS_2-WS_2 and WS_2-MoS_2 heterostructures as well as MOCVD of WS_2 and MoS_2 onto graphene previously deposited in another MOCVD reactor.

O 46.5 Tue 15:00 POT 81

Efficient Hot Electron Transfer at Graphene-WS2 van der Waals Bilayers — SHuai Fu and •Hai Wang — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Hybridization of (semi-)metallic and semiconducting monolayers, such as graphene and layered transition metal dichalcogenides (TMDs), enables efficient and sensitive photodetectors, by combing the synergetic properties of strong absorption at exciton resonances in TMDs, efficient charge transfer cross the interfaces and ultrahigh charge mobility in graphene. In spite of the great advance in devices, the fundamental understanding of the mechanism underlying the ultrafast charge flow across the heterostructures lags far behind, and effective means of controlling its efficiency have not been established.

Employing Terahertz spectroscopy, we shed light on the fundamentals of ultrafast interfacial nonequilibrium dynamics in graphene-WS2 van der Waals bilayers. We report an efficient and ultrafast hot electron injection from graphene to WS2, which competes with hot carrier heating process in graphene. We will discuss the mechanism underlying the hot electron charge transfer process, and factors governing its efficiency and lifetime of interfacial charge states, which are critical for efficient optoelectronics (i.e. photodetectors) based on van der Waals heterostructures.

O 46.6 Tue 15:15 POT 81

Excitation Induced Dephasing in Monolayer Transition Metal Dichalcogenides — •Florian Katsch, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, 10623 Berlin, Germany

Exceptionally strong Coulomb interactions in atomically thin transition metal dichalcogenides lead to tightly bound electron-hole pairs (excitons) dominating their linear and nonlinear optical response. The latter involves bleaching [1], energy renormalizations [2], and higher-order Coulomb correlation effects like biexcitons [3] and excitation induced dephasing (EID) [4]. Whereas bleaching, energy renormalizations, and biexcitons are widely investigated, EID in exciton dominated semiconductors so far lacks microscopic calculations. Within a Heisenberg equations of motion formalism we identify the coupling between excitons and exciton-exciton scattering continua as the most prominent process causing EID and sideband formation. Evaluating the EID for single-layers of transition metal dichalcogenides, we find a good agreement with recent experiments [5,6].

[1] M. Selig *et al.*, Physical Review Research **1**, 022007 (2019).
[2] J. Shacklette and S. Cundiff, Physical Review B **66**, 045309 (2002).
[3] E. Sie *et al.*, Physical Review B **92**, 125417 (2015).
[4] H. Wang *et al.*, Physical Review Letters **71**, 1261 (1993).
[5] G. Moody *et al.*, Nature Communications **6**, 8315 (2015).
[6] E. Martin *et al.*, arXiv preprint arXiv:1810.09834 (2018).

O 46.7 Tue 15:30 POT 81

Dirac physics in honeycomb semiconductors — •Christiaan Post[1], Nathali Franchina Vergel[2], Tomas Meerwijk[1], Jesper Moes[1], Xavier Wallart[2], Guillaume Fleury[3], Ludovic Desplanque[2], Ingmar Swart[1], Christophe Delerue[2], Bruno Grandidier[2], and Daniel Vanmaekelbergh[1] — [1]Debye Institute for Nanomaterials Science, Utrecht, The Netherlands — [2]Institute of Electronics, Microelectronics and Nanotechnology (IEMN), Lille, France — [3]Laboratory for Chemistry of Organic Polymers (LCPO), Bordeaux, France

III-V semiconductor quantum wells have obtained a central place in advanced logics and opto-electronics. In more recent research, the effects of a nano scale geometry forming a periodic scattering potential in the lateral directions of the quantum well have been discussed and calculated. In case of a nano-scale honeycomb geometry, Dirac cones are formed similar as for graphene, creating massless fermions while the semiconductor quantum well band gap remains nearly unaltered.

In this research, we report on the electronic characterization of a modulated InGaAs quantum well with a honeycomb symmetry. The honeycomb symmetry is fabricated by perforating the quantum well with a triangular symmetry using nano-scale lithography. By performing scanning tunneling microscopy experiments, the electronic properties of the sample are intensively investigated, showing the combined electronic properties of a two-dimensional material and Dirac-like features. Muffin-tin calculations support the obtained experimental results, revealing the exciting properties of these novel materials.

O 46.8 Tue 15:45 POT 81

Structural and electronic properties of twisted MoS_2 bilayers — •Somepalli Venkateswarlu, Andreas Honecker, and Guy Trambly de Laissardière — Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Université de Cergy-Pontoise, France

Vertically stacked transition metal dichalcogenides of multilayer structures have gained increasing attention because of their fascinating features in electronics and optical properties [1]. We performed calculations of structural and electronic properties of nontwisted and twisted MoS_2 bilayers using first-principle calculations [ABINIT][2] and the tight-binding (TB) method. Our results reveal significant differences in the band structures of twisted and nontwisted ones: the appearance of a crossover between direct and indirect band gap, gap variation, and atomic relaxations. For rather large angles, the band structures are very similar for different rotation angles [3]. For the smallest angles, TB calculations predict some flat bands in the valence band and conduction band. As in twisted bilayer graphene, the corresponding states are localized in the AA stacking region of the Moiré pattern.

[1] E. S. Kadantsev, P. Hawrylak, Solid State Comm. **152**, 909 (2012).

[2] X. Gonze *et al.*, Comp. Mat. Sci. **25**, 478 (2002). https://www.abinit.org.

[3] Z. Wang *et al.*, J. Phys. Chem. C **119**, 4752 (2015).

O 47: Poster Session - 2D Materials: Electronic Structure, Excitations, etc.

Time: Tuesday 18:15–20:00 Location: P2/EG

O 47.1 Tue 18:15 P2/EG

Time-resolved and spatially resolved exciton dynamics in a microstructured WSe$_2$ monolayer investigated by 2D nanoscopy — •Daniel Fersch[1], Sebastian Pres[1], Victor Lisinetskii[1], Robert Schneider[2], Johannes Kern[2], Matthias Hensen[1], Rudolf Bratschitsch[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute of Physics and Center for Nanotechnology, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Atomically flat layers of transition metal dichalcogenides, e.g., WSe$_2$, are a fascinating material class with potential optoelectronic applications due to their direct bandgap and large exciton binding energies. Mechanical strain on the monolayer can lead to the formation of localized single-photon sources, which are of large interest for quantum-optical applications [1].

As these single-photon emitters are highly localized, it is beneficial to bypass the optical diffraction limit to investigate their physical nature. In this work, we therefore want to employ two-color time-resolved photoemission electron microscopy (TR-PEEM) on a WSe$_2$ monolayer to inspect local differences in the excited-state dynamics. Furthermore, we plan to use 2D nanoscopy [2,3] to directly probe the electronic structure of the material on a nanometer scale.

[1] J. Kern et al., Adv. Mater. **2016**, 28, 7101.
[2] M. Aeschlimann et al., Science **2011**, 333, 1724.
[3] B. Huber, S. Pres et al., Rev. Sci. Instr. **2019**, 90, 113103.

O 47.2 Tue 18:15 P2/EG

Develop strain manipulation techniques for STM measurement — •Jz-Yuan Juo[1], Bong Gyu Shin[1], Jack Maughan[1], Charlie Shaw[1], Soon Jung Jung[1], and Klaus Kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, DE-70569Stuttgart, Germany — [2]Institut de Physique, École Polytechnique Fédérale deLausanne, CH-1015 Lausanne, Switzerland

An atomic-scale understanding of how strain affects the electronic properties is essential for the implementation of two-dimensional (2D) materials into flexible electronics. However, the combination of low temperature scanning tunneling microscopy (STM) and strain-tunable devices remains challenging due to its technical limitations. The strain controller should fit in the STM sample holder with a maximum size of 1 cm^3 and function at ∼4 K. It should also be compatible with ultrahigh vacuum. Here, we developed a motor-based strain controller, which enabled us to apply uniaxial bending strain in situ. The polyimide film with surface roughness of ∼0.5 nm was chosen to minimize the substrate roughness induced strain. The 2D materials grown by chemical vapor deposition were transferred onto the polyimide film and tighten by clamps to deliver the strain to the 2D material effectively. The uniaxial deformation was confirmed by phonon shifts measured in Raman spectroscopy.

O 47.3 Tue 18:15 P2/EG

Highly ordered metallic phase of Indium on SiC(0001) — •Jonas Erhardt, Maximilian Bauernfeind, Victor Rogalev, Jörg Schäfer, and Ralph Claessen — Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany

Indium thin films attract attention due to diverse electronic properties, which feature for instance a two-dimensional electron gas (2DEG) [1] and superconductivity [2] in the 2D limit or Dirac-electrons in a triangular lattice. Here, we present a combined angle-resolved photoelectron spectroscopy (ARPES) and scanning tunneling microscopy (STM) study of highly ordered indium (≈ 2 monolayer) on silicon carbide (SiC). STM reveals a Kagome-like superstructure with a lattice constant of approximately 2.1 nm assigned as a $(4\sqrt{3} \times 4\sqrt{3})$R30° reconstruction. Additionally, ARPES as well as scanning tunneling spectroscopy (STS) show a metallic band structure with a pronounced electron pocket, indicative of an 2DEG. Interestingly, STS further reveals negative differential conductance (NDC), which is in contrast to the textbook interpretation as local density of states and is possibly related to substrate effects.

[1] E. Rotenberg *et al.*, Phys. Rev. Lett. **91**, 246404 (2003).
[2] T. Zhang *et al.*, Nat. Phys. **6**, 104 (2010).

O 47.4 Tue 18:15 P2/EG

Ab-initio simulation of angle-resolved photoemission spectra for transition metal dichalcogenides — •Christoph Dösinger and Peter Puschnig — Universität Graz, Universitätsplatz 5, A-8010 Graz

Angle-resolved photoemission spectroscopy (ARPES) is the most direct experimental technique to investigate the electronic structure of layered materials. ARPES band maps are routinely compared to results from ab-initio band structure calculations. However, simulations of photoemission cross sections including transition matrix element effects which provide additional insights are rare.

In this work, we perform ARPES simulations for single layers of transition-metal dichalcogenides (TMDs). Starting from density functional calculations including spin-orbit coupling, we have computed ARPES intensities within the plane wave final state approach which has proven to work surprisingly well for two-dimensional (mono)-layers of organic molecules adsorbed on metal surfaces. By comparing our simulated band maps and constant binding energy momentum maps with available experimental data for prototypical TMDs, WS2 and WSe2, we assess to what extent the simple plane wave approach can also be applied to this class of materials.

O 47.5 Tue 18:15 P2/EG

Modification of 2D materials by ultra-low energy ion implantation — •Manuel Auge[1], Michael Hennessy[2], Ursel Bangert[2], and Hans Hofsäss[1] — [1]II. Institute of Physics, Georg-August-University Göttingen, 37077 Göttingen, Germany — [2]Bernal Institute, University of Limerick, Limerick, Ireland

A new group of direct semiconductors are monolayer transition metal dichalcogenides (ML TMDs) of the form MX$_2$ (M = transition metal and X = chalcogen). The high interest in ML TMDs is based on their promising applications in nanoelectronics and photonics [1]. In order to exploit the great potential of the material, it is important to develop a controllable method for modifying the physical properties.

In our study, a unique mass selected ion beam deposition system is used to incorporate low energy ions into two dimensional (2D) lattices. Therefore, a 30 keV ion beam is decelerated in a UHV-chamber down to energies as low as 10 eV. A beam sweep ensures a uniform profile over an area of 1 cm^2 up to 2.5 cm^2. Here, we demonstrate the successful incorporation of Cr into the MoS$_2$ lattice. The integration of Cr could be verified by energy-dispersive X-ray spectroscopy (EDX) as well as by core loss electron energy loss spectroscopy (EELS). In addition, low loss EELS enables the investigation of the doping effect on the band gap of the material. Financial support by the Volkswagen Stiftung is gratefully acknowledged.

[1] K.F. Mak *et al.*, Phys. Rev. Lett. **105**, 136805 (2010)

O 47.6 Tue 18:15 P2/EG

Optoelectronic properties of point defects in hBN — •Alexander Kirchhoff, Thorsten Deilmann, Peter Krüger, and Michael Rohlfing — Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

While pristine hexagonal boron nitride (hBN) is a wide-gap insulator, its point defects are discussed as light emitters in the visible optical spectrum. In this study, we examine two substitutional carbon impurities, $\mathrm{C_N}$ and $\mathrm{C_B}$, the nitrogen vacancy $\mathrm{V_N}$ and the divacancy $\mathrm{V_{NB}}$ in a hBN monolayer from an *ab initio* approach, via the *GW*/BSE approximation. Our results show deep defect states and defect-related excitations with energies in the visible regime. We present a detailed analysis of their spatial structure and energetic composition.

O 47.7 Tue 18:15 P2/EG

p Orbital flat band and Dirac cone in the electronic honeycomb lattice — •Thomas Gardenier[1], Jette van den Broeke[2], Jesper Moes[1], Ingmar Swart[1], Christophe Delarue[3], Marlou Slot[1], Cristiane Morais Smith[2], and Daniel Vanmaekelbergh[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands — [2]Institute for Theoretical Physics, Utrecht University, The Netherlands — [3]Université de Lille, CNRS, Centrale Lille, Yncréa-ISEN, Université Polytechnique Hauts-de-France, UMR 8520 - IEMN, F-59000 Lille, France

Honeycomb systems have generated much interest in experimental and theoretical physics due to their interesting band structures. The architypical example of a honeycomb lattice is graphene. The electronic structure of graphene close to the Fermi level can be understood by only considering C 2pz orbitals. Bands due to coupling of sp2 hybrid orbitals are either much higher or lower in energy. It has been shown that in the absence of hybridisation, the band structure of honeycomb lattices features a topologically non-trivial flat band, as well as Dirac cones formed by px and py orbitals.

We patterned a Cu(111) surface with CO molecules to confine the surface state electrons into a honeycomb geometry. By careful tuning of the lattice parameters, we created a honeycomb lattice where s- and p-orbital bands are separated. Scanning tunneling spectroscopy and wavefunction mapping are used to determine the band structure and visualise the electron densities. The results are complemented by theoretical muffin-tin and tight-binding calculations.

O 47.8 Tue 18:15 P2/EG

Ultrafast microscopy of charge density wave phase transitions using pump-probe imaging ellipsometry — •Sebastian Rohrmoser, Julius B. Peters, Tobias Heinrich, Murat Sivis, and Claus Ropers — IV. Physical Institute, Georg-August-University Göttingen, Germany

Transition metal-Dichalcogenides (TMDC's) have long been studied as effectively 2D layered systems exhibiting interesting ordering phenomena such as charge density waves (CDW). A variety of experimental techniques in a pump probe fashion have been used to disentangle the fundamental processes leading to the charge ordering including electron diffraction [1], photoemission spectroscopy [2] and transient optical reflectivity [3]. However, spatiotemporal behaviour like domain growth and movement is not well studied.

In this contribution, we present an all-optical approach to measure the complex refractive index of optically excited 1T-TaS2 on a femtosecond temporal and micrometer spatial scale. Specifically, using a pump probe ellipsometry setup with a rotating polarizer we detect the optically driven phase transition between the nearly commensurate (NC) and incommensurate (IC) CDW phase. The scheme will be applied to study the spatiotemporal dynamics of excited CDW states and phase transitions for inhomogeneous excitations.

[1] M. Eichberger et. al., Nature 468, 799-802 (2010)
[2] J.C. Petersen et.al., Phys. Rev. Lett. 107, 177402 (2011)
[3] N. Dean et.al., Phys. Rev. Lett. 106, 016401 (2011)

O 47.9 Tue 18:15 P2/EG

In-plane anisotropy of the elastic properties of monolayer transition-metal dichalcogenides — •Juliane Mörsel, Pasquale Pavone, and Claudia Draxl — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Germany

Monolayer transition metal dichalcogenides are characterized as two-dimensional materials with hexagonal symmetry. Therefore, the linear elastic properties of these materials are isotropic along the in-plane directions and can be described by only two independent second-order elastic constants (SOECs). The anisotropy of the structure influences, nevertheless, the non-linear elastic properties, which at small values of applied strain can be described in terms of three independent third-order elastic constants (TOECs). In this work, we present an *ab-initio* investigation of the anisotropic behavior of the elastic properties of MoS_2, $MoSe_2$, WS_2, and WSe_2 monolayers. The SOECs and TOECs are obtained from numerical derivatives of the total energies with respect to the applied Lagrangian strain. For this purpose, total-energy calculations are performed using density-functional theory as implemented in the full-potential all-electron package `exciting` [1]. In order to explicitly exploit the anisotropic elastic behavior of these systems, we calculate the SOECs for non-equilibrium reference structures which are obtained by modifying the equilibrium configuration with uniaxial strains along the principal in-plane directions. Analysis of these results allows us to distinguish different regimes of nonlinearity.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26** (2014) 363202

O 47.10 Tue 18:15 P2/EG

Local electronic properties of monolayer and bilayer VS_2 on Au(111) — •Jannik Dornseiff, Sabina Simon, Felix Förschner, Julia Tesch, and Mikhail Fonin — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

The recent discovery of ferromagnetism in VSe_2 [1] boosted the interest in two-dimensional transition metal dichalcogenides (TMDs), which show peculiar magnetic properties. In this work we discuss the structure and local electronic properties of VS_2 monolayer on Au(111). By means of low-temperature scanning tunneling microscopy we analyze the exact atomic arrangement of VS_2. In spectroscopic measurements we observe a dominant peak at E_F, whose shape and position are dependent on the spatial position within the Moiré unit cell. Bilayer VS_2 islands show the same atomic structure as the monolayer. However, the electronic structure is distinctly different showing a gapped behaviour around E_F. We discuss our findings in conjunction with electron correlation effects in VS_2.

[1]. M. Bonilla et al., Nature Nanotechnology **13**, 289 (2018).

O 47.11 Tue 18:15 P2/EG

***In Operando* Soft X-Ray Photoemission Spectroscopy of 2D Materials** — Sanjoy K. Mahatha[1], •Alena Nierhauve[2], Sebastian Rohlf[3], Benedikt Schulte[4], Florian Diekmann[3], Jens Buck[3,5], Matthias Kallåne[3,5], Gregor Praedel[2,4], James McIver[4], and Kai Rossnagel[1,3,5] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]Fachbereich Physik, Universität Hamburg, 20355 Hamburg, Germany — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [4]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [5]Ruprecht-Haensel-Labor, Christian-Albrechts-Universität zu Kiel und Deutsches Elektronen-Synchrotron DESY, 24098 Kiel und 22607 Hamburg, Germany

2D materials provide a fruitful platform for the realization of novel forms of electronics including "Mottronics", "valleytronics", and "twistronics". Specifically, the combination of sub-micrometer position-resolved angle-resolved photoemission spectroscopy (ARPES) with *in operando* electrical control of device-like structures made from 2D materials opens a new avenue toward the direct probing and engineering of novel band-structure and transport phenomena underlying device functionality [1]. Here, we present first *in operando* results obtained from graphene and transition-metal dichalcogenides at our new sub-micrometer ARPES endstation at the soft X-ray beamline P04 of PETRA III.

[1] P.V. Nguyen *et al.*, Nature **572**, 220 (2019).

O 47.12 Tue 18:15 P2/EG

Strain tunable Photodetectors based on 2D materials: A case study of MoS2 monolayers — •Mohammad Bahmani[1], Mahdi Ghorbani-Asl[2], and Thomas Frauenheim[1] — [1]Bremen Center for Computational Materials Science, Department of Physics, Bremen University, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany

In monolayers of transition metal dichalcogenides (ML-TMDs), direct band-gap, weak screening of charge carriers, and a large surface-to-volume ratio facilitate the light-matter interactions in such materials, leading to noticeably high optical absorptions. Synthetic samples usually contain some fraction of intrinsic defects with significant effects on their electrical and optical properties. The localized defect levels have been observed to improve the photoresponsivity of MoS2 MLs by trapping the photoexcited charge carriers, thus increasing the photocurrent. Considering high resilience of ML-TMDs towards mechanical deformations, it was shown that biaxial strain improves the device properties of MoS2-based photodetectors. Recently, we showed the shift of the mid-gap levels of the defects inside MoS2 MLs as a function of various applied strains which could explain the observed improvements in photodetector devices. We study the properties of flexible photodetectors based on phase-engineered MoS2 MLs (1T-2H-1T) under strain. Using sisl tool, we employ a linear response regime to add the electron-photon interactions as a perturbation to the pristine Hamiltonian calculated by TranSIESTA/TBtrans.

O 47.13 Tue 18:15 P2/EG

Modulation of the excitonic behaviour of MoS_2 on gold electrodes with external potential: a sum frequency spectroscopy study — •Tao Yang[1], Erik Pollmann[2], Marika Schleberger[2], Yujin Tong[1,2], and Richard Kramer Campen[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]University of Duisburg-Essen, Faculty of Physics,Lotharstr. 1, 47057 Duisburg, Germany

Two dimensional (2D) materials have recently attracted significant attention because of their unique electronic and optical properties. In particular MoS_2, a transition metal dichalcogenide, has been intensively studied due to its dramatically layer-dependent properties and potential application in electrocatalysis, field-effect transistors and optoelectronics. While the fundamental physics of MoS_2 are increasingly well understood, less attention has been devoted to, and virtually all of these applications require, charge transfer between some other material, often a metal electrode and the MoS_2. Here we use final state resonant sum frequency spectroscopy to study the optical response of MoS_2 deposited on a gold electrode in aqueous solution as a function of applied bias. The data show the evolution of the A and B exciton with electron doping. Together with Raman and electrochemical characterisation, the current study provides important insights into understanding the relationship between electronic structure, atomic configuration and electron transfer at an MoS_2 electrochemical interface.

O 47.14 Tue 18:15 P2/EG

Hot electron dynamics in Stanene/Au(111) — •Marten Düvel[1], Germaine Arend[1], Daniel Franz Walter Marx[1], Jan Philipp Bange[1], Jonas Fredrik Pöhls[1], Marco Merboldt[1], Mahalingam Maniraj[2], Daniel Steil[1], Marcel Reutzel[1], Sabine Steil[1], and Stefan Mathias[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Stanene, the graphene analog with Sn, was recently predicted and has subsequently motivated intense research on the realization of Sn-based ultrathin materials. In our previous work [M. Maniraj et al., Comm. Phys., 2:12, 2019], we found a two-atomic honeycomb superstructure of Sn on Au(111) that shows a Dirac-like band centered at the $\Gamma-$point with anti-parallel spin polarization similar to a topological insulator. Here, we use time- and angle-resolved photoelectron spectroscopy to study the electronic structure and dynamics in the unoccupied regime of the band structure of this stanene-like material system.

O 47.15 Tue 18:15 P2/EG

Metal insulator transition studied with transport on H on epitaxial graphene — •Diana Slawig[1], Markus Gruschwitz[2], and Christoph Tegenkamp[1,2] — [1]Leibniz Universität Hannover, Germany — [2]TU Chemnitz, Germany

The ability of atomic hydrogen to chemisorb on graphene makes it a quite interesting system for hydrogen storage and sensor applications. The introduction of scattering centers via atomic hydrogen chemisorption, the concomitant spin polarization and the opening of a bandgap due to symmetry breaking of the sublattice symmetry makes it particularly interesting for electronic transport measurements.

In this study we performed systematic transport investigations on hydrogen adsorption on epitaxial monolayer graphene on SiC by means of 4-tip STM/SEM. Conductance values were investigated for various surface H-coverages up to the saturation coverage of 0.4 ML, well below the percolation limit. As a function of the H coverage, we observed a metal-insulator transition. Thereby, the sheet resistance increases by three orders of magnitude up to 37 kΩ□. Temperature dependent measurements on these hydrogen terminated graphene show activated transport behavior with an activation energy of 30 meV. We suspect that upon adsorption of the saturation coverage, the monolayer is neutralized and gapped due charge transfer and breaking of the lattice symmetry.

O 48: Poster Session - Electronic Structure of Surfaces: Spectroscopy, Surface States

Time: Tuesday 18:15–20:00 Location: P2/EG

O 48.1 Tue 18:15 P2/EG

Rashba-split surface state on Re(0001) investigated by STM — •Johannes Regel[1], Torge Mashoff[1], Jan Minar[2], Jürgen Braun[3], Hubert Ebert[3], and Hans-Joachim Elmers[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz — [2]University of West Bohemia, Pilsen, Czech Republic — [3]Department Chemie, Ludwig Maximilians-Universität, München

The electronic structure of surfaces differs significantly from the bulk structure. Due to the broken symmetry, surface states and resonances are formed at the surface. A strong spin-orbit coupling, as given for Re, leads to Rashba spin splitting of these states. Although the strong spin momentum coupling should suppress backscattering, Re(0001) shows quantum interference patterns in the proximity of defects and step edges.

We investigate the electronic states of the Re(0001) surface using low temperature scanning tunneling microscopy and spectroscopy. Differential conductivity measurements lead to an energy-dependent analysis of wavelength, phase and damping of the surface states. Additionally, we use molecular beam epitaxy to deposit pseudomorphic submonolayers of Au and Ni and study their influence on the complex reflection coefficient of the surface wave function. The dispersion relations of the surface states are compared with theoretical results and show good agreement.

O 48.2 Tue 18:15 P2/EG

Magnetic adsorbates on W(110): A comparative study of the electronic structure — •Pascal J. Grenz[1], Marcel Holtmann[1], Koji Miyamoto[2], Eike F. Schwier[2], Shiv Kumar[2], Taichi Okuda[2], and Markus Donath[1] — [1]Institute of Physics, Westfälische-Wilhelms-Universität Münster, Germany — [2]Hiroshima Synchrotron Radiation Center, Japan

We used spin- and angle-resolved photoelectron spectroscopy to study the electronic structure of ultrathin Ni and Co films on W(110) and compare the results with those of Fe/W(110) [1]. W(110) exhibits a Dirac-cone-like surface state [2] which is topologically non-trivial and protected by mirror symmetry [3]. Magnetic adsorbates on W(110) are a model system to study the influence of exchange interaction on topologically protected surface states. In this contribution, we show that Co and Ni have a distinctly different influence on the Dirac-cone-like surface state than Fe. Additionally, we investigated the dispersion and spin structure of interface states for sub-monolayer and monolayer coverages of Co/W(110) and Ni/W(110).

[1] K. Honma *et al.*, Phys. Rev. Lett. **115**, 266401 (2015). [2] K. Miyamoto *et al.*, Phys. Rev. Lett. **108**, 066808 (2012). [3] D. Thonig *et al.*, Phys. Rev. B **94**, 155132 (2016).

O 48.3 Tue 18:15 P2/EG

Capability of an ultra-low work function electride material for ion thrusters as neutralizer insert — Fabian Michel[1,2], Daniel Zschaetsch[1,2], Malina Reitemeyer[1,2], •Jurek Lange[1,2], Limei Chen[1,2], Detlev M. Hofmann[1,2], and Peter J. Klar[1,2] — [1]Institue of Experimental Physics I, JLU Giessen, 35392 Giessen — [2]Center for Material Research (ZfM/LaMa), JLU Giessen, 35392 Giessen

Due to its low workfunction for electrons electride materials have many advantages for applications for space flight propulsions. For this reason C12A7:e$^-$ is a promising insert candidate to be used in cold-cathode designs. By tuning the reduction process of C12A7 (12 CaO-7 Al_2O_3) it is possible to achieve electron concentrations up to $10^{21}/cm^3$. The concentrations can be determined by electrical measurements, and complementary by electron paramagnetic resonance (EPR) and Raman spectroscopy. In addition the later give information about impurities in the material. We further correlate the EPR and Raman results to photoelectron spectroscopy (XPS), to obtain a deeper understanding of the material properties. The task of the investigation is to contribute to the improvement of charge neutralizer materials for space applications.

O 48.4 Tue 18:15 P2/EG

The role of the final state in dichroic spin- and angle-resolved photoemission on the Au(111) surface state — •Maximilian Ünzelmann[1], Hendrik Bentmann[1], Tim Figgemeier[1], Raphael Crespo Vidal[1], Thiago R. F. Peixoto[1], Henriette Maass[1], Chul-Hee Min[2], and Friedrich Reinert[1] — [1]Experimentelle Physik 7, Universität Würzburg — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel

The Shockley surface state of the Au(111) surface is a paradigmatic example for a Rashba-type spin-splitting of two-dimensional electronic states. By means of spin- and angle-resolved photoemission we have investigated the photoelectron spin polarization and the linear dichroism (LD) in dependence on the photoelectron final state. To this end we conducted measurements in a photon-energy range from 18 eV to 30 eV and compare our results to previous findings for the giant Rashba systems $\mathrm{PbAg_2}$/Ag(111) and $\mathrm{BiAg_2}$/Ag(111) [1]. In all systems the LD changes its sign between energies of roughly 22 eV and 26 eV, likely due to a band gap in the similar final-state band structure of Ag(111) and Au(111). Interestingly, the measured spin polarization of the Shockley surface state is almost constant at these photon energies, in stark contrast to the case of $\mathrm{BiAg_2}$ [1]. We will discuss these results by comparing the different influence of inversion symmetry breaking and spin-orbit coupling on the spin-split electronic wave functions.

[1] Bentmann et al., Phys. Rev. Lett. 119, 106401 (2017).

O 48.5 Tue 18:15 P2/EG

Towards ultrafast time-resolved orbital imaging using a ToF-based momentum microscope and photoelectrons extracted by HHG light — •Wiebke Bennecke, Matthijs Jansen, Sabine Steil, Marius Keunecke, David Schmitt, Marten Düvel, Christina Möller, Daniel Steil, and Stefan Mathias — I. Physikalisches Institut, Georg-August-Universität Göttingen

Orbital imaging (OI) is a powerful method to visualize molecular orbitals in molecules-metal interfaces using angle-resolved photoemission spectroscopy (ARPES) data and phase retrieval algorithms [Puschnig *et al., Science* **326**, 702-706 (2009)]. On this poster, we will report on our progress towards a demonstration of time-resolved imaging of optically excited orbitals. OI requires the precise preparation of a few highly ordered monolayers of molecules on a monocrystalline metallic substrate. We achieve this by thermal evaporation from a Knudsen cell in combination with LEED and UV photoemission measurements to verify the sample quality. Our photoemission setup consists of a momentum microscope and a high harmonic generation beamline at 26.5 eV, which yields the full momentum- and energy-dependent photoelectron spectrum of the absorbed molecules in a single measurement. We combine this setup with UV, visible and IR pump beamlines, which allows us to induce a wide range of optical excitations on a femtosecond time scale. The measured time-resolved photoelectron spectra are analysed using a sparsity-driven phase retrieval algorithm, which enables us to visualize the molecular orbitals in real space while requiring only limited prior knowledge of the molecular orbital.

O 48.6 Tue 18:15 P2/EG

Improved numerical reconstruction method for Metastable Induced Electron Spectra of molecules — •Wichard J. D. Beenken[1], Tobias B. Gäbler[2,3], Erich Runge[1], and Stefan Krischok[1] — [1]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — [2]Friedrich-Schiller-Universität Jena, Institut für Angewandte Physik, Jena, Germany — [3]Fraunhofer Institut für Angewandte Optik und Feinmechanik IOF, Jena, Germany

Metastable Induced Electron Spectroscopy (MIES) is arguably the most surface-sensitive spectroscopic method. Thus, it has been used, e.g., to study molecular layers of organic molecules [1] and the composition of ionic liquids [2,3]. Of particular interest are the orientations of the molecules and ions to the surface plane. In order to obtain this information, detailed reconstructions of the MIES spectra based on quantum-chemical calculations of the molecule in combination with a simulation of many trajectories of the impinging metastable helium atoms including shadowing effects are required. The latter makes such an analysis numerically very costly. We present recent progress in the numerical simulation of MIES spectra. [1] J. Günster, G. Liu, V. Kempter, D.W. Goodman, Surf. Sci. 415 (1998) 303-311. [2] T. Ikari, A. Keppler, M. Reinmöller, W.J.D. Beenken, S. Krischok et al., Surf. Sci. Nanotech. 8 (2010) 241-245. [3] A. Ulbrich, M. Reinmöller, W.J.D. Beenken, S. Krischok, Chem. Phys. Chem. 13 (2012) 1718-1724.

O 48.7 Tue 18:15 P2/EG

Revisiting the Quantum Corral with combined atomic force and scanning tunneling microscopy — •Fabian Stilp, Julian Berwanger, Nadine Mundigl, and Franz Josef Giessibl — University of Regensburg, 93040 Regensburg, Germany

Cu(111) exhibits a surface state that is scattered by adsorbates, defects and step edges, leading to pronounced interference patterns visible by scanning tunneling microscopy (STM) [1]. In 1993, Crommie et al. [2] confined these surface state electrons into a circular symmetric Quantum Corral with a diameter of about 15 nm assembled from 48 single Fe adatoms. They investigated the Bessel-type eigenstates with scanning tunneling microscopy and tunneling spectroscopy [2]. Afterwards, also elliptic, square and triangular Quantum Corrals [3] were created which lead e.g. to the observation of Quantum Mirages [4]. While STM is only able to image the Quantum Corral's states close to the Fermi level, atomic force microscopy (AFM) probes all occupied states. We revisit Quantum Corrals with combined STM and AFM using monoatomic metal and CO-terminated tips, probing whether the eigenstates of the Quantum Corral also lead to signatures in the AFM signal.

[1] Crommie et al. Nature **363**, 524 (1993)
[2] Crommie et al. Science **262**, 218 (1993)
[3] Crommie et al. Physica D **83**, 98 (1995)
[4] Manoharan et al. Nature **403**, 512 (2000)

O 48.8 Tue 18:15 P2/EG

Influence of strong spin-orbit coupling in strong electron correlated Bi/Sb:CeAg$_\mathbf{x}$ on Ag(111) — •Hendrik Bostelmann-Arp, Katharina Kissner, Simon Müller, and Friedrich Reinert — Experimental Physics VII, Julius Maximilians University of Würzburg, 97074 Würzburg

Correlated electron systems show unique ground state properties. Ce-based compounds play a particular role in the investigation of strong correlation effects due to the single 4 f-electron occupation. At low temperatures the interaction of strongly localized 4 f-electrons with itinerant conduction electrons can lead to distinct features in the electronic structure such as the Kondo-Resonance and the formation of a hybridization band gap at the Fermi edge. The hybridization gap at the Fermi level is connected to the possibility of realising a Topological Kondo-Insulator by introducing additional elements with strong spin-orbit coupling [1].

In order to understand the influence of strong spin-orbit coupling on correlated systems we present results on the Kondo-System $\mathrm{CeAg_x}$ on Ag(111) alloyed with elements showing strong spin-orbit coupling i.e. Bi or Sb. We study the electronic structure by means of Angle Resolved and X-Ray photoemission spectroscopy (ARPES and XPS). Furthermore changes in the geometric surface structure are studied by Low Energy Electron Diffraction (LEED). [1] M. Dzero, et al.,Phys. Rev. Lett. 104, 106408 (2010)

O 48.9 Tue 18:15 P2/EG

eMIL: advanced emission Mössbauer Spectrometer — •Dmitry Zyabkin[1], Ulrich Vetter[1], Fredericus Linderhof[2], and Peter Schaaf[1] — [1]Ilmenau University of Technology, Gustav-Kirchhoff-Str. 5, 98693 Ilmenau, Germany — [2]Department of Experimental Physics, Palacký University in Olomouc, 17. Listopadu 12, Olomouc, Czechia

Mssbauer spectroscopy is one of the most powerful methods to locally probe structural and electronic properties in condensed matter. The method allows to analyse and quantify various atomic surroundings, magnetic states, in-field magnetic arrangements of magnetic moments and coordination symmetry [1]. This current work presents a contemporary design of an advanced emission Mössbauer Spectrometer (eMS) eMIL equipped with a parallel-plate avalanche counter. The setup is based on an emission geometry and provides numerous advantages over conversion electron, common emission or transmission Mössbauer spectroscopy. eMIL is designed to measure hyperfine interactions in solids under various exposures. The implemented design overcomes limitations and improves performance and handling. In the current revision the implantation chamber is supplied with an UV extension - allowing to perform studies of photo-catalytic materials under external light exposure. A specifically designed motorised lid-samples-holder is fully automatised, and makes it possible to study up to 4 samples loaded in a magazine within a temperature range up to 1100 K and to perform angular-dependence-measurements in high vacuum.

[1] Gütlich *et al*, Mössbauer Spectroscopy, Springer (2010)

O 48.10 Tue 18:15 P2/EG

Ordered and disordered Tellurium surface alloys on Ag(111) and Cu(111) — •Andreas Raabgrund, Maximilian Ammon, Tilman Kisslinger, Lutz Hammer, and M. Alexander Schneider — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

The formation of (surface) metal alloys using Te achieved a lot attention lately, e.g. for photovoltaics [1] or for spintronics [2]. In this work the Te surface alloys on Cu(111) and on Ag(111) were studied by low temperature STM, STS, LEED (all at 80 K) and DFT. Evaporation of $\Theta = 1/3$ ML Te leads to the formation of a $(\sqrt{3}\times\sqrt{3})R30^\circ$ superstructure on Ag(111) [3] and a $(2\sqrt{3}\times\sqrt{3})R30^\circ$ superstructure on Cu(111), respectively. By reducing the Te coverage we observe for both substrates patches of a disordered phase instead of a phase separation into ordered structure and clean surface. The reduced order below 1/3 ML Te coverage manifests itself as an increased background

signal in LEED and is shown by STM to arise from a disordered Te lattice. Investigating those surface alloys by STS shows for both ordered structures a strong signal above the Fermi energy with onsets at 0.6...0.7 eV for AgTe and at 1.3...1.4 eV for CuTe, respectively. These features are also found by DFT and are the result of the longe-range order since they are absent on the disordered structures.
[1] Ibers J., Nat. Chem. 1, 508 (2009)
[2] Eremeev et al., Phys. Rev. Lett. 108, 246802 (2018)
[3] Liu et al, J. Phys. Chem. Lett. 2019, 10, 1866-1871 (2019)

O 48.11 Tue 18:15 P2/EG

Angle-resolved photoemission spectroscopy measurements from thin film manganites — •Jonas Pöhls, Marten Düvel, Cinja Seick, Vitaly Bruchmann-Bamberg, Jan Philipp Bange, Marco Merboldt, Henrike Probst, Marius Keunecke, Sabine Steil, Daniel Steil, and Stefan Mathias — 1st Physical Institute, University of Göttingen

Strongly correlated oxide perovskites, e.g. the manganite $La_{1-x}Sr_xMnO_3$ (LSMO), have a very rich magnetic phase diagram [1]. This is closely linked with the electronic structure of the material. Angle-resolved photoemission spectroscopy (ARPES) provides an opportunity to study this structure. Due to the surface sensitivity of this technique, the study of thin films produced by metalorganic aerosol deposition (MAD) in atmosphere is challenging. We have developed a two-step cleaning process to prepare the samples in UHV for the ARPES studies. For this purpose we simulate in a first step the conditions during the production in the MAD for cleaning. In the second step we use a reaction with ozone to remove the remaining adsorbates. We will present our setup and discuss the influence of our cleaning process on the material properties. Furthermore, first photoemission data on the band structure of MAD-grown manganites will be presented.

[1] Moshnyaga et al., Ann. Phys. 523, 652 (2011)

O 48.12 Tue 18:15 P2/EG

Designing High Energy Resolution Laser-Based Tunable Pump and Probe ARTOF Workstations — Alexander Forsman, •Viktor Jonsson, Luca Piazza, Magnus H. Berntsen, Jonas Weissenrieder, and Oscar Tjernberg — Materials Physics, KTH Royal Institute of Technology, Electrum 229, SE-16440 Kista, Stockholm, Sweden

We present recent upgrades of a laser-based angle-resolved time-of-flight spectrometer including our plans to move our system to modern facilities, add time-resolving capabilities and radically improve the optical design. The current system is driven by a 45W fiber laser 300 fs pulses at 1030 nm. The 9^{th},15^{th} and 21^{st} harmonic is generated in an argon-gas jet, separated by a horizontal groove grating and focused by 2 toroidal mirrors to around 0.1mm at the sample position. We demonstrate an energy resolution of 20 meV at space charge limited flux. In the new lab a Tangor Amplitude laser will generate 500 fs to 2 ps pulses for the probe while feeding the fiber laser which will after an optical parametric amplification act as a tunable pump at wavelengths from 200 to 1000 nm. The new optical design relies on movable narrow bandwidth spherical mirrors inside a monochromator. Instead of using filters to separate the $5 \cdot 10^{-11}$ vacuum from the much lower 10^{-6} vacuum in the monochromator we use sets of turbo pumps and a XIA differential pump to enable a free path for the XUV to the sample position. Our new system will increase the flux making it feasible to probe using the additional 27^{th} harmonic.

O 49: Poster Session - Organic Molecules on Inorganic Substrates: Electronic, Optical and Other

Time: Tuesday 18:15–20:00 Location: P2/EG

O 49.1 Tue 18:15 P2/EG

Sum frequency spectroscopy of *o*-, *m*- and *p*-Methylbenzylphos-phonic acid on α-aluminium oxide — •Tim Lämmerzahl, Matthias Linke, Damian Firla, and Eckart Hasselbrink — Universität Duisburg-Essen, Essen, Germany

Self-assembled molecular monolayers (SAMs) are applied to engineer surface properties in a defined way which makes SAMs interesting for numerous applications. While there have been many studies on prominent SAMs e.g. thiols on gold, the existing knowledge on phosphonic acid (PA) SAMs still lacks behind. A very prominent substrate for PA SAMs is aluminum oxide, due to its use in a wide range of research applications like organic field-effect sensors and in different fields of industry e.g. aerospace. The surface sensitive vibrational sum frequency spectroscopy (vSFS) is well suited for the characterization of such surfaces. To this note we studied different isomers of methylbenzylphosphonic acid (MBPA) via vSFS in the spectral range of the C-H vibrations. We were able to show that due to the selection rules for sum frequency generation, different bands are observed for the three possible substitution patterns of MBPA in the spectral range of the aromatic C-H vibrations. When comparing the spectra in the spectral region of aliphatic C-H vibrations, a clear difference between the isomers can be shown. This study provides interesting insights into the orientation of different constitutional isomers on the surface.

O 49.2 Tue 18:15 P2/EG

Single-molecule vibrational progression on two-dimensional materials — •Alexander Mehler[1], Nicolas Néel[1], Johannes Halle[1], Marie-Laure Bocquet[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, Ilmenau, Germany — [2]École normale supérieure, PSL University, Sorbonne Université, CNRS, France

Probing genuine molecular properties even after adsorption on a surface requires the efficient reduction of the molecule-surface hybridization. Two-dimensional materials, such as graphene, hexagonal Boron Nitride (hBN) and stackings thereof, are promising buffer layers to this end. Scanning tunneling microscopy and spectroscopy at low temperature is used to explore molecular orbitals and vibrational quanta of the hydrocarbon molecule DBP (Dibenzotetraphenylperiflanthen) on graphene and hBN with submolecular resolution. Independent of the metal substrate, Ir(111), Pt(111) and Ru(0001), vibrational progression in both DBP frontier orbitals is observed for graphene and hBN, albeit with different numbers of vibrational quanta involved. Density functional calculations unveil that symmetry matching of electronic and vibrational excitations supports the observation of vibrational progression. The lifetime of the vibronic levels can be tuned by the molecular environment of a single DBP as well as by using different kinds and numbers of buffer layers.

O 49.3 Tue 18:15 P2/EG

Site selective adsorption and spin state locking of the spin crossover complex Fe(phen)2(NCS)2 on Au(111) — Sumit Beniwal[1], •Suchetana Sarkar[2], Felix Baier[2], Peter A. Dowben[1], and Axel Enders[1,2] — [1]Department of Physics, Universität Bayreuth, Universitätsstrasse 30, 95440 Bayreuth, Germany — [2]Department of Physics and Astronomy, University of Nebraska Lincoln, Lincoln, NE 68588, USA

The iron (II) spin crossover complex, Fe(1,10-phenanthroline)2(NCS)2, dubbed Fe-phen, has been studied with scanning tunnelling microscopy under ultra-high vacuum after adsorption on the "herringbone" reconstructed surface of Au (111) for sub-monolayer coverages. The Fe-phen molecules attach, through their NCS-groups, to the Au atoms of the fcc domains of the reconstructed surface only, thereby lifting the herringbone reconstruction. The molecules stack to form 1D chains, which run along the Au [110] directions. Neighboring Fe-phen molecules are separated by approximately 2.65 nm, corresponding to 9 atomic spacings in this direction. The molecular axis, defined by the two phen groups, is aligned perpendicular to the chain axis, along the Au [221] direction, thereby bridging over 5 atomic spacings, in this direction. Experimental evidence suggests that the molecular spins are locked in a mixed state in the sub-monolayer regime at temperatures between 100 K and 300 K. These results further the understanding of how interfaces could be leveraged to manipulate the spin state and the spin crossover in SCO complexes and demonstrate an avenue for the structural patterning of functional molecular films.

O 49.4 Tue 18:15 P2/EG

Decoupled or not decoupled? Investigation of charged organic molecules on a 2D insulator — •Maximilian Schaal, Iliyan Karadzhov, Marco Gruenewald, Felix Otto, Roman Forker, and Torsten Fritz — Friedrich Schiller University Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena

In the last years 2D materials have attracted much interest in fundamental research and practical applications because of their unique physical properties. One representative of the 2D materials is hexagonal boron nitride (h-BN), which is an insulator with a band gap of ≈ 6 eV [1]. h-BN is widely used as interlayer to decouple molecules from metallic surfaces [1]. This lead us to the question: Is one monolayer h-BN really efficient for decoupling PTCDA from the Ni(111) surface?

In this work we observed a charge transfer by differential reflectance spectroscopy (DRS) during the growth of PTCDA. The lateral structure was investigated in real as well as in reciprocal space by scanning tunnelling microscopy (STM) and low energy electron diffraction (LEED), respectively. Furthermore, the core states as well as the valence electron band structure was investigated by x-ray and angle resolved ultraviolet photoelectron spectroscopy (XPS and ARUPS), respectively. In the end we will discuss the origin of the charge transfer.

[1] W. Auwärter, Surf. Sci. Rep. **74**, 1-95 (2018).

O 49.5 Tue 18:15 P2/EG

DMEP-Ovalene as Precursor-Molecule for Nanographen on H:Si(100) — •Alexander Kölker, Leonid Shupletsov, Takashi Kumagai, Martin Wolf und Matthias Koch — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Electrically contacting single molecules is one of the biggest challenges in nanotechnology. Sophisticated techniques emerged such as break junction [1] and scanning probe microscopy (SPM) [2,3]. However, interpreting the electrical signal without knowledge of the precise chemical composition of the junction is difficult.

We have developed a SPM sample architecture with integrated subsurface electrodes in Si(001) for multi-terminal conductance measurements to fabricate robust molecular nano-circuits. To place molecules with highest precision between prior fabricated electrodes we will employ STM hydrogen lithography which enables the creation of reactive adsorption sites on the passivated silicon surface.

A first promising candidate to study is nanographene which localized electronic edge states are expected to be energetically located in the silicon band gap region.

Here we report a detailed structural and electronic characterizion of adsorption conformations of Dimethylphenyl-Ovalene (DMEP) on H:Si(001) as function of annealing temperature. STM and STS experiments at 4 K are supported by simulations for a free molecule in gas phase.

O 49.6 Tue 18:15 P2/EG

Adsorption and Electronic Properties of N-Heteropolycycles on Metal Surfaces — •Felix Landwehr[1], Mohsen Ajdari[1], Marvin Hoffmann[2], Hilmar Reiss[3], Hendrik Hoffmann[3], Uwe H. F. Bunz[3], Andreas Dreuw[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg — [2]Interdisziplinäres Zentrum für Wissenschaftliches Rechnen, Ruprecht-Karls-Universität Heidelberg — [3]Organisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg

Introduction of nitrogen atoms into the π-electron backbone of polycyclic hydrocarbons lowers the energy of the frontier orbitals and accordingly increases the electron affinity, while the optical gap remains almost constant. Thus, N-heteropolycycles possess a higher stability compared to the corresponding polyaromatic hydrocarbons.

Due to the increased electron affinity, aromatic N-heteropolycyclic compounds are n-type semiconductors and thus promising candidates for applications in field effect transistors. However, a detailed understanding of the adsorption and electronic properties of these molecules at interfaces and in thin films is needed to optimize the devices performance.

In this contribution, we used temperature-programmed desorption, electronic and vibrational high-resolution electron loss spectroscopy, as well as scanning tunneling microscopy/spectroscopy to elucidate the adsorption and electronic properties of N-heteropolycycles adsorbed on Au(111).

O 49.7 Tue 18:15 P2/EG

Application of multi-photon PEEM to a biological system: Geobacter sulfurreducens — •Franz Niklas Knoop[1], Hilke Sophie Wichmann[2], Gerhard Lilienkamp[1], and Winfried Daum[1] — [1]IEPT TU Clausthal — [2]IÖNC TU Braunschweig

Excitation of the molecular Soret transition of porphyrins by short tunable laser pulses has made possible multi-photon photoelectron emission microscopy (nP-PEEM) studies of porphyrin thin films and nanoplasmonic porphyrin hybrid systems with high molecular sensitivity [1]. More recently, we have also applied this method to films of the protein cytochrome c whose chromophoric group is a porphyrin. In this contribution we report on nP-PEEM results for a biological system, Geobacter sulfurreducens which is a promising candidate for microbial fuel cells. This bacterium as well as its extracellular matrix is rich of cytochrome c which is probed in our PEEM experiments using appropriates laser wavelengths. While films of porphyrin molecules such as MgTPP are very stable against irradiation with 100 fs laser pulses, photoemission from cytochrome c films as well as from Geobacter sulfurreducens shows substantial intensity and spectral changes upon laser irradiation. Our experiments point to thermal effects because moderate heating of the sample also increases the photoemission intensity from Geobacter sulfurreducens. We present and discuss Soret-resonant single-wavelength and laser-spectroscopic PEEM results obtained from single bacteria and bacteria films.

[1] K. Stallberg, G. Lilienkamp, W. Daum, J. Phys. Chem. C 121, 13833 (2017)

O 49.8 Tue 18:15 P2/EG

First Principles Studies of Electrical Conductance and Thermopower Properties of π-Conjugated Organometallic Complexes in Single Molecule Junctions — •Jannis Jung[1], Tatsuhiko Ohto[2], Hirokazu Tada[2], and Doreen Mollenhauer[1] — [1]Institute of Physical Chemistry, Justus Liebig University, Giessen, Germany — [2]Division of Frontier Material Science, Osaka University, Osaka, Japan

Single molecule junctions, consisting of a molecule connecting two bulk material electrodes, have a long history of research, which focuses on their electrical properties and uses in electronics. In particular, molecular junctions containing organometallic complexes showed high Seebeck coefficients and low thermal conductance, making them a promising thermoelectric material.

Here, the influence of the binding nature between a complex and differently structured gold surfaces as well as the influence of large side chains of the ligands to the electron transmission was investigated by density functional theory calculations using the Non-Equilibrium Green's Function (NEGF) method. Therefore, we studied junctions containing transition metal (Ru and Pt) complexes with highly π-conjugated ligands binding to different surface contacts. We showed a shift of the conductive (HOMO) orbitals towards the Fermi energy, effectively increasing the Seebeck Coefficient. Furthermore, intramolecular dispersion interactions can lead to a decrease of the electric conductance.

O 49.9 Tue 18:15 P2/EG

Surface spectroscopy of functionalized Si(001) surfaces — •Stefano Mazzei, Valérie Véniard, and Christine Giorgetti — Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA/DRF/IRAMIS, Institut Polytechnique de Paris

Understanding the mechanism of interaction between amino acids and peptides with surfaces opens new perspectives. Adsorption of DNA molecules on semiconducting surfaces is evoked for the design of biosensors or the production of bio-materials. The possibility to functionalize surfaces with bio-molecules, to create organized structures up to nanometers' distances depends on our capability to understand precisely the mechanisms which govern the deposition of molecular films onto different kinds of surfaces. For these reasons, this kind of systems have been intensively studied during last decades .

We present in this poster the results obtained for the Si(001) surface functionalized with two different molecules, the Thymine and the Uracil. The electronic structure has been obtained with a DFT approach, using Abinit . Using DP, which allows the calculation of the dielectric response of materials in the TDDFT framework, we computed several surface-related linear spectroscopy quantities (Reflectance Anisotropy Spectrum, adsorbance anisotropy...), that are compared with previous studies. Finally, the code 2Light, which has been recently extended to the case of surfaces, has been used to study the Second Harmonic Generation of the Si(001) functionalized with nucleobases, including local field effects.

O 49.10 Tue 18:15 P2/EG

Molecular chain formation at surfaces: PEEB/Au(111) - A High-throughput Study — •Lokamani Lokamani[1,2], Jeffrey Kelling[3], Jörg Meyer[1], Anja Nickel[1], Robin Ohmann[1], Gianaurelio Cuniberti[1], Jannic Wolf[4], Thomas Huhn[4], Peter Zahn[2], Francesca Moresco[1], and Sibylle Gemming[2,5] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Institute of Ion Beam Physics and Materials Research, HZDR, Germany — [3]Department of Information Services and Computing, HZDR, Germany — [4]Department of Chemistry, Uni Konstanz, Germany — [5]Institute of Physics, TU Chemnitz, Germany

The geometrical and electronic structure of 4-bis(phenylethynyl)-2,5-bis(ethoxy)benzene (PEEB) molecules adsorbed on the Au(111) is investigated by LT-STM and STS in conjunction with DFT based simulations. Due to low corrugation of the Au(111) surface, PEEB molecules can form quasi interlocked lateral patterns, as observed in experiments. We employ DFTB+ based high-throughput calculations including dispersion corrections via Lennard-Jones potential to evaluate an energy function, which incorporates the adsorption energy of single PEEB molecules on the metal surface and the interaction energy of a pair of PEEB molecules. Our calculations indicate, that the PEEB molecule is physisorbed on Au(111), with negligible distortion in geometry and moderate charge transfer of +0.14e. Furthermore, depending on coverage density specific types of pattern are preferred, which can be exploited to form 1D-molecular-wires on Au(111).

O 50: Poster Session - Plasmonics and Nanooptics: Fabrication and Characterization

Time: Tuesday 18:15–20:00 Location: P2/EG

O 50.1 Tue 18:15 P2/EG

Coupling of Quantum Emitters to Plasmonic Slot Waveguides — •Lok-Yee Yan, Mike Prämassing, Yuhao Zhang, Hans-Joachim Schill, and Stefan Linden — Physikalisches Institut, University of Bonn, Nußallee 12, D-53115 Bonn, Germany

Quantum emitters (QEs) coupled to plasmonic systems are considered as promising candidates for building blocks in quantum plasmonic circuits. So far, several plasmonic platforms such as silver nanowires and gold V-grooves have been exploited. The main idea behind those concepts is that one can easily tailor the electromagnetic density of states by shaping the geometry of the underlying metallic nanostructure. Here, we report on the fabrication of hybrid nanostructures consisting of colloidal semiconductor quantum dots or transition metal dichalcogenide (TMDC) monolayers, coupled to 80 nm wide slot waveguides in single-crystalline gold flakes. We use a two-step electron beam lithography process to deposit a controllable number of quantum dots on freely definable sites on the substrate while monolayers of TMDCs are prepared by mechanical exfoliation of the crystal bulk material. A focused ion beam allows us to mill the nanostructures into the gold film. Depending on the relative placement of the QEs and the plasmonic nanostructures, different coupling strengths can be achieved. We demonstrate this by imaging the fluorescence of the QEs onto an EMCCD camera and showing a reduction of lifetime as a result of an increase of the local photonic density of states.

O 50.2 Tue 18:15 P2/EG

Theoretical analysis on the plasmon-resonant optical response of silver nanoparticles with shapes of sphere, spheroid, and snipped trigonal prism — •Masafuyu Matsui and Hisao Nakamura — AIST, Tsukuba, 305-8568, Japan

Plasmon-resonant optical response of silver nanoparticles with shapes of sphere, spheroid, and snipped trigonal prism are investigated using an analysis method based on dipole–dipole interaction within discrete dipole approximation. In the analysis method, the induced dipole is decomposed into the contributions from incident-light electric field (an incident light term) and that from induced dipole oscillations (a dipole–dipole interaction term) to clarify microscpopic level mechanism of plasmon resonance and near-field effect. The analysis reveals that the diameter corresponding to the polarization direction of the incident light plays a crucial role in determining the optical response of the nanoparticles. In the plasmon resonance along the direction with small diameter, the incident light term is a dominant source of induced dipoles, resulting that the extinction peak appears close to the maximum of imaginary part of polarizability. In contrast, in the plasmon resonance along that with large diameter, the dipole–dipole interaction one is dominant and red-shifts the extinction peak. Therefore, shape control of nanoparticle with high anistropy, for example, nanoplate, is a key factor to exhibit the desired plasmon resonance with sharp peak, leading to development of effective plasmonic devices.

O 50.3 Tue 18:15 P2/EG

Generation of ultrashort laser pulses for nonlinear near-field imaging of plasmonic nanostructures — •Mike Prämassing, Felix Affeld, and Stefan Linden — Physikalisches Institut Universität Bonn, D-53115

Upon resonant excitation with ultrashort laser pulses, specially designed metallic nanoantennas faciliate the generation of light at higher harmonics of the excitation frequency. This effect can be used for example in metasurface designs to combine frequency conversion with other metasurface capabilities like beam fucusing or vortex beam creation.[1] In this work, we report on our progress towards nonlinear near-field imaging of plasmonic nanostructures. We utilize a pulsed tunable near-infrared light source at an operating wavelength of 1550 nm. The initial pulse has a temporal width of about 400 fs and is then spectrally broadened by a single mode fiber and further compressed in time domain by a prism compressor. We show interferometric linear optical near-field measuremetns of V-shaped nanoantennas utilizing a scattering type scanning near-field optical microscope (s-SNOM). As a further step, we plan to couple the compressed pulses into our s-SNOM setup. Thereby, we hope to measure the near-field intensity at the second harmonic frequency to be able to correlate the results with the linear measurements.

[1] Li, G., Zhang, S. & Zentgraf, T. Nonlinear photonic metasurfaces. Nat Rev Mater **2**, 17010 (2017)

O 50.4 Tue 18:15 P2/EG

Fabrication and near-field characterisation of plasmonic chiral couplers — •Hans-Joachim Schill, Mike Prämassing, and Stefan Linden — Physikalisches Institut Universität Bonn, D-53115

For particularly designed on-chip coupling structures the polarization properties of incident free-space radiation can steer the propagation direction in plasmonic waveguides.[1] Here we investigate an approach based on optical spin-orbit coupling utilizing a circularly polarized laser beam. Different planar coupler geometries, fabricated by focused ion beam milling and electron beam lithography are studied in order to yield switchable directional coupling depending on the helicity of the incident light. As a tool to investigate the properties and functionality of individual couplers we use scattering type scanning near-field optical microscopy (s-SNOM), where a sharp metallic tip is raster-scanned over the sample and scatteres the nearfield signal into the farfield. The obtained spatially resolved amplitude- and phase-information, reveal the intensity and propagation direction of the surface plasmon polaritons (SPPs). The experimental near-field measurements are compared with finite element simulations.

[1] Y. Lefier, T. Grosjean, Opt. Lett. 40, 2890-2893 (2015)

O 50.5 Tue 18:15 P2/EG

Near-Field characterization of sponge-like gold structures using optical frequencies — •Nicolai Grund, Mike Prämassing, and Stefan Linden — Physikalisches Institut Universität Bonn, D-53115

Three-dimensional nanoporous gold films exhibit strong, plasmonic "hot spots" with resonance frequencies ranging from the visible to the infrared regime, depending on the average pore size. This feature distinguishes these samples as promising substrates for chemical sensing applications in a broad spectral range[1]. We present an experimental near-field study of nanoporous gold films showing resonances from the visible to the near-infrared wavelength regime. To fabricate the nanoporous gold films, we make use of the composition of commercially available leaf gold. It consists of Gold (Au) and Silver (Ag), where a large fraction of the Ag can be etched away using salpeter acid (HNO_3). The average pore size can be controlled by choosing the initial ratio of Au and Ag. We utilize scattering-type scanning near-field optical microscopy (s-SNOM) in reflection mode in order to measure the near fields above the sample. The resulting two-dimensional near-field distributions allow to study the spatial distribution and density of plasmonic "hot-spots" on the film. Near-field imaging with different excitation wavelengths is used to determine the spectral occurrence and width of distinct hot spots.

[1] Wallace, Gregory Q., et al., Analyst 140.21 (2015): 7278-7282

O 50.6 Tue 18:15 P2/EG

Nanometer precise fabrication of electrically connected gold nanoantennas using a helium ion microscope — •Jessica Meier, René Kullock, Thorsten Feichtner, and Bert Hecht — Nano-Optics and Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany

Optical antennas can be used to control and enhance light-matter interaction on a nanometer scale and are therefore interesting for e.g. spectroscopy, optical sensing applications, and - if combined with electric connections - for electrically driven light emission. In all cases, a high fabrication accuracy, especially in the gap region, is mandatory for stable operation. Standard nanofabrication techniques including electron beam lithography and focused ion beam (FIB) milling using gallium (Ga) ions in combination with polycrystalline metal films achieve minimum feature sizes of 10 nm. The combination of Ga-FIB and helium ion microscope (HIM) based milling improves on that and allows to fabricate gap sizes down to 6 nm [1].

We present a Ga-FIB/HIM based milling approach combined with single-crystalline gold flakes, which already showed great improvements for pure Ga-FIB milling [2]. We are thus able to achieve nanometer precise antenna dimensions with high aspect ratios as well as gap sizes down to 3 nm. This opens the possibility to study field emission and nonlinear optical processes, namely second harmonic generation and two-photon photoluminescence.

[1] H. Kollmann et al., Nano Lett. **14**, 4778-4784 (2014)

[2] J.-S. Huang et al., Nat. Commun. **1**, 150 (2010)

O 50.7 Tue 18:15 P2/EG

Plasmonic nanoantennas embedded in zinc oxide — •Ruth Volmert, Nils Weber, Maximilian Albert, and Cedrik Meier — Department Physik, Universität Paderborn, 33098 Paderborn

Plasmonic nanoantennas for visible and infrared radiation can strongly enhance the interaction of light with nanoscale materials due to their strong near-field enhancement. In this work we show the effective generation of second harmonic generated light in zinc oxide (ZnO) by using double-resonant gold nanoantennas embedded in ZnO. By fully embedding the nanoantennas in the ZnO, the strong increase in the electric field between the antennas, triggered by their plasmonic resonance, is utilized for the frequency conversion. In order to embed gold nanoantennas in a ZnO environment, different approaches are demonstrated and analysed. The nanoantenna structure consists of three rods with two localized surface plasmon resonances at ω and 2ω. Two long antennas lead to strong localization of light at the fundamental frequency ω within the ZnO and the third antenna, placed between the two fundamental antennas, provides an improved reemission of the second harmonic generation (SHG) at 2ω into the far field. We show that embedding gold nanoantennas in ZnO is possible by MBE overgrowth of ZnO on the nanoantennas. In addition, nonlinear optical measurements show that the embedded structures lead to a significant enhancement of the SHG compared to the emission of nanoantennas placed on the ZnO substrate. These promising results demonstrate the potential of SHG emission from embedded metallic nanostructures and paves the way for further investigation on other fabrication parameters.

O 50.8 Tue 18:15 P2/EG

Tailoring energy and dimensionality of plasmonic nanostructures — •Hongdan Yan[1,2], Bo Liu[1,2], Dirk Wulferding[1,2], Frank Ludwig[2,3], and Peter Lemmens[1,2] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]EMG, TU-BS, Braunschweig, Germany

Novel routes for energy tuning and adaption of surface plasmon resonances within 3-dimensional Au nanowire arrays are presented. Based on a defect management of the substrate (anodic aluminum oxide, AAO) via annealing we demonstrate a tuning of the longitudinal resonance of plasmons towards higher energy [1]. To induce a 3D-1D crossover the Au nanowires are released in a self-controlled etching and annealing process. Optical absorption experiments demonstrate a very efficient coupling to molecular excitons with resulting "plexcitons" [2]. Theoretical modelling of the plasmonic spectrum supports our experimental findings. Work support by QUANOMET-NL4. [1] H. Yan, P. Lemmens, D. Wulferding, J. Shi, K. D. Becker, C. T. Lin, A. Lak, M. Schilling, J. Mat. Chem. Phys. 135, 206 (2012). [2] B. Liu, B. Thielert, A. Reutter, R. Stosch, P. Lemmens, J. Phys. Chem. C 123, 19119 (2019).

O 50.9 Tue 18:15 P2/EG

Manipulating single 3D plasmonic nanostructures with a focused helium ion beam — •Annika Bräuer, Christoph Dreser, Dieter P. Kern, and Monika Fleischer — Institute for Applied Physics and Center LISA+, Tübingen, Germany

Although particle plasmonics is a well-studied topic and quite well understood when it comes to confining light to the nanometer scale or tuning resonances, there still is ample scope in engineering nanostructures for higher near-field enhancements (NFE) [1] on the one hand and a better positioning and accessibility of hot spots on the other hand. In view of far-field properties, defining the directionality of the antenna emission is of strong interest.

Improvements in tuning such properties are mostly limited by fabrication processes. A helium ion microscope is a powerful tool for manipulating structures on a sub-5 nm-scale, offering a broad spectrum of features for NFE. By processing conical nanoantennas with a focused helium ion beam [2,3], we show that the resonant behavior can be changed as well as the emission characteristics, and near-field enhancement can be induced at defined positions.

[1] A. García-Etxarri et al., Optics Express 20, 25201-25212 (2012)

[2] M. Fleischer et al., Nanotechnology 21, 65301 (2010)

[3] F. Laible et al., Nanotechnology 30, 235302 (2019)

O 50.10 Tue 18:15 P2/EG

Nanostructuring with the aid of atomic layer deposition — •Benjamin Trzeciak[1], Eric N'Dohi[2], Florian Laible[1], Christoph Dreser[1], and Markus Turad[1] — [1]1Institute for Applied Physics and Core Facility LISA+, Eberhard Karls University Tübingen, Germany — [2]2University of Technology Troyes, France

Thin layers are indispensable in today's fabrication of nanostructures. In order to reduce the size of complex and innovative structures like MEMS sensors, fuel or solar cells it is not only necessary to produce smaller conductive structures. It is also crucial to be able to insulate the structures with even thinner layers. Atomic layer deposition (ALD) offers a solution for depositing ultra-thin layers with the accuracy of single layers. Their high aspect ratio, homogeneity, linear and isotropic growth are regarded as major advantages of this deposition technique.

In this work the technique of ALD is utilized in combination with plasmonic nanostructures, in particular silver nanodiscs. Non-passivated silver easily oxidizes or sulfidizes, which means that its optical properties are not stable over time. In order to guarantee long-term stability and maintain their optical properties, such as plasmonic resonances, the silver discs are passivate with a closed layer of minimal thickness. Building on this, ALD layers can be used as spacers with Angstrom distance control for hybrid structures such as dimers or nanostructure-quantumdot-systems.

The mechanism of ALD and the methods of ellipsometry and X-ray diffraction will be briefly discussed together with the preparation of silver nanodiscs and their spectra.

O 50.11 Tue 18:15 P2/EG

Comparison and analysis of ultra-narrow gaps fabricated by electron and helium ion beam lithography — •Hao HU[1,2], Monika Fleischer[2], and Pierre-Michel Adam[1] — [1]Universite* de Technologie de Troyes, 12 Rue Marie Curie, CS42060, 10004 Troyes Cedex, France — [2]Institute for Applied Physics and Center LISA+, Eberhard Karls University Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Metal nanostructures with ultra-narrow gaps, which enable strong field enhancements in plasmonic structures, have attracted widespread attention in physics, chemistry, and biology. However, fabricating ultra-narrow nanogaps is still challenging at present, and controllable gap size, accurate dimensions, and scalable fabrication are desired for further applications. The most common methods for fabricating nanogaps arrays are electron beam lithography (EBL) and focused ion beam

(FIB) milling. Depending on the difference of cross-linking reaction and degradation reaction occurring under the electron beam, the photoresist can be classified into two types: positive tone and negative tone. FIB can be divided into He-ion and Ga-ion beam depending on the ion source used. In this study, we provide a comparison of nanostructures fabricated with different methods including different types of EBL and FIB. By varying the fabrication methods of the nanostructures, we aim to find optimized approaches for fabricating ultra-narrow nanogaps.

O 50.12 Tue 18:15 P2/EG

Micro-ellipsometric Investigation of Ordered Plasmonic Nanostructures — •Jia Tang[1], Ilya Milekhin[2], Fang Dai[1], Eugene Bortchagovsky[3], Dietrich R. T. Zahn[2], and Monika Fleischer[1] — [1]Institute for Applied Physics, Eberhard Karls Universität Tübingen — [2]Semiconductor Physics, Technische Universität Chemnitz — [3]V. Lashkarev Institute of Semiconductor Physics of NAS of Ukraine

Nanoparticles of metals have size-dependent optical properties different from the corresponding bulk materials. Such properties originating from the ability of their conduction electrons to sustain collective oscillations known as plasmons, are key ingredients in applications including surface-enhanced spectroscopies, chemo- and bio-sensing, and holographic techniques. Here the interparticle interactions in plasmonic structures are focused on. Systems with strong coupling of localized modes or localized and propagating plasmons demonstrate hybridization of resonances. The main aim of this work is to investigate the influence of geometrical parameters and the form-factor of lattices on the plasmonic and optical properties by high spatial resolution ellipsometric measurements. This technique makes it possible to obtain detailed geometric as well as amplitude and phase information about the coupled systems, providing a better insight into the hybridization of plasmon modes. In this presentation, extinction spectroscopy and imaging spectroscopic ellipsometry with high spatial resolution are employed to investigate ordered metal-insulator-metal (MIM) nanostructures, which are prepared by electron beam lithography.

O 51: Poster Session - Metal Substrates: Adsorption and Reaction of Small Molecules

Time: Tuesday 18:15–20:00 Location: P2/1OG

O 51.1 Tue 18:15 P2/1OG

Electronic Structure of a Highly Ordered B_3N_3-Doped Nanographene Monolayer on Au(111) — •Axel Belser[1], Katharina Greulich[1], Holger F. Bettinger[2], Heiko Peisert[1], and Thomas Chassé[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tuebingen — [2]Institute of Organic Chemistry, University of Tuebingen

Electronic interface properties and the initial growth of hexa-*peri*-hexabenzocoronene with a borazine core (BN-HBC) on Au(111) have been studied by using X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). The results are compared to hexa-*peri*-benzocoronene (HBC). Both molecules form well-defined monolayers, in particular after annealing of 2-3 monolayers to 300 °C. Valuable information about the electronic structure is obtained by a variation of the tunneling voltage. The distribution of the HOMO and the LUMO determined tentatively by STM is in good agreement to DFT calculations.

O 51.2 Tue 18:15 P2/1OG

probing water overlayer on Pt(111) by noncontact atomic force microscopy — •Sifan You[1], Jing Guo[1,2], Duanyun Cao[1], Ji Chen[1], Xinzheng Li[1], Limei Xu[1,3], Enge Wang[1,3], and Ying Jiang[1,3] — [1]School of Physics, Peking University, Beijing 100871, P. R. China — [2]Beijing Normal University, Beijing 100875, P. R. China — [3]Collaborative Innovation Center of Quantum Matter, Beijing 100871, P. R. China

As a common and efficient catalyst in electrochemical reactions, platinum has attracted lots of attentions. Imaging the water structures at atomic level may help us to achieve a better understanding of electrical double layer near the electrode and active sites during the catalytic process. Using qPlus-based noncontact atomic force microscopy, here we were able to image partial dissociation of the first water overlayer on Pt(111) with unprecedented resolution. For the root square 37 structure, it is consistent with the previous results, showing a mixture of 5-6-7 water rings. Combined with X-ray photoelectron spectroscopy, we identify the structural evolvement of the water layer from intact *37**37 phase to a partially dissociated 3*3 phase after low-temperature annealing. Temperature and isotope dependent measurements clearly show that the transition involves a proton tunneling process, which is facilitated by a collective rearrangement of H-bonding network. This work reveals the key role of nuclear quantum effects in the surface-catalyzed water dissociation.

O 51.3 Tue 18:15 P2/1OG

Fusion of alkyl groups to form phenyl rings: a new on-surface reaction — •Amogh Kinikar[1], Marco Di Giovannantonio[1], Josè Ignacio Urgel[1], Kristjan Eimre[1], Carlo Pignedoli[1], Xiao-Ye Wang[2], Zijie Qiu[2], Akimitsu Narita[2], Klaus Müllen[2], Pascal Ruffieux[1], and Roman Fasel[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, 8600, Switzerland — [2]Max Planck Institute for Polymer Research, Mainz, 55128, Germany

On-surface synthesis allows for the design of carbon nanostructures such as graphene nanoribbons with atomic precision. However, the variety of conceivable structures critically depends on the number of available reactions. Here, we present a new surface-assisted reaction allowing for the controlled fusion of two alkyl groups to form a phenyl ring mediated by the activation of alkyl C-H bonds under ultra-high vacuum conditions. Scanning tunneling and non-contact atomic force microscopy images at different stages of the reaction along with DFT simulations allow us to elucidate the reaction mechanism. Furthermore, we study the influence of surface templating by comparing the reaction on Au(111) and Au(110). The selective formation of phenyl rings by the on-surface fusion of alkyl groups is unprecedented, and introduces a powerful new motif for the design of novel carbon nanomaterials while furthering our understanding of the reactive nature of the alkyl C-H bonds.

O 52: Poster Session - New Methods: Experiments

Time: Tuesday 18:15–20:00 Location: P2/1OG

O 52.1 Tue 18:15 P2/1OG

Design of an electron beam ion source for experiments with ultrafast timing resolution using SIMION simulations — •Johanna Fries[1], Anna Niggas[1], Gabriel L. Szabo[1], and Richard A. Wilhelm[1,2] — [1]TU Wien, Institute of Applied Physics, Vienna, Austria — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany

The interaction of ions with a solid surface is characterized by many different processes, such as sputtering, electron emission and nanostructuring. Time scales of these processes span from the sub-fs regime for charge exchange to the μs-regime for ion-induced defect diffusion. In order to investigate the dynamics of at least some of these processes in experiment, ion pulses with a pulse length and timing accuracy in the sub-ps range are necessary.

With the help of SIMION simulations we develop the design of an electron beam ion source (EBIS) capable of producing such ultrashort ion pulses. Our design uses a simple Ti:Sapphire oscillator as electron pulse trigger in contrast to high power or high harmonics laser systems for photo-ionization. Starting from the design of a commercial EBIS, several parts will be replaced with tailor-made components in SOLIDWORKS. The CAD drawing is then used for a particle trajectory simulation based on the code SIMION. To optimize the ion source performance with regard to pulse length, beam focus and output, parameters such as spatial dimensions and potentials are varied and systematically analyzed.

O 52.2 Tue 18:15 P2/1OG

Design of an ultrafast THz-STM — •Nils Bogdanoff, Sergey Trishin, Christian Lotze, Katharina J. Franke, and Tobias Kampfrath — Freie Universität Berlin, Department of Physics, Arnimallee 14, 14195 Berlin, Germany

Investigating the ultrafast dynamics of electronically excited systems is crucial for understanding its coupling to the environment. Most state-of-the-art ultrafast techniques are used to investigate isolated systems in gas-phase or applied to macroscopic surface areas of carefully tailored systems. However, many modern applications strive towards increasingly small, surface-coupled structures approaching the atomic scale. A standard technique for high electronic real-space resolution is scanning tunneling microscopy (STM). Its temporal resolution is limited by the bandwith of the amplifier, cabling and the junction capacity itself. In 2013 Cocker et al. demonstrated that applying a pulse of THz radiation to the junction of an STM can act as a transient bias voltage opening a tunneling channel only for an ultrashort period of time [1]. Using this in a pump-probe scheme and recording changes in the average tunneling current makes ultrashort timescales accessible by STM [1,2]. Here we present first steps on the way to constructing and characterizing a THz-STM using a tilted-pulse-front pumping scheme to generate THz-pulses in a lithium niobate (LN) crystal.

[1] Cocker, T. et al. An ultrafast terahertz scanning tunnelling microscope. Nature Photon 7, 620-625 (2013)

[2] Cocker, T. et al. Tracking the ultrafast motion of a single molecule by femtosecond orbital imaging. Nature 539, 263-267 (2016)

O 52.3 Tue 18:15 P2/1OG

Low Energy Positron Beam for Near-Surface Doppler-Broadening Spectroscopy — •Lucian Anton Joshua Mathes, Sebastian Vohburger, Vassily Vadimovitch Burwitz, and Christoph Pascal Hugenschmidt — Physics Department E21 and Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München

A new positron lab beam setup has been constructed for low energy Doppler-broadening experiments aimed at examining near-surface defect structures. Positrons are provided by a ^{22}Na source, then moderated in a thin tungsten foil from which they are guided to the sample chamber by a system of longitudinal and transverse magnetic fields. The positrons are accelerated electrostatically by a potential difference applied between moderator and sample to a kinetic energy from a few electronvolts up to 30 keV. Inside the UHV chamber the positron beam is focused onto the sample by an electrostatic single lens. This setup is intended to complement the positron instrument suite at NEPOMUC and expands capabilities in the field of defect studies close to the surface layer. First experimental results on oxides will be presented.

O 52.4 Tue 18:15 P2/1OG

Heat of Adsorption on Single Crystals: Microcalorimetry — •Ann-Katrin Baumann and Swetlana Schauermann — Max-Eyth-Str.2, 24118 Kiel

Rational design of new heterogeneous catalysts requires detailed understanding of the bonding interactions between the gaseous species and the catalytic surface. One of the crucial parameters in this interaction is the adsorption enthalpy of the involved surface species.

Adsorption enthalpies can be determined with high level of accuracy by a direct method of single crystal adsorption calorimetry (SCAC), which has a number of advantages over the commonly used indirect method of temperature programmed desorption. In contrast to indirect methods, SCAC provides heats of adsorption without relying on assumptions on the details of the desorption kinetics or reversibility of the desorption processes.

In this work, an improved experimental setup of SCAC is presented. In ultra high vacuum, a pulsed molecular beam is employed to dose a known amount of molecules on a well-defined thin metal single crystal (1-2 μm) or nanostructured model surfaces containing supported metallic nanoparticles. The arising heat of adsorption is detected by a pyroelectric material (β-PVDF) pressed against the back of the thin metal crystal. Simultaneously the sticking coefficient of the molecules is recorded in order to determine the amount of molecules contributing to the signal and the total amount of molecules remaining permanently adsorbed on the surface. We present the adsorption energies of simple molecules employing an improved design of SCAC setup.

O 52.5 Tue 18:15 P2/1OG

Temperature measurement by a pyrometer: Determination of the emissivity coefficient and influencing factors — •Robert Decke, Mate Puljiz, and Mathias Getzlaff — Institute of Applied Physics, University of Duesseldorf

Pyrometers represent an elegant tool for the contactless measurement of temperatures. This technique is especially important under vacuum or aggresive conditions. Additionally, high temperatures can be determined. For a correct procedure the emissivity coefficient must be known which is a measure for the difference of the emitted light intensity at a specific wave length between a black body and the real object. The goal of this study was therefore to investigate the influencing factors of this coefficient.

Here we report on the investigation of a W(110) crystal at different temperatures with pyrometers working at two different wave lengths. The real surface temperature was monitored using a thermocouple. The influence of the setup, the focus condition of the pyrometer optics, the wave length and the angle between the surface normal and the detection direction will be shown.

O 52.6 Tue 18:15 P2/1OG

Towards a high-intensity ion source for preparative mass spectrometry — •Paul Fremdling[1], Laurent Bernier[2], Loukas Kyriakidis[2], Julius Reiss[2], and Stephan Rauschenbach[1] — [1]Department of Chemistry, University of Oxford, UK — [2]Institut für Strömungsmechanik und Technische Akustik, Technische Unversität Berlin, DE

Preparative Mass Spectrometry (pMS) is an ion beam deposition technique producing highly purified, mass-filtered homogeneous samples of non-volatile compounds such as metal ion clusters(1), sugars(2) or intact Proteins in vacuum(3). High-intensity ion sources are a prerequisite to apply pMS to produce technological coatings on a macroscopic surface as well as to selectively mass-filter and land low-abundance ionic species.(4) However, in current mass spectrometers the transmission efficiency from electrospray to high vacuum is less than a tenth and the maximum ion current achievable is limited to the low nA range(4). We want to overcome this barrier by developing a novel vacuum interface combining a high-capacity transfer capillary(5, 6) with an ion funnel system optimised under fluid dynamics aspects.

1. M. A. Röttgen et al., Rev. Sci. Instrum. 77, 013302 (2006). 2. S. Abb et al., Angew. Chem. Int. Ed. 58, 8336-8340 (2019). 3. J.-N. Longchamp et al., Proc. Natl. Acad. Sci. 114, 1474-1479 (2017). 4. S. Rauschenbach et al., Annu. Rev. Anal. Chem. 9, 473-498 (2016). 5. M. Pauly et al., The Analyst. 139, 1856 (2014). 6. L. Bernier et al., J. Am. Soc. Mass Spectrom., 1-13 (2018).

O 52.7 Tue 18:15 P2/1OG

Femtosecond point-projection microscopy and holography – electron source coherence and spatial resolution — Faruk Krečinić and •Ralph Ernstorfer — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Femtosecond point-projection microscopy (fs-PPM) is a technique for visualizing ultrafast charge motion in real space. A nanotip electron source is brought close to the sample such that the diverging electron beam projects a magnified image of the sample onto the detector. Due to the use of low-energy electrons, the PPM image is highly sensitive to local (nanoscale) electric fields. At high magnification, one observes an in-line holographic projection of the sample that is sensitive enough to visualize a single elementary charge [1]. By triggering the emission of electrons from the nanotip with an ultrafast laser it is possible to perform pump-probe PPM, visualizing the ultrafast dynamics of charge carriers with nanometer resolution [2,3]. However, the photoemission process can also lead to a decrease in the spatial resolution. Using a semi-classical model we show how spatial and temporal coherence, as well as electron-optical aberrations and the apex geometry, affect the spatial resolution of the PPM technique. The introduced semi-classical model is in principle more generally applicable to investigations of the wave-optical properties of (photo)electron sources for electron microscopy.

[1] T. Latychevskaia, et al., Nano Letters, 16(9), 5469-5474, (2016). [2] M. Müller, et al., Nat. Comm., 5, 5292 (2014). [3] F. Krečinić, et al., arXiv:1803.01766, (2018).

O 52.8 Tue 18:15 P2/1OG

New 100-kHz User Beamline Based on High-Harmonic Gen-

eration for Time-Resolved Photoemission — •Charlotte E. Sanders, Yu Zhang, Adam S. Wyatt, Gabriel Karras, Richard T. Chapman, Gregory M. Greetham, Michael Towrie, and Emma Springate — Central Laser Facility, STFC Rutherford Appleton Laboratory, Harwell OX11 0QX, UK

The UK's Central Laser Facility (CLF) Artemis Laboratory offers open access to pump-probe angle-resolved photoemission spectroscopy (ARPES), whereby ultrafast dynamics in solid-state systems can be probed using high-harmonic generation. Our beamline supports the study of dynamics ranging from the femtosecond to the picosecond regimes, with tuneable polarization in both the pump and probe. We have recently upgraded our capabilities to include a 100-kHz laser system. In our first user call, in 2020, we plan to offer temporal and spectral resolution of around 50 fs and 100 meV, respectively, and probe photon energies of 25–40 eV, combined with pump photon energies of 0.48 or 0.73 eV (1.7 or 2.6 μm). In the future, with further development, we will offer additional options such as tuneable pump energy and probe energies up to 100 eV. The high repetition rate will permit favourable statistics and space charge conditions relative to lower-repetition rate systems.

O 52.9 Tue 18:15 P2/1OG

Extracting Protein Collision Cross Sections (CCSs) from Pre-Fourier Transform Mass Spectrum Transients — •Dhiren De Silva, Paul Fremdling, Tim Esser, Joseph Gault, and Stephan Rauschenbach — Department of Chemistry, Oxford University, UK

The collision cross section (CCS) of a molecule gives a sense of its size and shape and is defined as the area of a circle with radius equal to the sum of the radii of two colliding molecules. Protein CCSs have conventionally been measured through Ion Mobility experiments with dedicated instruments. More recently, procedures involving analysis of mass spectrum transients have been used to determine protein CCSs. These new methods make use of the fact that the transient signal, which is an oscillating signal due to the motion of ions in the trap, displays beating due to the superposition of the individual signals and decays in amplitude over time mainly due to ion-neutral collisions. Transients of several model proteins such as ubiquitin, cytochrome C and myoglobin in various charge states were recorded with the QE UHMR Orbitrap Mass Spectrometer. An algorithm was developed to extract the decay lifetime and calculate the CCS using ubiquitin in charge state 9 as a calibrant. We explore monitoring the CCS during native protein deposition ES-IBD experiments in a modified QE Orbitrap Mass Spectrometer. This will allow online monitoring of shape during protein deposition for imaging applications.

O 52.10 Tue 18:15 P2/1OG

Selective Preparation of Electron Micrsocopy grids via Native Electrospray Ion-Beam Deposition — •Sam Britton, Tim Esser, Paul Fremdling, Stephan Rauschenbach, and Dhiren De Silva — University of Oxford

Due to the close relationship of structure and function, structural determination of proteins is an enormously important area of biochemistry. Cryo-electron microscopy (EM) can generate highly resolved structures by averaging many low contrast, single particle images of proteins embedded in vitreous ice; however, TEM is typically unable to reach high resolution for heterogeneous samples. Here we outline an alternative approach of preparing samples for single-particle EM, which is based upon native electrospray ion-beam deposition (ES-IBD). Samples are prepared using a modified commercial mass spectrometer (Q Exactive UHMR - Thermo Fisher) and subsequently imaged with atomic force microscopy and TEM. We explore the ability of this instrument to mass select single species followed by focused, soft deposition onto a TEM grid, thereby eliminating the issue of sample heterogeneity.

O 52.11 Tue 18:15 P2/1OG

Following the motion of a charged conducting sphere by electrostatic induction in a parallel plate capacitor — Mirco Kaponig, •Andre Mölleken, Doris Tarasevitch, Detlef Utzat, Hermann Nienhaus, and Rolf Möller — Fakultät für Physik/Cenide, Universität Duisburg-Essen, Germany

The charges induced in the plates of a parallel plate capacitor due to a conducting charged moving sphere have been measured up to the mechanical contact. For larger distances the induced charge scales linearly with the distance. However, when the sphere approaches the plate further the charges on the sphere are attracted by the induced charges in the plate and move on the surface of the sphere towards the plate. This leads to a further increase of the induced charge. The experimental results compare well to an approximate formula which will be discussed in detail.

O 52.12 Tue 18:15 P2/1OG

Statistical evaluation of the switching current in a STM Josephson junction — •Martina Trahms[1], Rika Simon[1], Nils Bogdanoff[1], Olof Peters[1], Gaël Reecht[1], Clemens B. Winkelmann[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Univ. Grenoble Alpes, Institut Neél, 25 Avenue des Martyrs, 38042 Grenoble, France

The intrinsic order of the superconducting ground state is given by the superconducting order parameter. In a Josephson junction this order parameter can be determined by measuring the junction's critical current. A Josephson junction is formed in a scanning tunneling microscope (STM) using a superconducting tip in close proximity to a superconducting surface. In the I-V characteristic of this junction the transition from the Cooper pair to the quasi particle tunneling regime is specified by the switching current. In a purely thermal activated system the switching current follows a Poisson distribution around the critical current. However, the distribution of the switching current might also be sensitive to other energy fluctuations, e.g. quantum noise and spin related excitations induced by magnetic adatoms. To investigate these activation processes we statistically analyse the switching current in a Josephson junction formed between a Pb tip and Pb(111) surface.

O 53: Poster Session - Oxides and Insulators: Adsorption and Reaction of Small Molecules

Time: Tuesday 18:15–20:00 Location: P2/1OG

O 53.1 Tue 18:15 P2/1OG

Investigation of Proton Conductivity in Yttria Stabilized Zirconia Thin Films by Electrochemical Impedance Spectroscopy — •Lars-Erik Maurer, Erdogan Celik, and Matthias T. Elm — Center for Materials Research, Gießen, Germany

Dense and porous yttria stabilized zirconia (YSZ) thin films were fabricated using pulsed laser deposition in order to investigate the influence of the layer thickness on the electrical and protonic transport properties under dry and wet atmospheres. For that purpose, electrochemical impedance spectroscopy was performed at different temperatures, oxygen partial pressures and relative humidities. Under dry atmospheres, the total conductivity of the thin films is dominated by oxygen vacancies and increases with increasing grain size due to the blocking behavior of the grain boundaries. At wet conditions, the total conductivity of the dense films is reduced which is attributed to an annihiliation of the oxygen vacancies at the surface due to adsorbed water molecules. Only the porous layers exhibits a proton conductivity in wet atmosphere at low temperature and high relative humidity revealing the importance of the pore structure on the surface protonic conductivity of oxide materials.

O 53.2 Tue 18:15 P2/1OG

IRRAS study of CO adsorption on the calcite (10.4) surface — Weijia Wang, •Alexei Nefedov, Stefan Heissler, Yuemin Wang, and Christof Woell — Karlsruhe Institute of Technology, Institute of Functional Interfaces, Eggenstein-Leopoldshafen, Germany

The atomic structure of natural cleavage (10.4) calcite surface is a precondition to gain an understanding of its surface properties. To date, the atomic-level understanding of the structure is still under controversy. Therefore, in the present investigation, the (10.4) calcite surfaces were explored by the FTIR Spectroscopy with polarized infrared light in an ultrahigh vacuum (UHV) apparatus with the use of CO as a probe molecular. In order to achieve clean (10.4) calcite surface in UHV, dedicated devices (wobble stick, sample holder) are designed to perform the UHV cleavage. At low exposure, the adsorption of CO on the fresh cleaved (10.4) calcite surface at relatively low temperature of 62 K leads to a sharp negative C-O stretching band located at $2175.8\ \mathrm{cm}^{-1}$ using the p-polarized infrared light. This band represents a coverage-induced frequency redshift trend before reaching to the saturated coverage. This observation provides the direct spectroscopic evidence that the cleaved calcite surface is a well-ordered surface.

O 53.3 Tue 18:15 P2/1OG

LEED Analysis of CO on NaCl(100) under Optical Excitation — •Liam Shelling Neto, Hannes Böckmann-Clemens, and Claus Ropers — 4th Physical Institute - Solids and Nanostructures, University of Göttingen, Göttingen, Germany

Vibrational energy transfer between adsorbates and solid surfaces is of fundamental interest in surface science and has been explored in multiple contexts. In this regard, CO adsorbed on NaCl is a prominent model system, as its long vibrational lifetime allows for studying the energy flow between molecules via dipole-dipole interactions, which leads to the extreme concentration of vibrational energy at individual molecules. However, the structural modifications that accompany this process remain largely unknown and challenging to explore, for a lack of a direct probe to observe their dynamics. Here, we use an ultrafast LEED setup to monitor the surface structure under optical excitation. The presented results constitute a preliminary step towards the understanding of the structural dynamics accompanying the vibrational energy transfer.

O 53.4 Tue 18:15 P2/1OG

Quantitative LEED studies of acetylene physisorbed on ionic surfaces – significance of electron scattering from hydrogen — •Jochen Vogt — Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

C_2H_2 physisorption on ionic substrates is characterized by comparably soft interaction, leaving the internal structure of the molecules largely undistorted. On the KCl(100) surface, the first layer has $(\sqrt{2}\times\sqrt{2})R45^\circ$ symmetry [1], while on the NaCl(100) surface, $(3\sqrt{2}\times\sqrt{2})R45^\circ$ and even $(7\sqrt{2}\times\sqrt{2})R45^\circ$ phases have been observed [2]. In principle, a complete structure determination of such systems is possible using LEED I(V) analysis [3,4]. Due to the weakness of electron scattering from hydrogen, this element was not included in a LEED study of C_2H_2-(2×2)/MgO(100) [4]. The contribution addresses the possible systematic error resulting from the neglect of hydrogen scattering in these systems. In the case of C_2H_2/KCl(100), calculated I(V) curves of the very weak superstructure spots are significantly affected by the neglect of hydrogen with respect to both intensity and the position of maxima, the latter implying notable changes of the Pendry R-factor. [1] A. L. Glebov et al., Phys. Rev. B61(2000), 14028 [2] S. Picaud et al., Phys. Rev. B57 (1998), 10090 [3] J. Vogt, H. Weiss, Phys. Rev. B77 (2008), 125415 [4] D. Ferry et al., Phys. Rev. Lett. 78 (1997), 4237

O 53.5 Tue 18:15 P2/1OG

Theoretical characterization of the surface and adsorption properties of water on titanium dioxide surfaces — •Holger-Dietrich Sassnick[1,2], Sebastien Groh[3], Joachim Dzubiella[1,3], and Victor G. Ruiz[1] — [1]Research Group for Simulations of Energy Materials, Helmholtz-Zentrum Berlin, Berlin, Deutschland — [2]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Deutschland — [3]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Deutschland

Water splitting is a process for clean energy with promising technological applications to reduce environmental pollution an mitigate climate change. Rutile TiO_2(110) has become the prototypical oxide surface in surface science and its interaction with water a model system for the water-oxide interface. Even though extensive experimental and theoretical studies at the single-molecule level exist, the preferred adsorption state of water is still highly debated [U. Diebold, JCP 147, 040901 (2017)]. We present a thorough theoretical characterization of the surface and adsorption properties of water at the single-molecule level on the rutile (110) and the anatase (101) surfaces using density-functional theory including collective many-body effects in the dispersion interactions and a quantification of self-interaction error. In addition, we investigate coverage effects from the single-molecule to the monolayer regimes and quantify the dissociation barrier of a single water molecule. Our work aims to include all relevant effects at the electronic-structure level to quantify subtle changes on the water dissociation process and pave the way to more complex simulations of solid-liquid interfaces.

O 54: Poster Session - Semiconductor substrates: Adsorption and Reaction of Small Molecules

Time: Tuesday 18:15–20:00 Location: P2/1OG

O 54.1 Tue 18:15 P2/1OG

Vibrational Sum Frequency Generation Spectroscopy Study for Alcohol Adsorption on TiO_2 Thin Film — •Anupam Bera, Denise Bullert, and Eckart Hasselbrink — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

The surface chemistry of TiO_2 is most intensely studied as it is seen as a prototype system for its photocatalytic properties in particular in the context of water splitting and pollutant degradation. However, the interaction of TiO_2 with alcohols has attracted less interest although oxidation of the latter is of large industrial relevance. A thorough understanding of the photochemistry requires the fundamental knowledge of composition, structure of the adsorbed alcohols to TiO_2 surface in an ambient alcohol atmosphere at room temperature. However, extracting this important information is the limiting step in the most cases due to the challenges in probing the interfacial molecules at near ambient conditions. To address this limitation, we use vibrational sum frequency generation spectroscopy (vSFS) as it allows to solely detect surface species and discriminates against spurious signals from ambient gas phase. Our present study reveals important adsorption behaviour of the various alcohol (methanol, ethanol and isopropanol) systems on TiO_2 anatase nano thin film under ambient condition. A systematic study utilizing various polarizations and pressure combinations, allowing us to unambiguously assign the adsorbed species. Our findings reveal key insights into the initial mechanistic steps towards heterogeneous alcohol oxidiation reactions at near ambient condition.

O 54.2 Tue 18:15 P2/1OG

Controlled Manipulation of Diethyl Ether on Si(001)via Tip-Induced Electronic Excitation — •Alexa Adamkiewicz[1], Gerson Mette[1], Tamam Bohamud[1], Michael Dürr[1,2], and Ulrich Höfer[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, Germany — [2]Institut für Angewandte Physik, Justus-Liebig-Universität Giessen, Germany

Tip-induced electronic excitation via STM can give access to alternative reaction channels beyond thermal activation. Recently, we showed for the cleavage of tetrahydrofuran (THF) on Si(001) that excitation by the tunneling electrons leads to new final products, which can be selectively addressed by the type of excitation [1].

Here, we present the influence of the detailed configuration of the adsorbates on tip-induced ether cleavage. Due to the linear molecular structure of diethyl ether (Et_2O), the adsorbates undergo fragmentation when cleaved, thus leading to a higher degree of freedom compared to the ring-shaped THF. The final products differ significantly for Et_2O and THF. These differences do not only represent the influence of the different molecular structures of the adsorbates, but also provide insight with respect to the influence of the local electronic structure of the substrate on the reaction and the competition between electronic structure and steric constraints.

[1] G. Mette *et al.* Angew. Chem. Int. Edit. **58**, 3417 (2019).

O 55: Poster Session - Nanostructured Surfaces and Thin Films

Time: Tuesday 18:15–20:00 Location: P2/2OG

O 55.1 Tue 18:15 P2/2OG

Dynamic contact angles on adaptive surfaces — •Xiaomei Li, Simon Silge, Hans-Jürgen Butt, and Rüdiger Berger — Max-Planck-Institut for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Adaptive surfaces change their physical-chemical properties due to the presence of a liquid or its vapor. Surface adaptation is predicted to be one cause for contact angle hysteresis [1]. We measured the dynamic advancing and receding contact angles of sliding drops on 1H,1H,2H,2H-perfluorooctyltriethoxysilane (PFDTES) surfaces and on polystyrene-poly(acrylic acid) (PS-PAA) copolymer surfaces using a home-built tilted plane setup. PFDTES surfaces as example for a non-adaptive surfaces were prepared by chemical vapor deposition. PS-PAA copolymer surfaces as adaptive surfaces were fabricated by spin-coating. Two modes of adaptation were investigated: velocity dependent contact angles which reflect adaptation time scales from 5 ms to 2 s and drop-wise adaptation for adaptation time scales $>$10 s. The velocity dependent contact angles are compared to predictions from the hydrodynamic and molecular kinetic theories. The latter potentially allows modeling of dynamic contact angles and contact angle hysteresis caused by adaptation processes. [1] Hans-Jürgen Butt, Rüdiger Berger, Werner Steffen , Doris Vollmer, Stefan A. L. Weber, Langmuir, 34, 11292 - 11304 (2018).

O 55.2 Tue 18:15 P2/2OG

Surface Modifications by Ion-Induced Plasma Expansion — •Ayman Sherif El-Said[1] and Waleed Moslem[2] — [1]Physics Department, Dhahran 31261, Saudi Arabia — [2]The British University in Egypt (BUE), Cairo, Egypt

The development of ion sources and accelerators technology offers a new window for the creation of surface nanostructures in an efficient and accurate way. These nanostructures are fabricated without any further chemical treatment, which is common in the traditional lithographic methods. The driving force for the production of nanostructures by single ion impact is mainly the energy deposition of the incident ion in the utilized material [1, 2]. Therefore, it is found that MeV C60 cluster ions enables the creation of nanohillocks of size larger than the ones produced by GeV monoatomic ions. Furthermore, slow highly charged ions were able to create nanostructures similar to the ones created by swift heavy ions [3, 4]. Here, we introduce plasma expansion as a new approach for elucidating the formation mechanism of ion-induced nanostructures [5]. The role of both potential energy and kinetic energy of the impinging ions for the creation of nanostructures by ion-induced plasma is discussed.

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[2] O. Ochedowski, O. Osmani, M. Schade, B. K. Bussmann, B. Ban-d'Etat, H. Lebius, and M. Schleberger, Nat. Comm. 5, 3913 (2014).
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[5] W.M. Moslem, A.S. El-Said, R. Sabry, A. Shalouf, S. K. El-Labany, H. Phys. Lett. A 381, 102 (2017).

O 55.3 Tue 18:15 P2/2OG

Growth of ultrathin single crystalline Bi(111) on Si(111) — •Jesper Moes, Jan Cuperus, Daniël Vanmaekelbergh, and Ingmar Swart — Utrecht University, Debye Institute for Nanomaterials Science, Utrecht, The Netherlands

The spin-orbit derived surface states of bismuth films are of great interest for spintronic applications. STM techniques are ideal for the investigation of its electronic properties. We have grown ultrathin Bi(111) films on a Si(111) substrate with atomically flat areas of up to 100nm x 100nm. The surface states were observed via differential conductance spectroscopy and scattering by point defects. Further insight is obtained by combining quasi-particle interference and density functional theory calculations.

O 55.4 Tue 18:15 P2/2OG

Rapid Water Permeation through Carbon Nanomembranes: Variation of Precursor Molecules and Substrates — •Dario Stierl, Hoang Linh Le, Michael Westphal, Niklas Biere, Yang Yang, André Beyer, Dario Anselmetti, and Armin Gölzhäuser — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

Carbon nanomembranes (CNMs) of $\sim$1 nm thickness are produced by electron-induced crosslinking of self-assembled monolayers (SAMs). Recently, a remarkably high water permeance in combination with a high selectivity has been achieved by 1.2 nm thick free-standing CNMs which originate from p-terphenylthiol (TPT) SAMs on gold substrates [1]. All tested organic solvents were blocked by this type of CNM down to the detection limit, which results in selectivity values of above 100. This contribution reports on water permeation measurements which investigate the effect of preparing CNMs on different substrates as well as varying the CNM precursor molecules. In particular, CNMs from TPT-SAMs on silver as well as p-quaterphenylthiol (QPT) monolayers on gold were studied by X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), helium ion microscopy (HIM) and liquid permeation measurements with the mass-loss method.

[1] Y. Yang *et al.*, *ACS Nano* **2018**, 12, 4695.

O 55.5 Tue 18:15 P2/2OG

Real-time observation of ion-induced surface nanopatterning on crystalline Ge(001) by in-situ GISAXS — •Denise Erb[1], Peco Myint[2], Kenneth Lutterodt-Evans[3], Karl Ludwig[2], and Stefan Facsko[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Boston University, USA — [3]Brookhaven National Laboratory, USA

As a contact-less technique, GISAXS is well suited for in-situ and real-time investigation of surface self-assembly processes. We implemented a custom-made UHV sample environment for GISAXS at the ISR beamline of the NSLS-II synchrotron and observed the nanoscale pattern formation kinetics on a crystalline Ge(001) surface under ion irradiation. The Ge(001) surface is known to develop a nanoscale pit-and-mound pattern of faceted pyramidal structures under irradiation with 1 keV Ar+ ions at normal incidence. The edges of the pyramidal structures are aligned along the <100> and <010> direction, while their sidewall facets have a uniform polar tilt from the <001> direction. Such a regular surface morphology results in a GISAXS intensity distibution with distinct features. From the development of these features with ion fluence, we can conclude on the corresponding development of the surface morphology. Thereby, we directly monitor the lateral characteristic length as well as the polar facet angle as indicators of the kinetics of this ion-induced self-assembly process. The temporal development of these quantities is found to be in good agreement with results of numerical integration of the established continuum equation for surface height evolution under ion irradiation.

O 56: Poster Session - Nanostructures at Surfaces: Dots, Particles, Clusters

Time: Tuesday 18:15–20:00 Location: P2/2OG

O 56.1 Tue 18:15 P2/2OG

UV-light printing on APTES functionalized SiO2 surfaces: New approach for nanoparticle assembly — •Sergii Snegir[1], Olivier Pluchery[2], Thomas Huhn[1], and Elke Scheer[1] — [1]University of Konstanz, Konstanz, Deutschland — [2]Institut des Nano-Sciences de Paris (INSP), Sorbonne Universités, CNRS, Paris, France

The (3-Aminopropyl)trimethoxysilane (APTES) terminated SiO2 surface allows creating self-assembled monolayers (SAMs) of gold nanoparticles (AuNPs) if they are stabilized with trisodium citrate molecules. However, further functionalization of AuNPs with thiol-containing molecules leads to their strong aggregation on the surface due to the appearance of uncompensated dipole moments on the AuNP. Therefore, we developed a UV-light fixation method, which anchors AuNPs on their initial positions on the APTES surface prior to the process of AuNP functionalization. Herein, we present detailed studies of the passivation efficiency as the function of UV light wavelength, time of exposure, concentration of O2, N2, O3 gases. We have found that the combination of O3 and UV light under ambient atmospheric conditions leads to complete passivation of APTES terminated glass already after 2 min of UV exposure (26.1 mW/cm2). We have tested also the possibility to use the UV-light passivation for printing on APTES terminated surfaces by using different chromium masks. With this method, we can create SAMs of AuNP with different geometry and size (current resolution limit is several um) on a SiO2 surface (glass/quartz/silicon).

O 56.2 Tue 18:15 P2/2OG

Annealing behavior of FeNi alloy nanoparticles deposited on a W(110) surface: influence of the Stoichiometry — •Dennis Jagenburg, Mahboobeh Ravankhah, and Mathias Getzlaff — Institute of Applied Physics University Düsseldorf

Properties of metallic nanoparticles significantly differ from that of the corresponding bulk material. This has led to an increasing importance of investigating nanometer-sized metallic particles. From a technological point of view it is necessary to study the nanoparticles at higher temperatures due to heating and altering of structural components in devices during fabrication; thus, the functional performance may change. Therefore, the goal of this study is to analyze the influence of the stoichiometry and annealing temperature on the shape and structure of alloy nanoparticles.

Different sized-selected iron-nickel alloy nanoparticles are produced by a Magnetron-Based Nanocluster Source under UHV conditions and are deposited on a W(110) surface. Scanning Tunneling Microscopy (STM) is used to determine the behavior of $Fe_{0.25}Ni_{0.75}$ and $Fe_{0.75}Ni_{0.25}$ nanoparticles after deposition and subsequent tempering.

O 56.3 Tue 18:15 P2/2OG

Irradiation of Au-nano-islands with slow highly charged ions and characterization with AFM and SEM — •Gabriel L. Szabo[1], Janas Arkadiusz[3], Benedykt R. Jany[3], Franciszek Krok[3], and Richard A. Wilhelm[1,2] — [1]Institute of Applied Physics, TU Wien, 1040 Vienna, Austria — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Institute of Physics, Jagiellonski University, 30-348 Kraków, Poland

Impacts of slow highly charged ions (HCIs) onto a target surface can lead to a change of the material's structure, such as e.g. phase transitions and nano-structures. Responsible for this transformation is the excitation of electrons of the target material due to the neutralization of the ion in the area of the ion impact and subsequent lattice heating mediated by electron-phonon coupling. So far, potential energy effects have not been observed on metallic target materials. This is due to the high electronic conductivity of conductors, which results in a fast dissipation of the electrical excitations induced by the potential energy of the impinging HCI. For a better understanding of this processes, single metallic nano-islands were irradiated. Special emphasize is put on the lateral size of those structures below which the electronic excitation cannot dissipate fast enough and stays confined for a longer period of time. In case of an existing size threshold, nano-structuring due to potential energy effects can be expected. In this work, Au-nano-islands were irradiated by 180 keV Xe^{40+} ions. The samples were measured on the same spot with AFM and SEM, before and after irradiation.

O 56.4 Tue 18:15 P2/2OG

Electronic structure of a carbon dot monolayer on TiO2(110) — •Jan Beckord[1], Matthias Hengsberger[1], Andrea Cannizzo[2], and Jürg Osterwalder[1] — [1]Department of Physics, University of Zurich, CH-8057 Zürich — [2]Institute of Applied Physics, University of Bern, CH-3012 Bern

Carbon dots are nanometer-sized particles with a carbon core and a functionalized organic shell. Our research focuses on their observed photocatalytic properties: for example, they significantly improve the oxygen evolution reaction at titanium dioxide surfaces under visible light irradiation. To elucidate the electronic structure of this system, we adsorbed a single layer of carbon dots with an average size of 4 nm on a clean rutile TiO2(110) surface from aqueous solution in vacuo. We will present the full characterization of these surfaces using XPS, UPS and 2PPE. Our measurements revealed an increased upward band bending of the n-doped substrate and a lowered work function. A continuum of additional occupied states is found at binding energies between 6 eV and 11 eV due to the various molecular orbitals on the carbon dots, and some more occupied states are observed very close to the Fermi level at binding energies between 1 eV and 3 eV. 2PPE measurements revealed a continuum of unoccupied states as well, which pushes the band gap below 2 eV. These continua of electronic states therefore facilitate exciton generation from visible light, explaining the function of carbon dots as effective photosensitizers. Additionally, we found excellent long-term stability even in ambient air and under strong light, making this system suitable for applications under ambient conditions.

O 56.5 Tue 18:15 P2/2OG

Fullerene arrangement by vapor deposition on a well-ordered thin Al_2O_3 film grown on Ni_3Al (111) crystal — •Alexander Kononov and Heinz Hövel — Fakultät Physik / DELTA, Technische Universität Dortmund, 44227 Dortmund, Germany

A thin (∼0.5nm) Al_2O_3 film on a $Ni_3Al(111)$ surface that shows an well-ordered network structure in STM at a tunneling voltage of 3.2V presents a corresponding dot structure formation at 2.0V. The dot structure acts as nucleation pattern when metal islands are grown by atom deposition [1]. For mass-selected Cu clusters it provides thermal stabilization and a specific arrangement of the clusters with respect to the dot structure [2]. This initial situation offers a huge potential for film oxide functionalization with different mass-selected clusters. Due to its easy fabrication, fullerenes (C_{60}) with their properties represent a model system for the metal clusters (e.g. Pb-Clusters), which are planned to be used for future experiments in our surface science facility. We present experimental UPS and STM results for vapor-deposited submonolayers of C_{60} on the surface of well-ordered $Al_2O_3/Ni_3Al(111)$, which show different behavior (e.g. shift in UPS spectrum, island growth in STM images) for different surface temperatures during vapor deposition.

[1] S. Degen, C. Becker, K. Wandelt, Thin alumina films on Ni3Al(111): A template for nanostructured Pd cluster growth, Faraday Discuss. 125, 343 (2004). [2] D. Wolter, Mass selected copper clusters on well-ordered aluminum oxide layers, PhD thesis, TU Dortmund (2018).

O 57: Poster Session - Surface Dynamics: Phase Transitions and Elementary Processes

Time: Tuesday 18:15–20:00 Location: P2/2OG

O 57.1 Tue 18:15 P2/2OG

Phase transitions in geometrically disordered porous solids: from strong to weak disorder — •Henry R. N. B. Enninful, Dirk Enke, and Rustem Valiullin — Universität Leipzig, Leipzig, Germany

Mesoporous solids are widely used in various applications in catalysis, separations, adsorption, drug delivery, gas and energy storage, among others. Establishing their pore structure is therefore of direct practical relevance. While the state-of-the-art characterization approaches perform extremely well for ordered mesoporous solids, the occurrences of the cooperativity effects in phase transitions coupled with very complex morphological structures of the pore networks make these approaches not directly applicable for disordered materials. In this respect, better understanding of phase equilibria is needed.

In this contribution, we discuss the potentials of a recently developed serially connected pore model (SCPM) which intrinsically contains both the cooperativity effects and structural complexity. Notably, the governing equation derived within SCPM may be considered as an extension of the general adsorption isotherm (GAI) equation to include the network effects. We show the freezing and melting transitions (analogues of capillary evaporation and capillary condensation, respectively) complemented by the freezing scanning behavior (analogue of capillary evaporation scans) for a family of porous glasses with different pore sizes.

References [1] Scientific Reports, 7, 7216, 2017. [2] JPCC C, 123, 16239, 2019 [3] Frontiers in Chemistry, doi: 10.3389/fchem.2019.00230.

O 57.2 Tue 18:15 P2/2OG

Oxide formation during heat treatment of stainless steel AISI 446 — •Simon Homann[1,2], Cornelia Strauss[1,2], and Wolfgang Maus-Friedrichs[1,2] — [1]Institute of Energy Research and Physical Technology, Leibnizstraße 4, 38678 Clausthal- Zellerfeld, Germany — [2]Clausthal Centre of Material Science, Agricolastraße 2, 38678 Clausthal-Zellerfeld, Germany

Stainless steels are an important part of modern industry mainly because of their stability towards corrosion. The naturally forming oxide layer prevents a further degradation, which would otherwise lead to mechanical instability. At the same time, certain oxide layers also prevent the surface from wetting with braze used to join multiple workpieces, which is a known problem in the steel industry. The stainless steel used in this work (1.4762/ AISI 446) is a ferritic stainless chromium-steel containing aluminum (max. 3,3 at.%). Under heat treatment ($T > 450\ ^{\circ}C$) at normal pressure as well as typical vacuum brazing conditions ($p \sim 10^5$ mbar) this steel forms highly stable aluminum oxides which are mainly responsible for the inability to braze the workpieces. The aim of this work is to find a relationship between temperature and the formation of aluminium oxides in ultra-high vacuum ($p \sim 10^{-9}$ mbar) and to evaluate the chemical mechanism which explains the formation or lack of formation of those aluminum oxides. X-ray photoelectron-, auger- and energy dispersive x-ray spectroscopy and scanning electron microscopy were used for chemical and structural analysis.

O 57.3 Tue 18:15 P2/2OG

Time-resolved scanning electron microscope — •Simon Däster, Yves Acremann, and Andreas Vaterlaus — Laboratorium für Festkörperphysik, ETH Zürich, Schweiz

We develop a time-resolved SEM by energy-analyzing secondary electrons which provides a contrast mechanism for local potentials of a sample. This way, we intent to observe microwaves in electronic circuits in operando

O 58: Poster Session - Ultrafast Electron Dynamics at Surface and Interfaces

Time: Tuesday 18:15–20:00 Location: P2/2OG

O 58.1 Tue 18:15 P2/2OG

Photoinduced charge carrier dynamics and electron injection efficiencies in Au nanoparticle-sensitized TiO_2 determined with picosecond time-resolved X-ray photoelectron spectroscopy — Mario Borgwardt[1], Johannes Mahl[1], •Friedrich Roth[2], Lukas Wenthaus[3], Felix Brausse[1], Monika Blum[4], Klaus Schwarzburg[5], Guiji Liu[6], Francesca M. Toma[6], Wolfgang Eberhardt[3], and Oliver Gessner[1] — [1]Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA — [2]Institute of Experimental Physics, TU Bergakademie Freiberg, Leipziger Straße 23, D-09599 Freiberg, Germany — [3]Center for Free-Electron Laser Science / DESY, D-22607 Hamburg, Germany — [4]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States — [5]Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109, Berlin, Germany — [6]Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, California 94720, USA

We employ picosecond time-resolved x-ray photoemission spectroscopy to investigate photoinduced electron transfer in a plasmonic model system composed of 20 nm sized gold nanoparticles (NPs) attached to a nanoporous film of TiO_2. The measurement provides direct, quantitative access to transient local charge distributions selectively from the perspectives of the electron donor (AuNP) and electron acceptor (TiO_2). Back electron transfer from the perspective of AuNP is dominated by a fast recombination channel proceeding on a timescale of 60±10 ps and a minor contribution that is completed after ≈ 1 ns.

O 58.2 Tue 18:15 P2/2OG

Time resolved ARPES using femtosecond extreme ultraviolet laser pulses at 1 MHz repetition rate — •Jan Philipp Bange, Germaine Arend, Marten Düvel, Christina Möller, Marco Merboldt, Marcel Reutzel, Matthijs Jansen, Sabine Steil, Daniel Steil, and Stefan Mathias — I. Physikalisches Institut, Georg-August-Universität Göttingen, Germany

Angle-resolved photoemission spectroscopy (ARPES) is a powerful tool to map the momentum and energy dependent electron distribution of solids. Moreover, a time resolved ARPES setup is predestinated to investigate the ultrafast behaviour of electrons and the versatile couplings between electron and structural degrees of freedom. We apply femtosecond high harmonic generated (HHG) extreme ultraviolet (EUV) pulses at 21.6 eV as a probe. By generating the EUV pulses in a tight focusing geometry in an argon gas jet and by using a combination of reflective and transmissive optics we achieve both a small spectral bandwidth and a high photon flux of the probe beam. This enables us to capture distinct features in the photoemission spectra while keeping the integration time short due to a repetition rate of 1 MHz. The fundamental of the laser at 1.2 eV acts as pump resulting in a pump-probe setup. With this stroboscopic technique we investigate and capture the ultrafast electron dynamics in various material systems such as metal-organic hybrid interfaces, complex transition metal oxides and dichalogenides.

O 58.3 Tue 18:15 P2/2OG

Femtosecond time-resolved momentum microscopy on Graphene — •David Schmitt[1], Marius Keunecke[1], Christina Möller[1], Hendrik Nolte[1], Wiebke Bennecke[1], Davood Momeni Pakdehi[2], Klaus Pierz[2], Hans Werner Schumacher[2], Matthijs Jansen[1], Marcel Reutzel[1], Daniel Steil[1], Sabine Steil[1], and Stefan Mathias[1] — [1]I. Physikalisches Institut, 37077 Göttingen, Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

Recent experiments have shown that the photoexcitation of electrons in graphene leads to an ultrafast polarization-dependent anisotropy in the unoccupied Dirac cones[1]. To observe and analyze such anisotropies it is advantageous to employ a photoemission experiment that enables simultaneous access to all k-points with femtosecond resolution. We have built such a setup in recent years, which is based on time-of-flight momentum microscopy in combination with a 1 MHz femtosecond high-harmonic generation light source. The capabilities of the setup are evidenced by following the excitation and relaxation of the electronic structure in the whole Brillouin zone. In our poster, we will discuss our time-resolved experimental results regarding the hot electron dynamics in graphene.

[1] S. Aeschlimann et al., Phys. Rev. B 96, 020301 (2017)

O 58.4 Tue 18:15 P2/2OG

Ultrafast electronic heating and interband dynamics in bulk $1T$-VSe_2 — •Paulina Majchrzak[1,2], Deepnarayan Biswas[1], Alfred Jones[1], Klara Volckaert[1], Charlotte Sanders[2], Igor Marković[3], Byoung Ki Choi[4], Federico Andreatta[1], Raman Sankar[5], Yu Zhang[2], Gabriel Karras[2], Richard Chapman[2], Adam Wyatt[2], Emma Springate[2], Jill Miwa[1], Philip Hofmann[1], Phil King[3], Young Jun Chang[4], and Søren Ulstrup[1] — [1]Department of Physics and Astronomy, Aarhus University, DK — [2]Central Laser Facility, Rutherford Appleton Laboratory, UK — [3]School of Physics and Astronomy, University of St Andrews, UK — [4]Department of Physics, University of Seoul, ROK — [5]Institute of Physics, Academia Sinica, TW

Layered TMDCs are intensely studied model systems for understanding strongly-correlated materials. One such compound of interest is $1T$-VSe_2. In the bulk, it is metallic, and exhibits out-of-plane charge density wave (CDW) ordering. Its monolayer form, on the other hand, shows enhanced CDW transition temperature and perfect Fermi surface nesting. Here, we use TR-ARPES to trace out the response of the bulk VSe_2 system to an optical excitation on femtosecond timescales. The (E,k,t)-dependent ARPES spectrum is simulated with a spectral function model incorporating bare bands obtained from DFT. As a result, the transient electronic heating and the interband dynamics in the Se- and V-derived states around the Fermi level are deconvolved.

These findings lead to a more comprehensive understanding of the photoexcited behaviour in lesser-explored family of metallic TMDCs.

O 58.5 Tue 18:15 P2/2OG

Determining the orientation of transition dipoles of direct and indirect optical transitions in metals — •Tobias Eul, Michael Hartelt, Eva Prinz, Benjamin Frisch, Martin Aeschlimann, and Benjamin Stadtmüller — Department of Physics and Research Center Optimas, University of Kaiserslautern

Understanding the hot electron dynamics and their energy and momentum dissipation mechanisms paves the way to enhance the performance of next-generation electronic and spintronic devices. This understanding can be obtained by the combination of time-resolved photoemission spectroscopy and the recently developed momentum microscopy. However, to properly determine the electron dynamics with these techniques, it is crucial to clearly identify the orbital character of the initial, intermediate and final states that lead to the emission of a photoelectron.

Here, we propose a theoretical framework to predict the nature of the involved electronic states from the cross-correlation signal of a monochromatic 2PPE experiment. Our theory is based on the density matrix formalism, showing a dependence of the ratio between minimum and maximum of the cross-correlation trace and the orientation of the transition dipole with respect to the polarization of the incident light. Our calculations are then compared to momentum microscopy results for direct and indirect optical transitions in Ag(110), using both a phase-averaged and a phase-resolved pump-probe setup with a photon energy of 3.1eV. The comparison shows that the transition dipoles for direct transitions align along the ΓL-direction of the crystal.

O 58.6 Tue 18:15 P2/2OG

Towards realtime analysis of charge transport using a THz-pump photoemission-probe experiment — •Hamed Abbasi, Ping Zhou, Martin Mittendorff, and Uwe Bovensiepen — Faculty of Physics, University of Duisburg - Essen, Lotharstr. 1, 47057 Duisburg, Germany.

Investigation of electron transport is of fundamental interest in the field of charge carrier dynamics. Real-time experimental access can be obtained by exploiting the THz light pulse in a pump-probe experiment [1]. Here we report on generation and optimization of the THz field by using a photoconductive antenna [2], with which we obtained a field with 400 V/m amplitude with the near-IR laser of energy per pulse 1.4 nJ. As next steps, we plan to increase the field by an order of magnitude by exploiting a laser with higher energy per pulse (4 μJ), and synchronize it with an ultrashort UV pulse for time-resolved angle-resolved photoemission spectroscopy.

We thank the German Research Foundation for funding through CRC 1242.

[1] J. Reimann et al. Nature **562**, 396 (2018).

[2] A. Dreyhaupt et al. Applied Physics Letters **86**, 121114 (2005).

O 58.7 Tue 18:15 P2/2OG

Electron-Phonon Coupling in Metals at Elevated Temperatures. — •Tobias Held[1], Sebastian T. Weber[1], Jan Vorberger[2], and Baerbel Rethfeld[1] — [1]Fachbereich Physik and Research Center OPTIMAS, TU Kaiserslautern — [2]Helmholtz-Zentrum Dresden-Rossendorf

In the case of a solid being irradiated by a short-pulsed visible light laser, the energy is almost entirely absorbed by the electrons while the lattice remains cold. The resulting energy flow between electrons and phonons is commonly described by the electron-phonon coupling parameter G_{ep} in most temperature-based models.

Recent density functional theory (DFT) calculations accompanied by experimental results [1] indicate that a phonon mode-resolved approach is necessary to fully capture the process as opposed to the common assumption that the coupling is dominated by the longitudinal mode.

The coupling parameter can be calculated using analytical methods like a plane-wave approximation [2] as well as via DFT. Here we contrast these approaches and identify each one's advantages.

[1] L. Waldecker, R. Bertoni, R. Ernstdorfer and J. Vorberger, PRX 6, 021003 (2016)

[2] B. Y. Mueller and B. Rethfeld, PRB 87, 035139 (2013)

O 58.8 Tue 18:15 P2/2OG

Simulation of spatially resolved CDW dynamics — •Kurt Lichtenberg[1], Mohamad Abdo[1,2], Shaoxiang Sheng[1], Luigi Malavolti[1,2], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Charge-density waves (CDWs) feature collective excitations. They can, for example, be observed as an oscillatory collective response of the material's electron system to a fast optical stimulus [1]. On the other hand, scanning probe measurements reveal highly localized interaction with atomic defects [2]. Here we developed an empirical model for one-dimensional CDWs that treats the ultrafast dynamics of a CDW in real space and at the intrinsic time scale of the CDW motion. The model is based on time-dependent Ginzburg Landau Theory and motivated by former approaches [3,4]. Simulations based on this model enable the exploration of 1D CDW systems. We see a strong dependence of the collective mode behaviour on temperature, the impurity constellation and excitation intensity.

References [1] M.-A. Méasson et. al, PRB 89, 060503(R) (2014) [2] C. J. Arguello et. al, PRB 89, 235115 (2014) [3] W. L. McMillan, PRB 12, 1187-1196 (4) (1975). [4] G. Grüner, Density Waves in Solids. Perseus Publishing - Cambridge, Massachusetts, (2000).

O 59: 2D semiconductors and van der Waals heterostructures V (joint session HL/DS/O)

Time: Wednesday 9:30–13:00 Location: POT 81

O 59.1 Wed 9:30 POT 81

Impurity effects in graphene: resonances, localized states and Mott-transitions — Yuriy G. Pogorelov[1], •Denis Kochan[2], and Vadim M. Loktev[3] — [1]1IFIMUP-IN, Departamento de Física, Universidade do Porto, Porto, Portugal — [2]Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany — [3]N.N. Bogolyubov Institute of Theoretical Physics, NAS of Ukraine, Kyiv, Ukraine

Impurities modify electronic spectrum of graphene in several ways. For example, they can shift charge neutrality point, tilt the Fermi level, open spectral (quasi)gaps, form resonances, and localized states.

In the presentation we discuss formation of resonances, and localized states in graphene for Anderson-like impurities (Hydrogen, Copper, Fluorine) in top, bridge and hollow positions. Particularly, we focus on spectral transition between resonant and localized states, and Mott mobility edges, tracing dependencies on graphene Fermi energy, concentration of impurities, their sub-lattices distribution, and impurity hybridization strength.

Employing the group expansion of the Green's functions we calculated reconstructed band structure of graphene hosting Anderson impurities. Applying Ioffe-Regel-Mott criterion, we obtained system-specific critical concentrations at which system undergoes resonance-to-bound-state transition.

O 59.2 Wed 9:45 POT 81

Twisted Bilayer Graphene Produced by Atomic Force Microscopy Techniques — •Lina Bockhorn, Lucas Gnörich, Johannes C. Rode, Christopher Belke, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

The electronic properties of bilayer graphene strongly depend on relative orientation of the two atomic lattices. The rotational mismatch between both layers opens up a whole new field of rich physics, especially around the magic angle.

Twisted bilayer graphene can be obtained by different methods. Here, we use atomic force microscopy techniques to generate twisted bilayer graphene. A diagonal cut is applied at high contact force through a monolayer graphene. Several folds spread from the newly created edge. The self-assembled twisted bilayer graphene is separated in folds with one or two rips.

We estimate the relative orientation of twisted bilayer graphene which is prepared by folding monolayer graphene [1, 2, 3].

[1] H. Schmidt, J. C. Rode, D. Smirnov, R.J. Haug, Nature Communications 5, 5742 (2014)
[2] J. C. Rode, D. Smirnov, C. Belke, H. Schmidt, R.J. Haug, ANNALEN DER PHYSIK 529 (11), 1700025 (2017)
[3] J. C. Rode, D. Zhai, C. Belke, S. J. Hong, H. Schmidt, N. Sandler, R. J. Haug, 2D Materials, 6(1), 015021 (2019)

O 59.3 Wed 10:00 POT 81

Magneto-Raman Spectroscopy for Probing Electron-Phonon and Electron-Electron Interactions in Graphene — •Jens Sonntag[1,2], Sven Reichardt[1,3], Ludger Wirtz[3], Mikhail Katsnelson[4], Bernd Beschoten[1], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany — [3]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [4]Radboud University, Institute for Molecules and Materials, Nijmegen, Netherlands

We present charge carrier density-dependent magneto-Raman spectroscopy measurements on suspended graphene and hBN/graphene heterostructures to investigate electron-phonon and electron-electron interactions, both without applied magnetic field and within the quantum Hall regime. Strikingly, at $B = 0\,\mathrm{T}$ we do not observe the expected strong renormalization of the G-mode energy as a function of charge carrier density n. We identify Laser induced heating and a limited electron-hole lifetime as possible origins.
Utilizing gate-tunable magneto-phonon resonances, we extract the charge carrier density-dependence of the Landau level transition energies and the associated effective Fermi velocity v_F. In contrast to the logarithmic divergence of v_F at zero magnetic field, we find a piecewise linear scaling of v_F as a function of n, due to a magnetic field-induced suppression of the long-range Coulomb interaction. Furthermore, we can estimate the excitonic correction to the energies of the Landau level transitions to $\approx 6\,\mathrm{meV}$.

O 59.4 Wed 10:15 POT 81

Tip-enhanced Raman spectroscopy combined with other Scanning Probe Microscopy Methods: Focus on 2D Materials — •Jana Kalbacova[1], Marc Chaigneau[2], and Andrey Krayev[3] — [1]HORIBA Jobin Yvon GmbH, Germany — [2]HORIBA Scientific, France — [3]HORIBA Scientific, USA

New two dimensional materials are on the rise. After the wonder material graphene, new materials such as MoS2, MoSe2, WSe2 have an intrinsic bandgap and as such are opening new doors for semiconductor applications. Raman spectroscopy offers information on the chemical structure of materials but cannot provide information on the electronic properties such as surface potential or photocurrent of our sample. Co-localized measurements combining scanning probe microscopy (SPM) with Raman spectroscopy can already bring a wealth of information; however, further improvements can be obtained by a tip that will act as an antenna and amplify the Raman signal and thus breaking the diffraction limit in a method called Tip-enhanced Raman spectroscopy (TERS). Typically spatial resolution of 10 - 20 nm can be achieved. In this contribution, we investigate different 2D materials by a combination of TERS, tip-enhanced photoluminescence, Kelvin probe microscopy, and other SPM methods to show very locally for example doping variations or defects that would otherwise go unnoticed with other macro- and microscopic techniques.

O 59.5 Wed 10:30 POT 81

Edge photogalvanic effect driven by optical alignment in bilayer graphene — •Susanne Candussio[1], Mikhail V. Durnev[2], Jun Yin[3], Artem Mishchenko[3], Helene Plank[1], Vasily V. Bel'kov[2], Sergey A. Tarasenko[2], Vladimir Fal'ko[3], and Sergey D. Ganichev[1] — [1]University of Regensburg, 93040 Regensburg, Germany — [2]Ioffe Institute, 194021 St. Petersburg, Russia — [3]University of Manchester, Manchester M13 9PL, UK

We report on the observation of the edge electric current excited in bi-layer graphene by terahertz laser radiation. We show that the current generation belongs to the class of second order in electric field phenomena and is controlled by the orientation of the THz electric field polarization plane. Application of a magnetic field normal to the graphene plane leads to a phase shift in the polarization dependence. In strong magnetic field the current exhibit 1/B-magnetooscillations with a period consistent with that of the Shubnikov-de-Haas effect and amplitude by an order of magnitude large as compared to the current at zero field measured under the same conditions. The developed microscopic theory shows that the current is formed in the edges vicinity limited by the mean-free path and originates from optical alignment of free carriers and scattering at the edges, which naturally break the P-symmetry. The observed magnetooscillations of the photocurrent are attributed to the formation of the Landau levels.

O 59.6 Wed 10:45 POT 81

Electronic Properties of Two-Dimensional $ZrSe_3$-Films — •Lars Thole[1], Christopher Belke[1], Sonja Locmelis[2], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

The family of 2d materials offers a big variety of different material classes [1]. This includes the transition metal trichalcogenides (TMTC) of the form MX_3, where M is a transition metal and X is a chalcogen [2, 3]. Here we exfoliated $ZrSe_3$ into thin films and contacted them with electron beam lithography. These thin flakes were investigated by means of optical microscopy, atomic force microscopy and electrical measurements. During this, it was shown that the material degrades in ambient condition. Furthermore, an activation energy of about 0.6 eV was measured. Inducing charge carriers showed the samples to be n-doped semiconductors. Finally, a mean free path for the bulk material was determined.

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30 min. break

O 59.7 Wed 11:30 POT 81

ultraviolet photodetectors based on mechanically exfoliated few-layer FePS3 and ZnO quantum dots with high responsivity — •juanmei duan[1,2], liang hu[3], yujia zeng[3], manfred helm[1,2], shengqiang zhou[1], and slawomir prucnal[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany — [2]Technische Universität Dresden, D-01062 Dresden, Germany — [3]College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, P. R. China

Metal-phosphorus-trichalcogenides (MPTs), FePS3, are newly developed 2D wide-bandgap semiconductors and have been proposed as excellent candidates for ultraviolet (UV) optoelectronics. In this work, few-layer FePS3/ZnO quantum dots heterojunction were studied with Transmission electron microscopy (TEM), scanning electron microscope (SEM), X-ray photoelectron spectroscopy (XPS), and Raman measurement. The photoresponse characteristic of UV detectors based on FePS3/ZnO were investigated under 365nm, 405nm illumination and bias voltages. The high photoresponse property paves the way for the further development of 2D MPTs/ZnO quantum dots in high-performance UV photodetectors.

O 59.8 Wed 11:45 POT 81

Selectively grown Topological Insulator Nanodevices — •Daniel Rosenbach[1], Abdur Rehman Jalil[1], Jonas Kölzer[1], Nico Oellers[1], Michael Schleenvoigt[1], Tobias Werner Schmitt[2], Peter Schüffelgen[1], Gregor Mussler[1], Hans Lüth[1], Detlev Grützmacher[1], and Thomas Schäpers[1] — [1]Peter Grünberg Institut (PGI-9) and JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich, 52425 Jülich, German — [2]JARA-FIT Institute Green IT, RWTH Aachen University, 52062 Aachen, Germany

1-dimensional topological insulator nanoribbons in close proximity to elemental superconductors can be utilized to create localized Majorana modes for topological quantum computation architectures. We employ a selective area growth method using molecular beam epitaxy in order to define topological insulator nanodevices without harmful post processing steps. Using the transmission line method the interface of Bi_2Te_3 nanorribons towards ex situ applied Ti/Au contacts is probed at low temperatures. Furthermore, magnetotransport measurements on nano-Hallbars of down to 50 nm wide Bi_2Te_3 nanoribbons show indications of highly mobile charge carriers originating from 2-dimensional, topological surfaces. Finally, making use of a stencil mask on-chip, elemental superconductors like Nb and Al are deposited to define in situ, lateral topological Josephson junctions. Superconducting properties of proximitized topological nanoribbons are presented and discussed.

O 59.9 Wed 12:00 POT 81

Investigation of one-dimensional materials — •Hadeel Moustafa, Peter Larsen, Morten Gjerding, and Karsten Jacobsen — Technical University of Denmark (DTU), department of physics.

1D materials are an interesting subset of materials with promising applications in batteries, photonic crystals and as electronic interconnects. 1D materials also present the possibility of combining them with other 1D materials or higher dimensional materials to create new hetero-structures with novel physical properties. Another potential application could be in heterogeneous catalysis, where the restricted geometry of 1D materials might lead to new types of atomic sites with different chemical characteristics. We identify potential 1D materials through a screening procedure applied to the ICSD and the COD. We employ the dimensionality scoring parameter defined in ref [1], which is based exclusively on the atomic geometry. The algorithm extract one-dimensional components from periodic three-dimensional crystals. So far around 300 compounds have been studied. Their basic properties like atomic structure, stability (heat of formation and convex hull), band structure, density of states and work function have been calculated. They are furthermore characterized using symmetry and grouped together using a clustering algorithm based on the root-mean-square-distance. In the future we expect to construct new potential 1D materials by element substitution in the constructed database. [1] http://doi.org/10.1103/PhysRevMaterials.3.03400.

O 59.10 Wed 12:15 POT 81

Proximity exchange effects in excitons of TMDC/ferromagnet van der Waals heterostructures — •Paulo E. Faria Junior, Klaus Zollner, and Jaroslav Fabian — Universität Regensburg, Germany

Proximity effects in two-dimensional van der Waals heterostructures are an efficient way to modify intrinsic electronic properties[1]. In particular, proximity exchange offers the possibility of inducing magnetic properties in nominally nonmagnetic materials. Furthermore, this induced synthetic Zeeman splting exhibits strong signatures in the optical spectra. Combining ab initio calculations with tight-binding modeling and the effective Bethe-Salpeter equation for excitons, we investigate the proximity exchange in TMDC/ferromagnet systems: (i) (Mo,W)Se2 on the ultrathin van der Waals ferromagnet CrI3[2] and (ii) (Mo,W)S2/hBN on ferromagnets Co and Ni[3]. Since stacking different 2D materials requires adjusting the lattice parameters to obtain commensurate supercells, we also discuss the impact of biaxial strain in monolayer TMDCs[4]. We show the evolution of different optical transitions and the role of excitonic effects in the direct transitions. [1] Zutic et al., Mater. Today 22, 85 (2019). [2] Zollner, Faria Junior, Fabian, PRB 100, 085128 (2019). [3] Zollner, Faria Junior, Fabian, arXiv:1910.13223 (2019). [4] Zollner, Faria Junior, Fabian, PRB 100, 195126 (2019). Supported by: Alexander von Humboldt Foundation, Capes, DPG SFB 1277.

O 59.11 Wed 12:30 POT 81

Decreasing Activation Energies with Thickness of Thin $HfTe_5$ layers — •Christopher Belke[1], Sonja Locmelis[2], Lars Thole[1], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

Hafnium pentatelluride ($HfTe_5$) is a layered two dimensional material from the class of Transition Metal Penta Chalcogenide with the chemical formula MX_5, where M is a transition metal and X a chalcogenide [1]. $HfTe_5$ shows a resistivity anomaly and is expected to be a topological insulator [2] with a bulk band gap of about 22 meV [3]. In addition, theory predicts that a single layer should show a band gap of about 400 meV and should be a quantum spin hall insulator [1].

We present that the electronic properties of $HfTe_5$ drastically change with decreasing thickness. We prepared samples with different thicknesses under 100 nm and made temperature dependent measurements to determine the activation energy in an Arrhenius plot. We found that the band gap increases with decreasing thickness. Conductivity measurements also show an anomaly due to a mobility change at around 120 K.

[1] H. Weng et al., Phys. Rev. X 4, 011002 (2014)
[2] S. Liu et al., APL Materials 6, 121111 (2018)
[3] H. Wang et al., Phys. Rev. B 93, 165127 (2016)

O 59.12 Wed 12:45 POT 81

Tailoring of electronic and magnetic properties of hematene: a computational study — •Yidan Wei, Mahdi Ghorbani, and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Exfoliation of non van der Waals materials has established new class of two dimensional materials, such as hematene btained from hematite. In order to exploit and design potential applications, understanding the electronic and magnetic properties is crucial. Using density functional theory calculations, the atomic structures, electronic and magnetic properties of hematene are systematically investigated. Bare hematene in the ferromagnetic states is less stable than that in the anti ferromagnetic states, and it has a direct band gap. The stability, electronic and magnetic properties of hematene can change significantly with different terminations. Hematene covered with OH is a semiconductor with surface states removed, while hematene covered with H changes from semiconductor to half metal. Further, changes in the electronic characteristics are possible under with mechanical deformation. Applying strain causes significant changes in the electronic properties of hematene. In case of non-terminated hematene, both compressive and tensile strain can result in a reduction of the band gap in the anti-ferromagnetic state under biaxial and uniaxial deformation, and the band gap increases in case of OH terminated hematene. The band gap also increases under tensile strain in the ferromagnetic states. The deformation can lead to the enhancement of polarization.

O 60: Overview Talk: Leo Gross

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

Topical Talk O 60.1 Wed 9:30 TRE Phy

On-surface reactions and charge transitions by atomic manipulation — •Leo Gross — IBM Research - Zurich, Säumerstr. 4, 8003 Rüschlikon, Switzerland

Molecules can be created using atomic manipulation to break and to form covalent bonds. High-resolution atomic force microscopy (AFM) with functionalized tips provides insights into the structure, geometry, aromaticity, charge states and bond-order relations of the molecules created and into the reactions performed [1]. Recently, we generated the molecular carbon allotrope cyclo[18]carbon and resolved its long debated structure [2].

On insulating substrates, we can control the charge state of molecules by deliberately attaching and detaching single electrons with the tip. We measured the reorganization energy of a molecule on an insulator [3] and resolved the changes within molecular geometry, adsorption and aromaticity related to its oxidation state [4].

References
[1] L. Gross et al. Angew. Chem Int. Ed 57, 3888 (2018)
[2] K. Kaiser et al. Science 365, 1299 (2019)
[3] S. Fatayer et al. Nat. Nano. 13, 376 (2018)
[4] S. Fatayer et al. Science 365, 142 (2019)

O 61: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions III (joint session O/HL/CPP/DS)

Time: Wednesday 10:30–13:30 Location: GER 38

Invited Talk O 61.1 Wed 10:30 GER 38

Hybrid Perovskites: polarons, excitons and phase diagrams — •Georg Kresse, Menno Bokdam, and Ryosuke Jinnouchi — University of Vienna, Faculty of Physics and Center for Computational Materials Sciences

Halide perovskites are very promising solar cell materials. The first part of this presentation studies the formation of polarons and excitons in MAPbI3. We show that both, polarons and excitons, possess about similar binding energies. To obtain accurate results, the calculations have to be carefully converged with respect to the k-point sampling, something that has been often "overlooked" in the past [1].

The second part of the talk presents studies on the finite temperature behavior of MAPbI3. To achieve the required long simulation time and large length scales, an on-the-fly machine learning scheme that generates force fields automatically during first principles molecular dynamics simulations is used. This force field opens up the required time and length scales, while retaining the distinctive chemical precision of first principles methods [2]. Using machine learned potentials, isothermal-isobaric simulations give direct insight into the underlying microscopic mechanisms of the phase transitions. We observe that MAPbI3 is an very dynamic material even at room temperature, putting some question marks on the hereto considered static models.

[1] M. Bokdam, T. Sander, A. Stroppa, S. Picozzi, D. D. Sarma, C. Franchini, G. Kresse, Scientific Rep. 6, 28618 (2016); [2] R. Jinnouchi, J. Lahnsteiner, F. Karsai, G. Kresse, M. Bokdam, PRL 122, 225701 (2019).

O 61.2 Wed 11:00 GER 38

Assessing ab-initio methodology to compute electronic properties of organic-inorganic metal halide perovskites — •Cecilia Vona, Dmitrii Nabok, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Organic-inorganic metal halide perovskites (HaPs) are materials widely studied for their light-harvesting properties. Owing to the interplay between strong electron-electron interaction and spin-orbit coupling, their theoretical investigation is still a challenge. Here we evaluate the methodology to compute their electronic structure. To this extent, we explore several approaches, within density-functional theory and many body perturbation theory, to compute the electronic structure of PbI$_2$, which is the precursor of many HaPs. Spin-orbit coupling effects are taken into account, and the hybrid functionals PBE0 and HSE are at the center of the investigation. We first explore several methods to determine the mixing parameter α, which in PBE0 and HSE defines the amount of Hartree-Fock exchange mixed with the semi-local functional PBE. We then use the results obtained from HSE and PBE0 for different values of α as starting point of G_0W_0 calculations. All the calculations are performed with the full-potential all-electron computer package `exciting`, in which LAPW+lo bases are implemented. We observed that hybrid functionals with a proper α value are most suitable to compute the electronic structure of PbI$_2$. Moreover, we show that the methodology is transferable to CsPbI$_3$, and we expect the same behavior for the lead-iodine perovskites.

O 61.3 Wed 11:15 GER 38

Rashba-Dresselhaus Effect in Two Dimensional Layered Halide Perovskites — •Benedikt Maurer[1,2], Claudia Draxl[1,2], and Christian Vorwerk[1,2] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin — [2]European Theoretical Spectroscopy Facility

It has been shown that huge spin-orbit coupling in bulk hybride organic inorganic perovskites in combination with broken inversion symmetry leads to Rashba-Dresselhaus splitting, which influences the optoelectronic properties. This indicates that such effects also affect the optoelectronic properties of their two dimensional layered relatives, which are promising candidates as new light emitting materials. In this work, we aim at understanding which inversion symmetry breaking can lead to the Rashba-Dresselhaus effect in those materials. For this purpose, we develop model structures, where we replace the organic compounds by Cs atoms and disregard possible distortions in the inorganic layers, resulting in the structural composition Cs$_{n+1}$Pb$_n$I$_{3n+1}$. Using the all-electron full-potential density-functional-theory code `exciting`, we systematically study how atomic distortions impact the band structure for n=1, 2 and ∞. We identify displacement patterns that yield Rashba-Dresselhaus splitting, and determine the size of the splitting as a function of the displacement. Furthermore, we analyze the spin textures in electronic states around the band gap to differentiate between Rashba and Dresselhaus effect. Our study reveals in-plane lead displacements as the origin of the Rashba-Dresselhaus splitting.

O 61.4 Wed 11:30 GER 38

Intrinsic polarons on polar surfaces — •Michele Reticcioli[1,2], Zhichang Wang[2], Igor Sokolovic[2], Michael Schmid[2], Ulrike Diebold[2], Martin Setvin[2], and Cesare Franchini[2,3] — [1]University of Vienna, Center for Computational Materials Science, Vienna, Austria — [2]Institute of Applied Physics, Technische Universitaet Wien, Vienna, Austria — [3]University of Bologna, Department of Physics and Astronomy, Bologna, Italy

Uncompensated charge at the surface boundary of polar materials is conventionally expected to form a two dimensional electron gas (2DEG), as a result of the alternating charged-plane stacking in the ionic crystals, interrupted by the surface cut. By means of density-functional theory calculations and surface-sensitive experiments, we propose a different paradigm able to accommodate the uncompensated charge in a more effective way, establishing a more favorable ground state for the system, that is the polaron formation (local lattice distortions coupled with charge localization). In fact, the intrinsic uncompensated charge tends to spontaneously localize and form polarons, rather than a 2DEG. Only beyond the critical polaron density, excess charge arising from external doping or defects starts to build dispersed electronic states. Here, we show how polarons and 2DEG compete on the polar KTaO3(001) surface.

O 61.5 Wed 11:45 GER 38

Polarons in extended p-conjugated systems: the role of electron correlation. — •Daniele Fazzi[1], Klaus Meerholz[1], and Fabrizia Negri[2] — [1]Institut für Physikalische Chemie, Universität zu Köln, Luxemburger str. 116, 50939 Köln, Germany — [2]Dipartimento di Chimica, Università di Bologna, via F. Selmi, 2, 40126 Bologna, Italy

Polarons play a crucial role in governing charge transfer in organic materials. An accurate description of their electronic structure and electron-phonon couplings is mandatory to understand their response and transport properties.

We report a comprehensive investigation of polarons in extended p-conjugated systems (ladder-type polymers, graphene nano-ribbons, and cyanine-based compounds [1-2]). We show how spin polarized DFT lead to solutions of the polarons wavefunction which are not the most stable ones. This aspect, can be traced back to the multireference character of polarons. Broken symmetry DFT can address the electronic and structural properties of polarons, providing a correct assessment of charge transport parameters, otherwise incorrectly computed [3]. Multi-reference wavefunction methods are also considered to take into account correlation effects in charged and excited states.

Our study calls for a careful assessment in the description of charged/excited states in conjugated materials.

[1] Wang, S., et al., Adv. Mater. 2018, 30, 1801898. [2] Medina, S. et al., Phys. Chem. Chem. Phys., 2019, 21, 7281-7288. [3] Fazzi, D. et al, J. Mat. Chem. C., 2019, 7, 12876-12885.

O 61.6 Wed 12:00 GER 38

Optical and x-ray absorption spectra of MgO from first-principles including many-body effects — •Vijaya Begum, Markus E Gruner, and Rossitza Pentcheva — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, Germany

We discuss the optical and x-ray absorption (XAS) spectra of MgO – a wide band gap oxide with versatile applications – in the framework of density functional theory (DFT) including many-body and excitonic corrections. The quasi-particle band gap improves over DFT with PBEsol as the starting exchange-correlation functional (4.58 → 7.52 eV) and is overcorrected with the hybrid functional HSE06 (6.58 →

8.53 eV) when compared to experiment (7.7 eV). Including excitonic effects by solving the Bethe-Salpeter equation (BSE) leads to excellent agreement with the experimental spectrum both for the real and imaginary part of the dielectric function, when starting with the HSE06 functional. Furthermore, the x-ray absorption spectra of the O and Mg K-edge calculated with the Exciting code exhibit good agreement with experiment regarding the positions of the prominent peaks, underlining the importance of including the core-hole and electron interactions within the G_0W_0+BSE. Projection of the electron-hole coupling coefficients from the BSE eigenvectors on the band structure allows to explore the origin of the peaks and identify the orbital character of the relevant contributions.

Funding by DFG CRC1242, project C02 is gratefully acknowledged.

O 61.7 Wed 12:15 GER 38

Strain effects on the lattice-dynamical properties of titanium dioxide — •Peter Weber, Sebastian Tillack, Pasquale Pavone, and Claudia Draxl — Humboldt-Univeristät zu Berlin, Physics Department and IRIS Adlershof, Germany

A fingerprint of temperature-related anharmonic effects in a crystal is the change of the phonon frequencies with the volume. For anisotropic crystals, this variation must be generalized by the introduction of the mode Grüneisen tensor, which expresses the change of the phonon frequencies with respect to any applied strain. In this work, we present the results of an *ab-initio* investigation of the strain effects on the lattice-dynamical properties of the rutile and anatase phases of TiO_2. In particular, we focus our attention to the determination of the generalized Grüneisen parameters at the Brillouin zone center. In order to obtain all independent components of the Grüneisen tensor for these phases, all polar and nonpolar phonon frequencies at the Γ point are calculated for several strained configurations. These calculations are performed using density-functional theory as implemented in the full-potential all-electron software package `exciting` [1]. The connection between the Grüneisen tensors of the acoustic branches and the elastic constants of these materials is analyzed and discussed. Our results are also compared with available Raman scattering data for strained TiO_2.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26** (2014) 363202

O 61.8 Wed 12:30 GER 38

Ab-initio phonon self-energies and fluctuation diagnostics of phonon anomalies: lattice instabilities from Dirac pseudospin physics in transition-metal dichalcogenides — •Jan Berges[1], Erik van Loon[1], Arne Schobert[1], Malte Rösner[2], and Tim Wehling[1] — [1]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Germany — [2]Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands

We present an ab-initio approach for the calculation of phonon self-energies and their fluctuation diagnostics, which allows us to identify the electronic processes behind phonon anomalies. Application to the prototypical transition-metal dichalcogenide 1H-TaS_2 reveals that coupling between the longitudinal–acoustic phonons and the electrons from an isolated low-energy metallic band is entirely responsible for phonon anomalies like mode softening and associated charge-density waves observed in this material. Our analysis allows to distinguish between different mode-softening mechanisms including matrix-element effects, Fermi-surface nesting, and Van Hove scenarios. We find that matrix-element effects originating from a peculiar type of Dirac pseudospin textures control the charge-density-wave physics in 1H-TaS_2 and similar transition-metal dichalcogenides.

O 61.9 Wed 12:45 GER 38

Toward a general non-local polarizability density functional for van der Waals dispersion interactions — •Szabolcs Góger, Dmitry Fedorov, Péter Szabó, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

Density functional theory (DFT), while being a workhorse for electronic structure calculations, struggles with describing long-range electron correlations including van der Waals (vdW) dispersion interactions. Various promising approaches have been developed to include vdW interactions in DFT, but a broadly applicable method is yet to be found [1,2]. The first key issue is developing a general density functional for non-local polarizability in molecules and solids. In this work, we use different known properties of atomic and molecular polarizabilites including the direct relation between the dipole polarizability and vdW radius unveiled recently [3]. Diverse methods starting with the Slater-Kirkwood approach [4] are applied to simple quantum mechanical systems like the Drude oscillator and the hydrogen atom under the effect of various electric fields. Our model studies along with prior work on semi-local polarizability functionals [5] pave the way toward developing a unified non-local polarizability functional for molecules and materials.

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O 61.10 Wed 13:00 GER 38

Insights into van der Waals interactions from the quantum Drude oscillator model — •Dmitry Fedorov, Martin Stöhr, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

The quantum Drude oscillator (QDO) model [1] represents the response of all valence electrons in an atom by a single Drude particle with its charge, mass, and characteristic frequency. Due to the simple form, this model serves as an insightful approach for the description of atomic response properties and van der Waals (vdW) interactions [2]. Recently, the QDO model helped to unveil a non-trivial relation between the dipole polarizability and the atomic volume, $\alpha_{\text{dip}} \propto V^{4/3}$, [3] as well as the surprising direct relation between the multipole polarizabilities and the equilibrium distances in vdW-bonded atomic dimers [4]. Here, we provide a detailed insight into the physical background of the aforementioned findings. The connection between different striking scaling laws obtained by diverse ways shows the inner consistency and power of this simple but efficient model. We discuss the importance of the revealed quantum-mechanical relations between response and geometric properties of atoms for computational models like the Tkatchenko-Scheffler [5] and the many-body dispersion [2] methods.

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O 61.11 Wed 13:15 GER 38

Conical intersections in molecular systems: 3D vs 2D models — •Erik Pillon, Dmitry Fedorov, Péter Szabó, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg

The molecular Aharonov-Bohm effect [1], covering various phenomena caused by the Berry (geometric or topological) phase in molecular systems, is an important playground for understanding fundamental quantum physics as well as for building quantum electronic devices. The related non-adiabatic effects, stemming from the coupling between the electron and nuclear degrees of freedom, are especially pronounced in systems possessing conical intersections (CI) in potential energy surfaces, ubiquitous in condensed matter and molecular physics. Many toy models have been introduced to study the influence of CIs on the nuclear dynamics from a general point of view. However, most of them, including the linear vibronic coupling model [2, 3] widely used in literature, employ two-dimensional (2D) real Hamiltonians. In our work, we check whether such models capture all the important features of real molecular systems. To this end, we perform a comparison of the conventional approaches with the general treatment of a CI within the three-dimensional (3D) complex Hamiltonian possessing SU(2) symmetry [4]. The features present within the 3D model but missing in the 2D case are identified and discussed.

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O 62: Focus Session: Big Data in Aquisition in ARPES (joint session O/CPP)

Due to the advancement of both electron detectors and light sources, ARPES data is increasing in volume and complexity. This applies to ARPES performed at 3rd and 4th generation light sources as well as lab-based sources. We have reached a point where data handling, workflow management, visualization and analysis is a severe challenge and potentially become the bottleneck in our workflows rather than data acquisition itself. Currently there exist mainly isolated, i.e. lab- or facility-specific, solutions for data acquisition and file formats, metadata definitions, data-processing workflows, and analysis approaches. A community-wide ARPES (meta)data schema in the quest for reproducible, scalable and transparent data analysis is not yet established. This focus session aims to reveal the great potential for speeding up our progress by attacking certain challenges in joint efforts.

Organized by: Ralph Ernstorfer (FHI Berlin), Michael Hartelt and Martin Aeschlimann (TU Kaiserslautern)

Time: Wednesday 10:30–13:15 Location: REC C 213

Invited Talk O 62.1 Wed 10:30 REC C 213

Towards FAIR experimental data — •Claudia Draxl — Humboldt-Universität zu Berlin — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Knowledge and understanding of materials is based on their characterization in terms of a variety of properties and functions. Surprisingly though, for only a very small number of materials this information exists. Making materials data available, opens avenues for data-driven research in terms of re-purposing (using materials for a different purpose than intended by the original work), detecting candidate materials for a given application, and finding descriptors by approaches of artificial intelligence. Prerequisite for all this is a FAIR (findable, accessible, interoperable, reusable) data infrastructure. In computational materials science, the NOMAD Laboratory (https://nomad-coe.eu) has set the stage for FAIR data [1], by offering services like free upload to the NOMAD Repository, the NOMAD Archive, the NOMAD Encyclopedia, and the NOMAD Analytics Toolkit. In this talk, I will address our concepts and first steps towards extension of this open-science platform towards experimental data and sample synthesis. Here, for instance, data volume and velocity are big issues for many measurement techniques, while large uncertainties may come from (often incompletely known) sample quality, instrumental resolution, or measurement conditions. These challenges are tackled within the non-profit association FAIR-DI (https://fairdi.eu) and FAIRmat (https://fairdi.eu/fairmat), a proposed consortium for the NFDI.

[1] C. Draxl and M. Scheffler, MRS Bulletin 43, 676 (2018).

O 62.2 Wed 11:00 REC C 213

NXarpes, the Data File Standard for ARPES in NeXus — •Moritz Hoesch[1], Pavel Dudin[2], and Tobias Richter[3] — [1]DESY Photon Science, Hamburg, Germany — [2]Synchrotron Soleil, Gif-sur-Yvette, France — [3]European Spallation Source, Lund, Sweden

NeXus is a common data format for neutron, x-ray, and muon science. It is being developed as an international standard by scientists and programmers representing major scientific facilities in order to facilitate greater cooperation in the analysis and visualization of neutron, x-ray, and muon data (cited from [1]). Diamond Light Source has adopted the NeXus standard, including for the instruments HR-ARPES and nano-ARPES on beamline I05 [2]. The specific NXarpes format, deliberately focusing on the essentials and thus expandable without deviation from the standard is available to the community [3]. In this presentation I will show examples of NXarpes data files and discuss the reception of this format by the community of ARPES users.

[1] https://www.nexusformat.org; [2] https://www.diamond.ac.uk/I05 ; [3] http://download.nexusformat.org/sphinx/classes/applications/NXarpes.html

O 62.3 Wed 11:15 REC C 213

Handling Big Multidimensional Experimental Data on Small Desktop Computers — •Michael Hartelt, Benjamin Frisch, Tobias Eul, Eva Prinz, Marten Wiehn, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany

In the pursuit of discovering new phenomena, photoemission experiments have evolved to capture ever more information about the electronic properties of materials. Major progress was made in the parallel detection of more degrees of freedom, which can include real- or k-space, energies and spin states of the emitted electrons. Additional dimensions of the parameter space are opened up by state-of-the-art experimental techniques that vary the sample temperature, the photon energy of the light source, or the time-delay between ultrashort laser pulses. As a result, experimental datasets of a single experiment can nowadays be 4-dimensional or even more. This makes the analysis of experimental data a non-trivial task, both conceptually and computationally.

We present our approach for the easy handling of these multi-dimensional, bigger-than-memory datasets on a conventional office computer. Using the Python programming language gives us access to powerful open-source packages like h5py, opencv, numpy, pint, and pycuda. Taking advantage of these, we integrated them into a toolbox package, which manages storage of large datasets for optimized I/O performance. The user is provided with an interface based on physical context, to perform data evaluation procedures with high efficiency.

O 62.4 Wed 11:30 REC C 213

Data Acquisition and Treatment on a Scientific and Industrial Level — •Stefan Böttcher, Christian Fleischer, and Thorsten Kampen — SPECS Surface Nano Analysis GmbH, Voltastrasse 5, 13355 Berlin

The recent developments in angular resolved photoemission and momentum microscopy let arise scientific instruments which produce enormous amount of raw data, easily exceeding several Tb of file size. Solutions or attempts of standard data- or transfer-formats are present in many fields, such as XPS or SPM. Here we present our approach on the data acquisition and processing in the acquisition and analysis software. We show the classes of metadata available to the experiment and the routes to export the data into usable formats. The data handling and the storage of transformation is a critical aspect with the present discussion. Finally an outlook into possibilities for DIN/ISO standardization can be given.

O 62.5 Wed 11:45 REC C 213

Challenges in data collection at a modern cw laser-driven spin-ARPES system — Tristan Heider[1], Peter Baltzer[2], Claus M. Schneider[1], and •Lukasz Plucinski[1] — [1]FZ Jülich PGI-6, Jülich, Germany — [2]MBS AB, Uppsala, Sweden

At PGI-6 in Jülich we operate a laser-driven angle- and spin-resolved photoemission (spin-ARPES) system, based on the *A*1 hemispherical analyzer with the lens deflector (MBS AB) and a single *k*-point *Ferrum* spin detector (Focus GmbH). The details of the system are described in a separate talk [1].

The typical data sets at our laboratory are 3D k_x vs. k_y vs. E_{kin} spin-integrated ARPES and 2D k_x vs. k_y spin maps. The size of a typical 3D dataset is approx. 100 MB, and for a complete measurement with the 6eV *cw* laser we take 4 of such sets, two with linear and two with circular light polarizations. The angular range of a single set is approx. 35°, therefore often more than one sample position needs to be measured, and a daily dataset exceeds 1 GB.

We will discuss the data collecting techniques, the data format, the data plotting, and the data storage and backup. We typically use MATLAB for data evaluation, however, we will discuss other options that might be more efficient for quick scanning through the large 3D datasets. We will use datasets from Fe-based superconductor and from 3D topological insulator as examples, and discuss challenges in evaluation of such data.

[1] T. Heider et al. this conference.

O 62.6 Wed 12:00 REC C 213

Single event data processing for multidimensional photoemission spectroscopy — •Steinn Ymir Agustsson[1], Rui Patrick Xian[2], Yves Acremann[3], Maciej Dendzik[2], Kevin Bühlmann[3], Davide Curcio[4], Dmytro Kutnyakhov[5], Federico Pressacco[6], Michael Heber[5], Shuo Dong[2], Philip Hofmann[4], Martin Wolf[2], Wilfried Wurth[5], Jure Demsar[1], Laurenz Rettig[2], and Ralph Ernstorfer[2] — [1]JGU Mainz — [2]FHI Berlin — [3]ETH Zurich — [4]Aarhus University — [5]DESY Photon Science, Hamburg — [6]Uni-Hamburg

The advent of novel electron detectors has opened up the field of photoemission spectroscopy to the single event detection regime. This significantly extends the accessible multidimensional parameter space for data acquisition, but also drastically increases the output of data from such experiments to the tens of MB/s regime. Handling such data therefore requires new approaches for data treatment, but also presents the opportunity for more advanced post-processing and analysis techniques. We present a distributed workflow for processing multidimensional photoemission data into an open source unified data structure. This allows, when combined with open source analysis algorithms, to directly apply such routines on data sets obtained from different experimental setups, from large scale facilities to table-top systems.

Invited Talk O 62.7 Wed 12:15 REC C 213

Reproducible data analysis with Snakemake — •Johannes Köster — Algorithms for reproducible bioinformatics, Genome Informatics, Institute of Human Genetics, University of Duisburg-Essen, Hufelandstr. 55, 45147 Essen Germany

Data analyses usually entail the application of many command line tools or scripts to transform, filter, aggregate or plot data and results. With ever increasing amounts of data being collected in science, reproducible and scalable automatic workflow management becomes increasingly important. Snakemake is a workflow management system, consisting of a clean, human-readable, text-based workflow specification language and a scalable execution environment, that allows the parallelized execution of workflows on workstations, compute servers, clusters and the cloud without modification of the workflow definition. Snakemake is hugely popular and was used to build analysis workflows for numerous high impact publications. With about 350 citations in the last two years, it is one of the leading frameworks for reproducible data science. This talk will show how Snakemake can be used to easily document, execute, and reproduce data analyses.

O 62.8 Wed 12:45 REC C 213

Concept for Handling of Photoemission Data at European XFEL — •Markus Scholz[1], Dmytro Kutnyakhov[2], Michael Heber[2], Manuel Izquierdo[1], Hans Fangohr[1], Yves Acremann[4], Kai Rossnagel[3], Anders Madsen[1], and Serguei Molodtsov[1] — [1]European XFEL Facility, Holzkoppel 4, 22869 Schenefeld, Germany — [2]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Ruprecht-Haensel-Labor, Christian-Albrechts-Universität zu Kiel and Deutsches Elektronen-Synchrotron DESY, 24098 Kiel and 22607 Hamburg, Germany — [4]Laboratorium für Festkörperphysik, ETH Zürich, 8093 Zürich, Switzerland

European X-ray Free Electron Laser (EuXFEL) is currently the world's biggest, brightest and highest repetition rate XFEL providing up to 27000 pulses/second. The planned open port named "Soft X-ray Port" (SXP), will allow time-resolved X-ray photoelectron spectroscopy (TR-XPES) experiments. In this contribution I will present how near-online analysis of photoemission data based on Jupyter notebooks could be realized and embedded in the EuXFEL software framework. For compute-intensive notebooks, it is possible to allocate dedicated nodes with user-specified hardware configuration from the Maxwell computer cluster to a running JupyterHub session. This is of particular value due to the size of data sets and the the remotely accessible analysis.

O 62.9 Wed 13:00 REC C 213

Processing workflow for band structure reconstruction from multidimensional photoemission data — R. Patrick Xian[1], Vincent Stimper[2], Shuo Dong[1], Maciej Dendzik[1], Samuel Beulieu[1], Bernhard Schölkopf[2], Martin Wolf[1], Stefan Bauer[2], Laurenz Rettig[1], and •Ralph Ernstorfer[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Max Planck Institute for Intelligent Systems, Tübingen, Germany

Recent advances in photoelectron detectors and light sources result in an increase of size and dimensionality of photoemission data, leading to new challenges in data preprocessing and analysis: the large number of adjustable parameters of modern electron optics require experiment-specific calibration and artifact correction [1]; visual inspection of multidimensional ARPES data may be hampered by the varying levels of contrast [2]. We discuss a workflow for conditioning volumetric three- and four-dimensional momentum microscopy data for band structure mapping from single-electron events to calibrated, reusable data [3].

[1] Xian et al., Ultramicroscopy 202, 133 (2019).
[2] Stimper et al., IEEE Access 7, 165437 (2019).
[3] Xian et al., arXiv 1909.07714.

O 63: Focus Session: Functional Molecules at Surfaces III

Time: Wednesday 10:30–13:45 Location: TRE Ma

O 63.1 Wed 10:30 TRE Ma

Molecular Nanotribology: Nanomanipulation & Dynamics of Single-Molecules at Surfaces. — •J.G. Vilhena[1], Remy Pawlak[1], Philipp D'Astolfo[1], Shi-Xia Liu[2], Silvio Decurtins[2], Justin A. Lemkul[3], Giacomo Prampolini[4], Thilo Glatzel[1], Alexis Baratoff[1], Rúben Pérez[5], and Ernst Meyer[1] — [1]University of Basel, Switzerland — [2]University of Berne, Switzerland — [3]Virginia Tech, USA — [4]ICCOM-CNR, Italy — [5]Universidad Autónoma de Madrid, Spain

Understanding the motion/dynamics of a single molecule over a surface is a problem of a paramount importance in designing advanced molecular nanostructures/assemblies. The interest is better realized by the broad spectrum of promising applications including molecular electronic devices, tribology/corrosion inhibition, and 3D nanopatterning. One possible route to achieve a higher control on molecular diffusion along predetermined pathways would be to access the single-molecule mechanics during their on-surface displacements.Twenty years after the first atomic-manipulation it became possible to record the time variations of mechanical forces as we manipulate a molecule over a surface –cryo-force-spectroscopy. In this talk I shall discuss how dedicated all atom molecular dynamics simulations (based in first-principles simulations) coupled with cryo-force-spectroscopy measurements provides a comprehensive understanding of complex on-surface dynamics of the molecules (terpyridine, pyrene chains and ssDNA) over gold surfaces and how dynamic balancing of intra-molecular mechanics and surface comensurability play out in a broad range of conditions.

Invited Talk O 63.2 Wed 10:45 TRE Ma

The art of molecular manipulation with the scanning tunneling microscope: controlled rotations — •Nicolas Lorente — Centro de Fisica de Materiales (CSIC-EHU) and DIPC, San Sebastian, Spain

Rotations are key to the functioning of molecular machines. Controlling how to induce and stop the rotation of a molecule about a well defined axle is a difficult task that needs to be mastered. This is an important part of the research undertaken by the EU-H2020 project MEMO (https://www.memo-project.eu/flatCMS/). In this talk I will rationalize the ingredients to obtain molecular rotations. Among them, dispersive forces seem to be a must for all molecular systems where rotations can be effected. I will show controlled rotations of two molecular systems. One is a supramolecule formed by aceto-byphenil molecules on Au (111) largely characterized by dispersive interactions [1-3], and the second systems is a radical 2-(2-methoxyphenyl)-1,3-dimethyl-2,3-dihydro-1H-benzoimidazole (o-MeO-DMBI) that binds covalently by a single bond and the rest of the interaction is given by van der Waals forces [4]. We have used density functional theory completed with dispersive forces [3]. We have furthered the study by unraveling the interaction between tunneling electrons and molecular rotations [5].

[1] Anja Nickel et al. ACS Nano 7, 191 (2013)
[2] Vladimir Zobac et al.
[3] Roberto Robles, et al.

[4] Frank Eisenhut et al.
[5] Alexander Croy et al.

O 63.3 Wed 11:15 TRE Ma

Functional molecular arrays constructed through the manipulation of single molecules at room temperature — •Chao Li[1,2], Li Wang[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Department of Physics, Nanchang University, Nanchang 330031, China

Molecular devices made via the manipulation of single molecules in scanning probe microscopes have usually been assembled at cryogenic temperatures. Only few related manipulation experiments have been demonstrated at ambient temperature, at which application of the molecular devices are more easily conceivable. Here, we present room-temperature intermolecular signal transfer and processing using SnCl2Pc molecules on a Cu(100) surface. The in-plane orientations of molecules, which were used as information carrier, were effectively coupled through a series of controlled manipulations. The resulting arrays of coupled molecules realize different functions including logical gates, a motor, and a signal transfer circuit. The results highlight a strategy for building functional molecular devices at room temperature.

O 63.4 Wed 11:30 TRE Ma

LT-STM investigation of transmitting rotation between molecular gears on Au(111) — •Kwan Ho Au Yeung[1,2], Tim Kühne[1,2], Frank Eisenhut[1,2], Michael Kleinwächter[3], Yohan Gisbert[3], Gianaurelio Cuniberti[2], Claire Kammerer[3], Gwénaël Rapenne[3], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, Germany — [2]Institute of Materials Science, TU Dresden, Germany — [3]CEMES, Université de Toulouse, CNRS, Toulouse, France

Molecular gear is an essential and elementary component for the construction of planar single-molecule mechanical machines, in which a refined design of molecules, a smart selected surface for anchoring, and a highly controllable rotation are desired. The family of pentaphenylcyclopentadiene (PPCP) molecules shows not only the appearance of macroscopic gears, but also the behavior of transmitting rotation from molecule to molecule. Under the investigation of LT-STM on the Au (111) surface, step-by-step, controlled, and transmitting rotations have been examined by lateral manipulation. Further, in order to achieve concentric rotations, and hence, the anchoring properties of molecules, the pristine and radical states of the molecules after tip-induced cleaving at the cyclopentadiene core have been studied.

O 63.5 Wed 11:45 TRE Ma

The role of the dipole moment in electric field induced manipulation of molecules and nanostructures — •Tim Kühne[1], Kwan Ho Au Yeung[1], Frank Eisenhut[1], Oumaima Aiboudi[3], Dmitry Ryndyk[2], Gianaurelio Cuniberti[2], Brigitte Voit[3], Franziska Lissel[3], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, Germany — [2]Institute for Materials Science, TU Dresden, Germany — [3]Leibniz Institute of Polymer Research, Dresden, Germany

Among the different mechanisms that can be used to drive a molecule on a surface by STM, we used voltage pulses to investigate the movement properties of di-tert-Butyl 2-isocyanoazulene-1,3-dicarboxylate (BCA) molecules. On the Au(111) surface, we observed single molecules and dimers, as well as the formation of metal-organic complexes with gold adatoms. Even if the pure molecule has a strong dipole moment in the gas phase, only metal-organic complexes could be moved by voltage pulses. Measurements at different bias and tip height conditions revealed the electric field effect as main driving force of this motion. In this talk, we discuss the observed movement properties with respect to the molecule dipole moment and the charge distribution of molecules and molecular nanostructures.

O 63.6 Wed 12:00 TRE Ma

Mechanical transmission of rotational motion between molecular-scale gears — •Huang-Hsiang Lin[1,2], Alexander Croy[1], Rafael Gutiérrez[1], Christian Joachim[3], and Gianaurelio Cuniberti[1,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01069 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]GNS and MANA Satellite, CEMES-CNRS, 29 rue J. Marvig, 31055 Toulouse Cedex, France — [4]Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany

Manipulating and coupling molecule gears is the first step towards realizing molecular-scale mechanical machines[1]. Here, we theoretically investigate the behavior of such gears using molecular dynamics simulations[2]. Specifically, for a single hexa (4-tert-butylphenyl) benzene molecule, we show that the rotational-angle dynamics corresponds to the one of a Brownian rotor. For two such coupled gears, we extract the effective interaction potential and find that it is strongly dependent on the center of mass distance. Finally, we study the collective motion of a train of gears.

[1]W.-H. Soe, S. Srivastava and C. Joachim, J. Phys. Chem. Lett., 6462 (2019)

[2]H.-H. Lin, A. Croy, R. Gutierrez, C. Joachim and G. Cuniberti, arXiv:1910.06644 (2019)

O 63.7 Wed 12:15 TRE Ma

Rotation and translation of molecular motors on a metallic surface — •Monika Schied[1], Peter Jacobson[1], Dongdong Liu[2], James M. Tour[2], and Leonhard Grill[1] — [1]Department of Physical Chemistry, University of Graz, Austria — [2]Department of Chemistry, Rice University, USA

Artificial molecular motors that convert an external energy input into controlled motion have seen great developments in the last decades [1]. While many studies exist in solution, little is known how such functional molecules behave on a surface. Molecules on surfaces have the advantage of a fixed point of reference and confinement in two dimensions making it easier to study the directionality of their motion.
The uni-directional rotation of the motors investigated in this study is based on a combination of double bond isomerisation and helix inversion. This so-called Feringa motor has already been implemented into molecular structures to enable or enhance their lateral translation on metal surfaces [2, 3].
Here, we image and manipulate single motor molecules on metallic surfaces by low-temperature scanning tunnelling microscopy (STM). Rotational and translational movements as well as changes in appearance are observed after voltage pulses with the STM tip.

[1] W. R. Browne and B. L. Feringa, Nat. Nanotech. 1, 25 (2006)
[2] T. Kudernac et al., Nature 479, 208 (2011)
[3] A. Saywell et al., ACS Nano 10, 10945 (2016)

O 63.8 Wed 12:30 TRE Ma

Weakly-bound supramolecular structures: calculations for understanding experiments with the scanning tunneling microscope — •Roberto Robles[1], Vladimír Zobač[1], Kwan Ho Au Yeung[2], Francesca Moresco[2], Dmitry Ryndyk[2], Christian Joachim[3], and Nicolás Lorente[1,4] — [1]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), San Sebastián, Spain — [2]Center for Advancing Electronics Dresden, TU Dresden, Germany — [3]Centre d'Elaboration de Matériaux et d'Études Structurales (CEMES), CNRS, Université de Toulouse, Toulouse, France — [4]Donostia International Physics Center (DIPC), San Sebastián, Spain

4-Acetylbiphenyl is a small aromatic molecule that binds via dispersive forces (van der Waals) with a gold surface. Experiments performed in the group of Dr. Moresco in TU Dresden showed that, under certain conditions of deposition, these molecules formed a 4-molecule superstructure nicknamed the "windmill" because of its cross-shaped structure. These "windmills" are reproducible, directional and resilient to external interactions. Closer inspection of the scanning tunneling microscope images (STM) reveals that the unique seemingly H-bond should take place between a methyl group and the O atoms. This is one of the weakest H bonds if it binds at all. We undertook density functional theory calculations completed by empirical van-der-Waals corrections to study the supramolecular structure. From the simulation of STM images, total energy calculations and Gibbs free-energy estimates, we reach the conclusion that windmills are likely to involve gold adatoms to join the four acetylbiphenyl molecules together.

O 63.9 Wed 12:45 TRE Ma

Bending and twisting of C-C bonds by mechanical lifting of surface-adsorbed polymers — •Philipp D'Astolfo[1], Guilherme de Vilhena[1], Carl Drechsel[1], Xunshan Liu[2], Silvio Decurtins[2], Shi-Xia Liu[2], Rémy Pawlak[1], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Basel, Switzerland — [2]Department of Chemistry and Biochemistry, University of Bern, Bern, Switzerland

The torsion and rotation about single carbon-carbon bonds is a natural process that is ever-present in Chemistry- and Surface-Sciences. Due to their small magnitude, measurements of force-induced conformational changes between units of a long polymeric chain have proven difficult until now[1]. To shed light on these processes, we performed lifting experiments using atomic force microscopy (AFM) at 4.8K of different cyclic carbon polymers adsorbed on a gold substrate. In the pulling curves we detected alternating periods related to successive unit detachments of the poly-pyrenylene units vertically lifted from the Au(111) surface. Molecular dynamic (MD) simulations attribute those spacing variations to symmetry-broken bent and rotated conformations of the sliding physisorbed segment and steric hindrance by the just lifted monomer[2]. In a second experiment, we pulled asymmetric cyclopentaaceanthrylene-polymers that revealed more complex detaching periods depending on the adsorption motif of the polymer units and the resulting steric hindrance between them.

[1] Kawai et al., PNAS, 2014, 11, 111, 3968-3972.
[2] Pawlak et al., Nano Lett., 2019 submitted.
[3] D'Astolfo et al., manuscript in preparation.

O 63.10 Wed 13:00 TRE Ma

DFTB based computational approach to STM imaging, spectroscopy and manipulation of single molecules — Seddigheh Nikipar[1,2], •Dmitry Ryndyk[1], Sibylle Gemming[2], Francesca Moresco[3], Thomas Frauenheim[4], and Gianaurelio Cuniberti[1] — [1]IfWW, TU Dresden — [2]HZDR, Dresden — [3]cfaed, TU Dresden — [4]BCCMS, University of Bremen

We present a new computational approach and open software realization for STM imaging, spectroscopy, and manipulation. The major motivation of the theoretical modeling is to understand the results of surface chemical reactions and nanoscale mechanical motion stimulated and controlled in the STM experiments on single molecules, polymers, and 2D organic materials at finite voltage bias. In our previous work, we showed that this method gives a good agreement between simulated and experimental STM images. Recently we tested it for STM analysis of polymers [1] and nanocarbons [2]. Especially, in the case of strong interactions between adsorbate (molecular motifs) and substrates, the simulated STM images support the experiment to get insight into the structural deformation of molecular motifs due to substrates. We develop our own open-source DFTB+XT package as a core of the TraNaS OpenSuite - integrated open software suite for nanoscale modeling [3], partially based on the DFTB+ [4] source code.

[1] D. Skidin, et al., Nanoscale 10, 17131 (2018).
[2] D. Skidin, et al., Chem. Commun. 55, 4731 (2019).
[3] TraNaS OpenSuite, tranas.org/opensuite, github:tranas-open.
[4] B. Aradi, et al., J. Phys. Chem. A 111, 5678 (2007); dftbplus.org.

O 63.11 Wed 13:15 TRE Ma

Controlling orientation, rotation, and translation of a single molecule by STM via an internal electrical dipole — •Grant J Simpson[1], Víctor García-López[2], A Daniel Boese[3], James M Tour[2], and Leonhard Grill[1] — [1]Department of Physical Chemistry, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria — [2]Departments of Chemistry and Material Science and NanoEngineering, and the Smalley-Curl Institute and NanoCarbon Centre, Rice University, Houston, TX 77005, USA — [3]Department of Theoretical Chemistry, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria

Controlling matter at the individual atom and molecule scale gives insight into basic physical and chemical properties which underpin the field of nanoscience. An interesting approach to controlling molecular mobility on a surface is to implement a strong dipole moment in a molecule which can then interact with the electric field of the tunnel junction. We have used a scanning tunnelling microscope (STM) running at low temperatures to induce and probe the motion of molecules adsorbed on a metal surface. Through interaction of the molecule dipole with the electric field of the tip, rotation with 100% directionality is demonstrated. By mapping the rotational behaviour, it was possible to assign a specific pivot point, which is precisely defined by the atomic composition of the molecule and the surface structure, and to visualise the internal dipole of the molecule [1]. Translation of these molecules can also be induced, revealing details about the molecular dynamics by systematic change of the experimental parameters.

[1] G. J. Simpson et al., Nat. Commun. 10, 4631 (2019)

O 63.12 Wed 13:30 TRE Ma

Characterizing Tip-Induced Motion and 3D Adsorption Conformations of Terphenyl Derivates on Metal Surfaces — •Qigang Zhong[1,2], Daniel Ebeling[1], Jalmar Tschakert[1], Shixuan Du[3], Doreen Mollenhauer[4], Hermann A. Wegner[5], Lifeng Chi[2], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig University Giessen, Germany — [2]Institute of Functional Nano & Soft Materials, Soochow University, China — [3]Institute of Physics, Chinese Academy of Sciences, China — [4]Institute of Physical Chemistry, Justus Liebig University, Germany — [5]Institute of Organic Chemistry, Justus Liebig University, Germany

Studying adsorption conformations and motion of single molecules confined on a 2D surface is essential for understanding surface catalysis, molecular reactions, or self-assembly at the atomic level. Due to site-specific molecule-substrate interactions the adsorption conformations are often non-planar, which can lead to characteristic dynamics of the adsorbed molecules. Here, we investigate the non-stationary features of two terphenyl-based molecules (4,4"-diamino-p-terphenyl, DATP and 4-bromo-3"-iodo-p-terphenyl, BrI-TP) on Cu(111) with single-bond resolution using noncontact atomic force microscopy[1,2]. Frustrated translational or rotational movements of the molecules between two metastable adsorption positions on Cu(111) are observed under the influence of the probe tip. Such non-stationary adsorption states can affect, e.g. the hierarchical dehalogenation of BrI-TP or the local binding affinity and the self-assembly process of DATP.

[1] Nat. Commun. 9, 3277 (2018). [2] ACS Nano 13, 324 (2019).

O 64: Organic Molecules on Inorganic Substrates IV: Adsorption, Growth and Networks

Time: Wednesday 10:30–13:45 Location: TRE Phy

O 64.1 Wed 10:30 TRE Phy

Interactions in STM-assembled molecular clusters — •Andreas Christ, Markus Leisegang, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The adsorption of organic molecules on metal surfaces has recently been studied intensive due to their potential application in electronic devices. For coverages up to a monolayer various self-assembled structures, including one-dimensional chains, Kagome lattices, or two-dimensional networks have been observed [1], which evolve from the delicate interplay of intermolecular and molecule-substrate interactions. To investigate these interactions more systematically, we employed STM manipulation of individual phthalocyanine molecules to manufacture molecular clusters and chains which vary in size and geometry. We observe that the tautomerization behavior of a single deprotonated phthalocyanine molecule changes as neighboring molecules are brought in close proximity. By changing the intermolecular distance and relative orientation we find that the tautomerization can be made asymmetric or hindered completely.

[1] Y. Wang *et al.*, AIP Advances **2**, 041402 (2012)

O 64.2 Wed 10:45 TRE Phy

Conformation controls mobility: 2H-Tetranaphthylporphyrins on Cu(111) — •Jan Kuliga[1], Stephen Masicot[1], Rajan Adhikari[1], Michael Ruppel[2], Norbert Jux[2], Hans-Peter Steinrück[1], and Hubertus Marbach[1] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany — [2]Lehrstuhl für Organische Chemie II, Universität Erlangen-Nürnberg, Henkestr. 42, 91054 Erlangen, Germany

The adsorption behavior and the mobility of 2H-Tetranaphtylporphyrin (2HTNP) on Cu(111) was investigated by scanning tunneling microscopy (STM) at room temperature (RT). The molecules adsorb in the *inverted* structure, like the structurally related 2HTPP, with the naphthyl plane restricted to an orientation parallel to the Cu surface. The orientation of the four naphthyl groups yields altogether 16 possible conformations. Due to the existence of rotamer pairs, 10 different appearances are expected on the surface, which could all be identified by STM at RT. Most interestingly, the orientation of the naphthyl groups significantly influences the diffusion behavior of the molecules on Cu(111). We could identify three different groups of conformers, which are either immobile, medium or fast diffusing at RT. The mobility seem to decrease with increasing size of the footprint of the conformers on the surface.

O 64.3 Wed 11:00 TRE Phy

Quantitative confirmation of the inverted adsorption structure for 2H-tetraphenyl porphyrin on Cu(111) — Paul T. P. Ryan[1,2], Paula L. Lalaguna[1,3], Felix Haag[4], Mona M. Braim[5], Pencheng Ding[5,6], David J. Payne[2], Johannes V. Barth[4], Tien-Lin Lee[1], D. Phil Woodruff[5], Francesco Allegretti[4], and •David A. Duncan[1] — [1]Diamond Light Source, Didcot, UK — [2]Imperial College London, UK — [3]University of Glasgow, UK — [4]Technical University of Munich, Germany — [5]University of Warwick, Coventry, UK — [6]Harbin Institute of Technology, China

The inverted model has been proposed as the adsorption structure for tetraphenyl porphyrin (2H-TPP) on Cu(111) in recent publications[1,2]. In this model two of the 2H-TPP pyrrole rings are tilted almost perpendicular to the surface, moving the iminic N atoms into a surface bridge site and breaking the aromaticity of the porphyrin macrocycle. Published X-ray standing waves (XSW) data [3] was used to justify this model, yet that study was dogged by radiation damage and did not probe the lateral adsorption site of the molecule. Here we present a XSW study without such damage, addressing the lateral adsorption site of the iminic N atoms. These atoms are indeed found to occupy bridge or near-bridge adsorption sites on the surface, displaced laterally by 1.1 ± 0.2Åfrom direct atop sites. This result is in excellent agreement with the predicted value for these parameters in the inverted model, from the DFT calculations of Lepper et al., of 1.18 Å. [1] Chem. Comm. 53, 8207 (2017); [2] Chem. Mater. 31, 3009 (2019); [3] J. Phys. Chem. C 118, 13659 (2014)

O 64.4 Wed 11:15 TRE Phy

Arrangement and electronic properties of cobalt phthalocyanine molecules on Si(111) $(\sqrt{3}\times\sqrt{3})$ R30°-B — •Milan Kubicki, Martin Franz, Susi Lindner, Holger Eisele, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

The formation of self-assembled monolayers of organic molecular materials on solid surfaces is an important subject because of their possible application in advanced optical and electronic devices. Here, the molecular arrangement and the interfacial electronic properties of cobalt phthalocyanine (CoPc) on the deactivated Si(111) $(\sqrt{3}\times\sqrt{3})$ R30°-B surface are studied by scanning tunneling microscopy and spectroscopy [1]. It is found that for submonolayer coverages the CoPc molecules lie flat on the Si surface with the Co d_{z^2} orbital of the molecule forming a hybrid state with the p_z orbital of the Si adatom at the surface. For multilayer coverages, in contrast, the CoPc molecules are tilted with respect to the Si surface forming highly ordered organic molecular films, and the electronic properties resemble those of pure CoPc.

[1] S. Lindner, M. Franz, M. Kubicki, S. Appelfeller, M. Dähne, and H. Eisele, Phys. Rev. B, in print (2019).

O 64.5 Wed 11:30 TRE Phy

Wetting of Porphyrin Multilayers on Rutile TiO2(110) — •Elmar Kataev[1], Daniel Wechsler[1], Federico Williams[2], Julia Köbl[1], Natalia Tsud[3], Kevin Prince[4], Hans-Peter Steinrück[1], and Ole Lytken[1] — [1]Friedrich-Alexander University Erlangen-Nürnberg, 91058, Erlangen, — [2]Universidad de Buenos Aires, Buenos Aires C1428EHA, Argentina — [3]Charles University, 116 36, Prague, Czech Republic — [4]Sincrotrone Trieste SCpA, Basovizza, Italy

Porphyrin/oxide hybrid materials find widespread applications in catalysis, sensors, organic electronics, and light-harvesting systems. However, molecular-level understanding of the interaction of porphyrins with oxides is missing. Here we report a photoemission study of the coverage- and temperature-dependent multilayer growth of cobalt(II) 5-monocarboxyphenyl-10,15,20-triphenylporphyrins (CoMCTPP) and cobalt(II) tetraphenylporphyrins (CoTPP) on a TiO2(110) surface. We find that CoTPP grows in layer-by-layer mode up to 3 layers, switching its behaviour to 3D growth afterwards. For CoMCTPP, we observe 3D growth directly after completion of the first layer. We describe this behavior by a roughness model consisting of a uniform film with sine-shaped islands on top of it. Subsequent annealing resulted in desorption without major rearrangement of the molecules. We conclude that a carboxylic group reduces the porphyrin mobility due to stronger molecular-substrate and molecular-molecular interactions. Supported by the DFG Research Unit FOR 1878 funCOS.

O 64.6 Wed 11:45 TRE Phy

Porous 2D networks formed by cyano-functionalized tetraphenyl porphyrins on Cu(111) — •Rajan Adhikari[1], Gretel Siglreithmaier[1], Jan Kuliga[1], Michael Lepper[1], Manuel Meusel[1], Helen Hölzel[2], Norbert Jux[2], Bernd Meyer[3], Hans-Peter Steinrück[1], and Hubertus Marbach[1] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr.3, 91058 Erlangen, Germany — [2]Lehrstuhl für Organische Chemie II, Universität Erlangen-Nürnberg, Nikolaus-Fiebiger-Str. 10 , 91058 Erlangen, Germany — [3]Computer-Chemistry-Center (CCC), Universität Erlangen-Nürnberg, Nägelsbachstr. 25, 91052, Erlangen, Germany

We investigated the adsorption of three related cyano-functionalized tetraphenyl porphyrin derivatives on Cu(111) by scanning tunneling microscopy in ultra-high vacuum with the goal to identify the role of the cyano group and the central Cu atom. The porphyrin derivatives studied were Cu-TCNPP, Cu-cisDCNPP, and 2H-cisDCNPP. Starting from different structures obtained after deposition at room temperature, all three molecules form the same long-range ordered hexagonal honeycomb-type structure with triangular pores, and three molecules per unit cell. For the metal-free 2H-cisDCNPP, this goes along with self-metalation. The structure-forming elements are pores with a distance of 3.1 nm, formed by triangles of porphyrins fused together by CN-Cu-NC interactions, with Cu adatoms. This finding leads us to suggest that the twofold cyano-functionalized at ”cis” conformation is the minimum prerequisite to form a highly ordered 2D porous pattern.

O 64.7 Wed 12:00 TRE Phy

Heteromolecular bilayers on a weakly interacting substrate: Interactions and molecular distortions of F16CuPc — •Qi Wang[1], Antoni Franco-Cañellas[1], Jiacheng Yang[2], Julian Hausch[1], Samuel Struzek[1], Mengting Chen[2], Pardeep Kumar Thakur[3], Alexander Gerlach[1], Steffen Duhm[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [2]Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou 215123, People’s Republic of China — [3]Diamond Light Source, Harwell Science and Innovation Campus, OX11 0DE Oxfordshire, United Kingdom

Heteromolecular bilayers of π-conjugated organic molecules (COM) on metals, which are considered as model systems for more complex thin film heterostructures, are investigated with respect to their structural and electronic properties [1]. By exploring the influence of the organic-metal interaction strength in such bilayer systems, we determine the molecular arrangement in the physisorptive regime for copper-hexadecafluorophthalocyanine (F16CuPc) on Au(111) with template layers of 5,7,12,14-pentacenetetrone (P4O) and perylene-3,4,9,10-tetracarboxylic diimide (PTCDI). Using the X-ray standing wave (XSW) technique to distinguish the different molecular layers, we show that these two bilayers are ordered following their deposition sequence. Surprisingly, F16CuPc as the second layer within the heterostructures exhibits an inverted intramolecular distortion compared to its monolayer structure.

[1] Q. Wang, et. al., J. Phys. Chem. C. (2018) 122, 9480-9490.

O 64.8 Wed 12:15 TRE Phy

Tailoring adsorbed porphyrins with reactive metal centers — •Francesco Allegretti[1], David Duncan[1,2], Peter Deimel[1], Alissa Wiengarten[1], Willi Auwärter[1], Ari Seitsonen[3], and Johannes Barth[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]Diamond Light Source, Didcot, OX11 0DE, UK — [3]Département de Chimie, École Normale Supérieure, F-75005 Paris, France

Endowing adsorbed metal complexes such as porphyrins and phthalocyanines with specific functionalities can be of paramount importance for a range of applications, including heterogeneous catalysis, solar cells, and chemical sensors. The exploitation of on-surface reactions following the adsorption of free-base macrocyclic species on metal substrates provides an elegant route to tailor reactive centers in clean environments. Here, we report on the formation of Titanium(II) tetraphenylporphyrin (TiTPP) molecules on a Ag(111) surface by on-surface metalation. Unlike other metalloporphyrins we have previously studied, these species are very reactive even in the monolayer limit, and readily react with molecular oxygen to form oxotitanium porphyrin (TiOTPP) molecules with Titanium(IV) centers. We characterize the TiTPP and TiOTPP products at the molecular scale by a combination of X-ray spectroscopy, scanning probe microscopy and density functional theory to unravel details of the self-assembly, the molecular conformation and the oxidation state of the metal centers. Both molecules are promising candidates for future studies into model catalytic and photocatalytic reactions at surfaces.

Invited Talk O 64.9 Wed 12:30 TRE Phy

On-surface Chemical Reactions of Heterocycles for Functional Nanomaterials — •Shi-Xia Liu — Department of Chemistry and Biochemistry, University of Bern, Switzerland

On-surface chemical reactions are of high interest and have been intensively investigated in order to obtain carbon-based functional nanomaterials which very often can not be synthesized by wet chemistry. Thus, tailor-made heterocyclic precursors are becoming quite crucial in the development of highly symmetric 2D-conjugated porous architectures and N-doped graphene nanoribbons (GNRs) with desired functions due to their intrinsic electronic properties. This presentation focuses on our collaborative work on self-assembly and C-C coupling reactions on different surfaces leading to the formation of a range of nanostructures including small clusters,1 molecular wires,2 fully fused porphyrin-GNR hybrids3 and 2D-conjugated porous networks with Kagome characteristics.4 All these atomically precise nanostructures can be directly visualized by scanning tunneling microscopy (STM) and noncontact atomic force microscopy (nc-AFM). Their electronic properties can be fine-tuned by chemical modification and will be discussed.

References 1. N. Kocic et al., J. Am. Chem. Soc. 2016, 138, 5585-5593. 2. S. Karan et al., Angew. Chem. Int. Ed. 2019, submitted. 3. L. M. Mateo et al., Angew. Chem. Int. Ed. 2019, DOI: 10.1002/anie.201913024. 4. R. Pawlak et al., manuscript in preparation.

O 64.10 Wed 13:00 TRE Phy

On-surface Synthesis of Porphyrin-GNR Hybrid Chains — •Joel Deyerling[1], Mathias Pörtner[1], Luka Dordević[2], Alexander Riss[1], Davide Bonifazi[3], and Willi Auwärter[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]Department of Chemical and Pharmaceutical Sciences, University of Trieste, Italy — [3]School of Chemistry, Cardiff University, U.K.

In recent years, the on-surface formation of hybrid structures combining porphyrins and graphene nanoribbons (GNRs) attracted increasing interest [1-3]. A control on the precise atomic structure of such covalently linked porphyrin-based heterosystems is highly relevant for the tuning of their electronic and functional properties.

Here, we address dehalogenative coupling reactions of a bromonaphthalene functionalized Zn-porphyrin derivative on Ag(111) and Au(111). This precursor, its reaction steps, and different coupling motifs are characterized by scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) using a CO functionalized tip. Porphyrin-GNR hybrid chains exceeding a length of 20 nm are achieved. Our experiments reveal atomistic details of different coexisting coupling motifs, which holds great promise for future investigations of the corresponding electronic structure.

[1] J. Li *et al.*, Sci. Adv. 4, eaaq0582 (2018)
[2] L.M. Mateo *et al.*, Angew. Chem. Int. Ed., (2019)
[3] F. Bischoff *et al.*, Angew. Chem. Int. Ed., 57, 16030 (2018)

O 64.11 Wed 13:15 TRE Phy

Adsorption and intercalation of Zn porphines at the *h*-BN interface on Cu(111) — •Aleksandr Baklanov[1], David Duncan[2], Martin Schwarz[1], Knud Seufert[1], Johannes Küchle[1], Paul Ryan[2,3], Ignacio Piquero-Zulaica[1], Francesco Allegretti[1], and Willi Auwärter[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]Diamond Light Source, Harwell Science and Innovation Campus, Didcot, UK — [3]Department of Materials, Imperial College London, South Kensington, London, UK

Two-dimensional *h*-BN is an insulating layer used frequently to decouple adsorbed (metal-)organic molecules from the underlying metal single crystal support, thus preventing the strong influence of the latter on the molecular geometric and electronic properties [1,2]. The adsorption of Zn-porphine molecules on *h*-BN/Cu(111) as well as intercalation by placing the molecules between the *h*-BN cover and the Cu(111) [3], reveals distinct differences compared to porphine adsorption on bare Cu(111) [4]. Here we address the molecular conformation, adsorption structure, functionality of adsorbed and intercalated porphines, combined with the electronic and geometric structure of the *h*-BN by means of X-ray standing waves (XSW), X-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy/spectroscopy (STM/STS).

[1] W. Auwärter, Surf. Sci. Rep. **74**, 1 (2019).
[2] M. Schwarz et al., Nanoscale **10**, 21971 (2018).
[3] J. Ducke et al., ACS Nano **12**, 2677 (2018).
[4] M. Schwarz et al., J. Phys. Chem. C **122**, 5452 (2018).

O 64.12 Wed 13:30 TRE Phy

Ultrathin ionic liquid layers and organic molecules on metal surfaces — •Stephen Massicot, Matthias Lexow, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Ionic liquids (ILs) are salts with melting points below 100°C and extreme low vapor pressure. Due to these properties, they have been studied extensively as promising candidates for various thin film applications, e.g in the fields of sensors, electrochemistry and catalysis. The interplay of ILs with organic molecules at metal surfaces in this context is highly important to understand and predict the behavior of these thin films applications.

In this study, we deposit ultrathin imidazolium IL layers and porphyrins by in-situ physical vapor deposition on a Ag(111) surface as model support. The structure and composition of the film at the solid and at the vacuum interface is studied by angle-resolved and temperature-programmed X-ray photoelectron spectroscopy on the molecular scale.

Supported by the European Research Council (ERC) through an Advanced Investigator Grant to HPS.

O 65: Plasmonics and Nanooptics IV: Waveguides and Antennas

Time: Wednesday 10:30–13:30 Location: WIL A317

O 65.1 Wed 10:30 WIL A317

Plasmonic nanfocusing spectroscopy: from local excitation to local detection of optical near fields — •Abbas Chimeh[1], Sven Stephan[1], Martin Esmann[2], Anke Korte[1], Jinhui Zhong[1], Martin Silies[1], Nahid Talebi[3], and Christoph Lienau[1] — [1]Universität Oldenburg, Oldenburg, Germany — [2]Centre de Nanosciences et de Nanotechnologies, Paris, — [3]Universität Kiel, Kiel, Germany

The nanofocusing of light in tapered plasmonic waveguides efficiently confines electromagnetic radiation into volumes far below the wavelength, breaking the diffraction resolution limit of optical microscopy [1]. Selective delivery of the optical excitation to a specific point near the sample surface has made plasmonic nanofocusing an effective tool for spatially resolved spectroscopy on the nanoscale [2]. Here, we show that a tapered plasmonic guide is also capable of not only nanofocusing of light into nanometric volumes but also detecting light from them. We show by full-wave analysis of electromagnetic fields how surface plasmon polaritons (SPPs) nanofocused onto the apex of a gold nanotaper excite the near fields of a nanorod. These near fields are coupled back to the taper apex and launch back propagating SPPs. We detect the local light scattering spectra of nanorods from these back propagating SPPs and quantify line broadenings and spectral shifts induced by tip-sample coupling. Our finite-difference time-domain simulations are in a good agreement with experimental results. [1] D. K. Gramotnev et al., Nature Photon. 8, 14 (2012). [2] M. Esmann et al., Nature Nanotechnol. 6, 6040 (2019)

O 65.2 Wed 10:45 WIL A317

Surface Polariton-Like s-Polarized Waveguide Modes in Switchable Dielectric Thin-Films on Polar Crystals — •Nikolai Christian Passler[1], Andreas Hessler[2], Matthias Wuttig[2], Thomas Taubner[2], and Alexander Paarmann[1] — [1]Fritz-Haber-Institute of the MPG — [2]RWTH Aachen University

Surface phonon polaritons (SPhP) and surface plasmon polaritons are fundamental building blocks of nanophotonics. These modes are unmatched in field enhancement and spatial confinement, and all-optical control is feasible with phase-change materials such as $Ge_3Sb_2Te_6$ (GST). However, the excitation of surface polaritons is limited to p-polarization. On the contrary, waveguide modes in high-permittivity films can couple to both p- and s-polarized light, and in thin films, their confinement can become comparable to surface polaritons.

For a thin GST film on SiC, we here [1] demonstrate that the s-polarized waveguide mode features a similar dispersion, confinement, and electric field enhancement as the index-shifted SPhP of SiC. Experimentally, employing the Otto geometry for prism coupling [2], we show that switching the GST film between its amorphous and crystalline phase grants non-volatile control over the SPhP and the s-polarized waveguide mode dispersions. Thus, polariton-like waveguide modes in dielectric thin films on polar crystal substrates provide a promising additional building block for actively tunable, low-loss, and omni-polarized nanophotonic applications.

[1] N. C. Passler et al., Adv. Opt. Mater., 1901056 (2019)
[2] N. C. Passler et al., ACS Photonics 4, 1048 (2017)

O 65.3 Wed 11:00 WIL A317

Single Molecule Nonlinearity in Plasmonic Waveguides — •Christian Schörner and Markus Lippitz — University of Bayreuth, Germany

Past room temperature experiments of single quantum emitters coupled to plasmonic waveguides have mainly focused on the highly efficient channeling of the spontaneous emission into waveguide modes. However, quantum emitters can interact with multiple optical fields leading to functional all-optical control capabilities in waveguide circuits. Here, we realize a nonlinear optical experiment, where a pump and a red-shifted depletion pulse interact fully remotely with a single molecule via propagating gap-plasmons. A saturation of the molecules' stimulated emission via confined gap-plasmons is found, that can be up to 50 times more efficient compared to a diffraction limited far-field focus.

O 65.4 Wed 11:15 WIL A317

Mode-selective electrical excitation of optical waveguides — •Maximilian Ochs, Luka Zurak, Enno Krauss, Jessica Meier, René Kullock, Monika Emmerling, and Bert Hecht — NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany

Downscaling light-based communication to the nanoscale, i.e. optical nanocircuitry, promises higher data transfer rates than currently available technologies. Waveguides, routing optical modes in a controlled way, are fundamental components in such circuits and have already been demonstrated utilizing optical excitation schemes [1]. However, the electrical driving - necessary to integrate these devices into common circuits and reduce their footprint - still remains a challenge.

Here, we demonstrate the mode-selective electrical excitation of optical waveguides using inelastic electron tunneling. The tunnel gap is fabricated with high accuracy and reproducibility by combining helium ion milled single-crystalline gold flakes and feedback-controlled dielectrophoresis [2]. Based on the position of excitation, specific modes can be launched and their interference enables control over the polarization of the out-coupled light. In this context, we propose an integrated system allowing to switch between the excitation of two different modes. This work paves the road for more complex optical nanocircuits, such as logic gates at optical frequencies.

[1] E. Krauss et al.,*Nano Lett. 19, 3364 (2019)*
[2] R. Kullock et al.,*Nat. Commun. accepted (2019)*

O 65.5 Wed 11:30 WIL A317

Limits of optical Yagi-Uda antennas — •René Kullock, Maximilian Ochs, Philipp Grimm, Monika Emmerling, and Bert Hecht — NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany

Yagi-Uda antennas are a promising building block for light-based on-chip data communication which allows much higher bandwidths than conventional electrical circuitry. On the macroscopic scale they provide a highly directed emission of radio waves and scaled down to the nanometer regime they do the same for light. Already a while ago optically driven Yagi-Uda antenna have been realized [1] and recently we were able to demonstrate the crucial electrical driving using inelastic electron tunneling [2].

Here we show how such antennas are fabricated using advanced focused-ion beam milling and feedback-driven dielectrophoresis. We compare the resulting directional antennas with FB ratios of up to 9 dB to conventional RF Yagi-Uda antennas, discuss their scalability and design limits. Despite increased losses of metals at optical frequencies we show that by utilizing dielectric guiding layers, which are only available in the optical domain, the antennas can actually outperform their RF counterparts.

[1] A. Curto et al., Science 329, 5994 (2010)
[2] R. Kullock et al., Nat. Comm. *accepted* (2019)

O 65.6 Wed 11:45 WIL A317

Strongly coupled, high-quality plasmonic dimer antennas fabricated using a sketch-and-peel technique — •Moritz Gittinger[1], Katja Höflich[2], Vladimir Smirnov[1], Heiko Kollmann[1], Christoph Lienau[1], and Martin Silies[1] — [1]AG Ultrafast Nano-Optics, Carl von Ossietzky University Oldenburg, Germany — [2]Helmholtz Zentrum für Materialien und Energie, Berlin, Germany

A combination of helium- and gallium-ion beam milling together with a fast and reliable sketch-and-peel technique is used to fabricate gold nanorod dimer antennas with an excellent quality factor and with gap distances of less than 6 nm. The high fabrication quality of the sketch-and-peel technique compared to a conventional ion beam milling technique is proven by polarization resolved linear dark-field spectromicroscopy of isolated dimer antennas. We demonstrate a strong coupling of the two antenna arms for both fabrication techniques, with a quality factor of more than 14, close to the theoretical limit, for the sketch-and-peel produced antennas compared to only 6 for the conventional fabrication process. The obtained results on the strong coupling of the plasmonic dimer antennas are supported by finite-difference time-domain simulations of the light-dimer antenna interaction. The presented fabrication technique enables the rapid fabrication of large-scale plasmonic or dielectric nanostructures arrays and metasurfaces with single-digit nanometer scale milling accuracy. [https://doi.org/10.1515/nanoph-2019-0379]

O 65.7 Wed 12:00 WIL A317

Comparative study of plasmonic antennas fabricated by electron and ion beam lithography — •Vlastimil Křápek, Michal Horák, Lukáš Kejík, Kristýna Bukvišová, Vojtěch Švarc, and Tomáš Šikola — CEITEC, Brno University of Technology, Purkyňova 123, 61200 Brno, Czech Republic

We present a comparative study of plasmonic antennas (gold nanodiscs) fabricated by electron beam lithography and focused ion beam milling. Plasmonic antennas were characterized using transmission electron microscopy including electron energy loss spectroscopy and energy dispersive X-ray spectroscopy, and atomic force microscopy. We have found stronger plasmonic response with better field confinement in the antennas fabricated by electron beam lithography, which is attributed to their better structural quality, homogeneous thickness, and only moderate contamination mostly of organic nature [1].

Further, we compare monocrystalline and polycrystalline plasmonic antennas (gold nanorods) fabricated by focused ion beam lithography. Interestingly, monocrystalline nanorods feature inclined facets due to anisotropic rate of focused ion beam milling, while the facets of the polycrystalline nanorods are upright. Electron energy loss spectroscopy revealed that the parameters of the localized surface plasmon modes (energies, Q factors, and peak loss probabilities) in both structures are within the experimental error identical. We conclude that the polycrystallinity does not deteriorate the optical properties of plasmonic antennas.

[1]. M Horák et al., Sci. Rep. **8**, 9640 (2018).

O 65.8 Wed 12:15 WIL A317

Generating ultra-narrow gaps in bow-ties utilizing break junctions — •Florian Laible[1], Kai Braun[2], Martin Eberle[2], Dieter P. Kern[1], Alfred J. Meixner[2], and Monika Fleischer[1] — [1]Institute for Applied Physics and Center LISA+, University of Tübingen, 72076, Tübingen, Germany — [2]Institute for Physical and Theoretical Chemistry and Center LISA+, University of Tübingen, 72076, Tübingen, Germany

Investigations on the interplay of localized plasmonics and electron tunneling require electrically contacted dimer nanoantennas with ultra-narrow, i.e. sub-1 nm, gaps. The realization of this configuration is a challenging task. It has been achieved in [1], but this experiment is hardly suitable for more general investigations.

We present an alternative approach to reach ultra-narrow gaps in the

focus of a confocal microscope. Gapless bow-tie antennas are integrated into mechanically controllable break junctions. The nanostructures are optically decoupled from the electrical leads. The gap is created by bending the substrate. Its size is measured (in situ) using the tunnel effect and controlled by increasing or decreasing the bending of the substrate.
Due to the decoupling of the nanostructures from the leads, localized plasmon polaritons are excited in the bow-tie when illuminated by the laser of a confocal microscope. Combined electrical and optical measurements will be presented alongside with the fabrication process.
[1] K. J. Savage, et al. Nature, 491(7425),574, 2012.

O 65.9 Wed 12:30 WIL A317

Electro-Chemistry of two closely spaced electrically-connected plasmonic antennas in air — •Luka Zurak, Bert Hecht, and Thorsten Feichtner — Nano-Optics & Biophotonics Group, Wilhelm-Conrad-Röntgen-Center for Complex Material Systems (RCCM), Experimental physics 5 - Universität Würzburg, Germany

It has been shown that small resonant plasmonic nano particles can be tuned by applying a voltage, when placed in an electro-chemical environment. Resonance shifts can be due to double-layer formation, surface chemistry or charging which are notoriously difficult to distinguish.

We have developed a system of two parallel electrically connected gold nanorods with unequal lengths and resonances. They are placed at a distance of 150 nm. We show by means of time dependent white light spectroscopy that the humidity of ambient air is sufficient to support electrochemistry at the rod surfaces when voltages of up to ±20 V are applied. Electrochemical processes reveal themselves by small shifts of the nanorod resonances with a slow time constant on the order of 10 seconds. When the same experiments are performed under a N_2 atmosphere, the resonance shifts nearly completely vanish.

O 65.10 Wed 12:45 WIL A317

Coupling of phosphorescent single molecules to plasmonic nanostructures — •Marcel Krumrein[1], Maximilian Rödel[1], Ulrich Müller[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Phosphorescent materials are widely used in OLED applications to improve the external quantum efficiency of these devices. After excitation, the intersystem crossing in such molecules converts the S_1 singlet state into a long-living T_1 triplet state where a radiative, phosphorescent decay into the S_0 ground state takes place on, typically, μs time scale. In this work we couple single molecules of the phosphorescent emitter Ir(piq)$_3$ to plasmonic nanostructures to influence their dynamics and, thus, their effective emissive rates. For this purpose, long-range ordered metallic nanoarrays were fabricated by means of shadow nanosphere lithography and the Ir(piq)$_3$-doped PMMA host-guest system was deposited via spin-coating on-top. Effects by coupling to the underlying plasmonic array were investigated by lifetime analysis and photon-correlation functions measured with a confocal microscope setup. By comparison with Ir(piq)$_3$:PMMA reference samples on glass we observe an enhancement of the emission intensity by more than an order of magnitude which indicates a change of the intramolecular transition rates in proximity to the metallic nanostructures. We will discuss these results in context to the implementation of metal-organic hybrid structures in electrically driven photonic devices.

O 65.11 Wed 13:00 WIL A317

Fourier-space microspectroscopy of disordered plasmonic metasurfaces — •Florian Sterl, Ediz Herkert, Steffen Both, Thomas Weiss, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

The optical properties of plasmonic nanoparticle ensembles are not only determined by the particle shape and their size, but also by the nanoantenna arrangement. We present computational and experimental approaches to gain a better understanding of the impact of disorder on the far-field behavior of complex plasmonic metasurfaces. We treat the nanoantennas as dipoles, and simulate the electric field based on dipole-dipole interaction. We can then extract the wavelength-resolved far-field response and convert it into real-space and Fourier space RGB images. A designated Fourier microspectroscopy setup allows us to record the real- and Fourier-space images of plasmonic metasurfaces.

We consider different types of spatial disorder. In the case of ‘frozen-phonon disorder’, each element is displaced from its initial lattice position by a random amount within a variable range. In the case of correlated disorder, the displacement of any element affects the surrounding elements with a certain correlation length and function. Our results show that the two classes of disorder can be clearly distinguished in real and Fourier space. These insights provide the possibility to design the visual appearance of a metasurface by tailored disorder.

O 65.12 Wed 13:15 WIL A317

Investigating Surface Plasmons and Photonic Bandgap of Ordered Nanoarray Constructed by Hierarchical Alumina Membranes — •Yi Wang, Yudie Huang, Jiaxu Chen, Fanzhou Lv, and Wenxin Wang — Photonic Materials Group, College of Physics and Optoelectronic Engineering, Harbin Engineering University, Harbin, China

The purpose to manipulate photonics and the trend of device miniaturization prompt people to design sophisticated ordered nanostructures with well practicability over large scale. Attributing to the inherent structure feature of ordered pore array, alumina membranes (AMs) are widely used in preparation of ordered nanoarrays for various device applications. For the reason that, artificial modulated AMs can offer porous membranes with uniform geometric parameters, in order to achieve controllable distribution of nanomaterials. Here, we demonstrate the idea to fabricate hierarchical alumina membrances (HAMs) with controllable subwavelength patterns as promising platform to construct plasmonic structures. By precisely controlling the anodization potential, sophisticated structures of AMs are regulated into distinctive patterns. After replicating HAMs with functional polymer and noble metal, hierarchical nanostructures (HNs) with unique surface plasmon resonance (SPR) properties are obtained, which is developed as dynamic plasmonic sensing device. In addition, the photonic bandgap brought by HNs are investigated in detail. This approach for elaborate HNs fabrication broadens the scope for the design and application of functional nanostructures in the field of nanophotonic devices.

O 66: 2D Materials IV: Interfacial Interactions (joint session O/HL/CPP)

Time: Wednesday 10:30–13:45 Location: WIL B321

O 66.1 Wed 10:30 WIL B321

Interplay between electronic instability and moiré structure of monolayer V_2S_3 on Au(111) — •Sahar Pakdel[1], Umut Kamber[2], Raluca-Maria Stan[1], Anand Kamlapure[2], Brian Kiraly[2], Fabian Arnold[1], Andreas Eich[2], Arlette S. Ngankeu[1], Marco Bianchi[1], Jill A. Miva[1], Charlotte Sanders[1], Philip Hofmann[1], Alexander A. Khajetoorians[2], and Nicola Lanata[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Aarhus, Denmark — [2]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

The formation of Moiré superstructures between 2D-materials and their substrates has attracted considerable attention, as it can influence their physical properties. Here we study monolayer V_2S_3 grown on an Au(111) substrate. Scanning tunneling microscopy experiments exhibit multiple domains with different Moiré structures. Comparing the calculated Fermi surfaces with angle resolved photo-emission spectroscopy data, we find that the substrate induces a substantial shift in the chemical potential. We show that the computed Lindhart function of V_2S_3 (at the measured chemical-potential) has a pronounced peak corresponding to a second-order reciprocal point of the prevalent Moiré structure. This suggests that the system tends to favor Moiré structures with modulations able to accommodate underlying electronic instabilities of V_2S_3. We speculate that this could be the manifestation of a more general mechanism and a promising route for tailoring the electronic structure of 2D-materials.

O 66.2 Wed 10:45 WIL B321

Probing the electronic structure of twisted transition metal dichalcogenide bilayers by photoemission — •bharti parashar[1], sven borghardt[2], kevin janssen[1], mateo jugovac[1], vitaliy feyer[1], dorota wilgocka slezak[3], józef korecki[3], lukasz plucinski[1], and claus m. schneider[1] — [1]PGI-6, FZ Jülich, Germany — [2]PGI-9, FZ Jülich, Germany — [3]Polish Academy of Sciences, Kraków, Poland

Moire bands in twisted transition metal dichalcogenide (TMDC) bilayers are predicted to host novel topological and correlated electronic phases [1]. We performed angle-resolved photoemission studies with few micrometer resolution (μ-ARPES) on several hetero- and homobilayers made from MoS$_2$ and WSe$_2$ by mechanical exfoliation and dry transfer technique. The twist angle between the layers was determined in a separate experiment by μ-LEED.

We determine the hybridization between the layers through monitoring the formation of new spectral features in normal emission spectra, that are not present in respected monolayers. The existence of hybridization indicates high quality of the interface that is critical to enable formation of interesting moire bands. Furthermore, our results allow to shed light on whether the valence band maximum is located at Γ or at K at various bilayers. This is improtant for predicted moire physics, since only at K the bands are spin-momentum locked.

[1] See e.g.: F. Wu, T. Lovorn, E. Tutuc, I. Martin, and A. H. MacDonald, Phys. Rev. Lett. 122, 086402 (2019), and refs. therein.

O 66.3 Wed 11:00 WIL B321

Electronic vs Structural Effects in the Moiré Pattern of MoS$_2$ on Au(111) — Caio C. Silva[1,2], Daniela Dombrowski[1,2], Nicolae Atodiresei[3], Wouter Jolie[2], Ferdinand Farwick zum Hagen[2], Jiaqi Cai[2], Paul T. P. Ryan[4], Pardeep Thakur[5], Vasile Caciuc[3], Stefan Blügel[3], David A. Duncan[5], Thomas Michely[2], Tien-Lin Lee[5], and •Carsten Busse[1,2,6] — [1]WWU Münster, Germany — [2]Universität zu Köln, Germany — [3]FZ Jülich and JARA, Germany — [4]Imperial College London, U. K. — [5]Diamond Light Source Ltd, U. K. — [6]Universität Siegen, Germany

The lattice mismatch between a monolayer of MoS$_2$ and its Au(111) substrate induces a moiré superstructure. The local variation of the registry between sulfur and gold atoms at the interface leads to a periodic pattern of strongly and weakly interacting regions. In consequence, also the electronic bands show a spatial variation.

We use scanning tunneling microscopy and spectroscopy (STM/STS), x-ray photoelectron spectroscopy (XPS) and x-ray standing wave (XSW) for a determination of the atomic structure and the resulting electronic properties. The experimental results are corroborated by density functional theory (DFT). We deduce the structure of the supercell with high precision, identify the fraction of interfacial atoms that are strongly interacting, and analyze the variation of the electronic structure in dependence of the location within the moiré cell and the nature of the band.

O 66.4 Wed 11:15 WIL B321

Complex moiré structures in rotated monolayer V$_2$S$_3$ on Au(111) — •Umut Kamber[1], Sahar Pakdel[2], Raluca-Maria Stan[2], Anand Kamlapure[1], Brian Kiraly[1], Fabian Arnold[2], Andreas Eich[1], Arlette S. Ngankeu[2], Marco Bianchi[2], Jill A. Miwa[2], Charlotte Sanders[2], Nicola Lanata[2], Philip Hofmann[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Aarhus, Denmark

Moiré superlattices have led to the emergence of tunable many-body states of matter like superconductivity and Mott insulator states absent in the individual layers [1,2]. For transition metal dichalcogenides (TMDCs), there has been a strong interest in how electronic structure is modified near the single layer limit and potentially affected by the dielectric environment. Here, we show spatially periodic modifications to the electronic structure of single layer V$_2$S$_3$ grown on Au(111) varying with the underlying moiré pattern [3]. Similar modifications were observed in multiple moiré patterns, each arising from a different relative orientation between the monolayer and the Au(111) substrate. We characterize these spatial variations in electronic structure with respect to the atomic and moiré lattices via scanning tunneling microscopy and spectroscopy, with the help of ab initio calculations.

[1] Y. Cao et al., Nature, 556, 43 (2018).

[2] Y. Cao et al., Nature, 556, 80 (2018).

[3] F. Arnold et al., 2D Mater. 5, 045009 (2018).

O 66.5 Wed 11:30 WIL B321

Screening effects at the internal interfaces of bulk-like MoS$_2$ — •Philipp Marauhn, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

The two-dimensional nature of TMDCs is intrinsically linked to reduced screening. This renders the materials sensitive to their dielectric environment. Quasiparticle calculations of MoS$_2$ deposited on different substrates have shown the importance to account for environmental screening [1]. In this talk we discuss how screening effects modify the electronic structure across the internal interfaces of bulk-like MoS$_2$.

In a first step we use a tight-binding model to reproduce the band structure on a level of density functional theory. To include polarization effects, we extend the model by introducing a self-energy operator constructed from layer-resolved quasiparticle corrections calculated within the framework of GW. Using this GW-tight-binding approach, we show that environmental screening has strong impact on the formation of the subbands which originate from interlayer interactions. Most striking, at the K-point, the surface layer decouples from lower lying layers forming a direct gap which is distinctly different from that of the total system.

[1] M. Drüppel et al., Nat. Commun. **8**(1), 2117 (2017)

O 66.6 Wed 11:45 WIL B321

Charge density wave and superconductivity of single-layer NbSe2 on different screening environments — •Wen Wan, Paul Dreher, Marco Gobbi, and Miguel M. Ugeda — Donostia International Physics Center and Centro de Física de Materiales, San Sebastián-Donostia, Spain

Superconductivity and charge density wave order, typical collective electronic phases of transition metal chalcogenides (TMD), are highly sensitive to external perturbations. In the 2D limit, the properties, and even the mere existence, of these phases in monolayers of TMDs become mostly dependent on the supporting substrate due to charge doping/screening and hybridization effects [1,2]. Here, we carry out low-temperature STM/STS (350 mK) measurements to study the electronic structure of single-layer NbSe2 grown on different substrates by molecular beam epitaxy. In particular, we explore and compare the fate and fundamental properties of the superconducting and CDW states of single-layer NbSe2 on both highly metallic, semi-metallic and insulating TMD substrates [3].

[1] M. M. Ugeda, et al. Nature Physics 12, 92 (2016).

[2] Stan, et al. Phys. Rev. Mat. 3, 044003 (2019).

[3] W. Wan, et al., in preparation.

O 66.7 Wed 12:00 WIL B321

Incorporation of K and Cs into hBN/Ir(111) and hBN/Ru(0001) — •Jiaqi Cai[1,2,3], Caio Silva[2,3], Wouter Jolie[2], Thais Chagas[1], Kai Mehlich[1], David Duncan[4], Christoph Schlueter[4], Tien-Lin Lee[4], and Carsten Busse[1,2,3] — [1]Department Physik, Universität Siegen, Walter-Flex-Str. 3, 57068 Siegen — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [3]Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [4]Diamond Light Source, Didcot OX11 0DE, Oxfordshire, United Kingdom

The bi-atomic unit cell of monolayer hexagonal boron nitride (hBN) makes its interaction with the substrate more complex in comparison with its famous cousin, graphene. To probe this interaction, we incorporate alkali metals into hBN/substrate systems. We choose alkali metals for two reasons: i) they tend to lose the electron in the out-most orbitals, thus introducing a strong electronic effect into the hBN/substrate system; ii) the alkali metal ions have full-shell structure, making them unlikely to chemically bond to hBN.

In this talk, we report our experimental results on K as well as Cs incorporation into epitaxial hBN on Ir(111) and Ru(0001). We rely on STM, LEED, XPS, and XSW for the determination of the atomic coordinates with high precision. We report a rich pool of structures (adsorption and/or intercalation of alkali metals), and find that the location of the alkali metal ions are determined by the hBN-substrate interaction strength, and the size of the alkali metal ions.

O 66.8 Wed 12:15 WIL B321

Control of interface alloying between silicene and a silver substrate — •Johannes Küchle[1], Aleksandr Baklanov[1], Felix Haag[1], David Duncan[2], Paul Ryan[2,3], Ari Seitsonen[4], Willi Auwärter[1], and Francesco Allegretti[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]Diamond Light Source, Didcot, UK — [3]Imperial College London, UK — [4]Département de Chimie, École Normale Supérieure, Paris, France

Silicene, the silicon analogue of graphene, is a promising material with unique structural and electronic properties, which has been the focus of intense research in the past decade. The epitaxial growth *via* deposition of silicon on solid substrates is an established strategy for silicene preparation, however, strong interfacial interactions may modify the functional properties of the resulting layer. On metal substrates, interfacial alloying may occur, but surprisingly, its role is often underestimated. Here, we present our recent experiments with soft X-ray photoelectron spectroscopy (SXPS) at various Si coverages, indicating that during the growth of the most commonly studied (4×4) superstructure of silicene on Ag(111) a Si-Ag surface alloy is formed. Our scanning tunneling microscopy studies resolve a yet unreported phase, which we relate to the Si-Ag alloy. Notably, we show that the alloy related component in SXPS can be largely suppressed by growing silicene on a GeAg$_2$ surface alloy on Ag(111). In this case, a number of distinct structures are observed by low-energy electron diffraction, which differ significantly from all previously reported superstructures of silicene.

O 66.9 Wed 12:30 WIL B321

Curvature-Induced Charge Baskets in Two-Dimensional Semiconducting Monolayers — •bong gyu shin[1], jz-yuan juo[1], soon jung jung[1], and klaus kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, DE-70569 Stuttgart, Germany — [2]Institut de Physique, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

The localized quantum states in two-dimensional (2D) materials are attractive for valley- and spin- related optoelectronics or other quantum applications. However, achieving these quantum states is still challenging due to technical difficulties. Here, we investigated strain-induced charge localization and quantum confinement in monolayer MoS$_2$ on a SiO$_2$/Si substrate using a gate-tunable home-built scanning tunneling microscope at $\sim$4.9K. Monolayer MoS$_2$ follows surface roughness of the substrate, which exhibits a bending strain with band gap reduction. This band gap reduction at a local regime acts like a potential well leading to charge localization. When the bending strain in MoS$_2$ is larger than 2% at a local region of $\sim$4 nm, quantum-confined energy levels are observed near the conduction or valence band edge due to the significant band gap reduction of $\sim$1 eV. Moreover, our theoretical results show that spatial flattening of the conduction (valence) band edge occurs by heavy electron- (hole-) doping of over $\sim 10^{13}$ cm^{-2}. The strain-induced quantum confinement in 2D materials can play an important role in the future development of quantum devices.

O 66.10 Wed 12:45 WIL B321

Long-range charge order induced by strain in layered IrTe$_2$ revealed by ARPES — •Chris W. Nicholson[1], Maxime Rumo[1], Geoffroy Kremer[1], Thomas Jaouen[1], Baptiste Hildebrand[1], Marie-Laure Mottas[1], Björn Salzmann[1], Aki Pulkinnen[2], Bernardo Barbiellini[2], Timur Kim[3], Saumya Mukherjee[3], Cephise Cacho[3], Matthias Muntwiler[4], Fabian von Rohr[5], Philipp Aebi[1], and Claude Monney[1] — [1]University of Fribourg, Switzerland — [2]LUT University, Finland — [3]Diamond Light Source, UK — [4]Swiss Light Source, Switzerland — [5]University of Zurich, Switzerland

Uniaxial strain combined with ARPES offers a relatively new route to studying the interplay between the lattice and electronic structure. The wide range of properties displayed by layered transition metal dichalcogenides makes them intriguing candidates for exploring this.

Here we present ARPES data revealing the influence of tensile strain on the electronic structure of IrTe$_2$, which exhibits a complicated mixture of one dimensional charge ordered phases at low temperatures but very broad electronic bands [1]. The application of strain induces a single, long-range ordered phase, with clear quasi-1D features at the Fermi level and sharp bands over a wide binding energy range. By comparison with electronic structure calculations, we will discuss the mechanism of this strain-induced stabilization with reference to the redistribution of charge between Ir and Te bonds [2].

[1] Ko et al, Nat. Comm 6, 7342 (2015)

[2] Nicholson et al, in preparation

O 66.11 Wed 13:00 WIL B321

Seeking 2D Ferromagnets among TMD materials — •Paul Dreher[1,2], Wen Wan[1,2], Adolfo O. Fumega[5], Md N. Huda[4], Shawulienu Kezilebieke[4], Santiago Blanco[2,3], Victor Prado[5], Hannu-Pekka Komsa[4], Marco Gobbi[2,3], Peter Liljeroth[4], and Miguel M. Ugeda[1,2] — [1]Donostia International Physics Center, San Sebastián, Spain — [2]Centro de Física de Materiales, San Sebastián, Spain — [3]CIC nanoGUNE, San Sebastián, Spain — [4]Department of Applied Physics, Aalto University School of Science, 00076 Aalto, Finland — [5]Departamento de Física Aplicada, Universidade de Santiago de Compostela, Campus Sur s/n, E-15782 Santiago de Compostela,Spain

We study the magnetic character of various monolayer TMD candidates (VSe2, CrSe2) grown by MBE on different substrates (NbSe2, graphene, graphite) by combining various characterization techniques. Our findings reveal that the substrate plays a crucial role on the magnetic order in the grown TMD monolayer. The CDW order in single-layer VSe2 causes a strong reduction in the DOS at EF incompatible with ferromagnetism. When grown on graphene substrates, the CDW persists VSe2 and it becomes paramagnetic [1]. Instead, the electronic structure of single-layer VSe2 on a superconducting substrate (NbSe2) shows features compatible with magnetism [2]. Finally, XMCD measurements on Cr-based TMD monolayers indicate the presence of an uncompensated spin in Cr, which retains a paramagnetic behavior even at low temperatures. [1] J.Phys.Chem.C, 123, 27802 (2019), [2] ArXiv:1909.10208 (2019).

O 66.12 Wed 13:15 WIL B321

Signatures of strong coupling between WS$_2$ excitons and surface plasmon polariton waves — Moritz Gittinger[1], Sven Stephan[1], Trung Nguyen[1], Antonietta deSio[1], •Martin Silies[1], Christoph Lienau[1], Alison Cadore[2], Ilya Goykhman[2], and Andrea Ferrari[2] — [1]Institute of Physics and Center of Interface Science, Carl von Ossietzky Universität Oldenburg — [2]Cambridge Graphene Centre, University of Cambridge, UK

All-solid-state strong coupling systems with large vacuum Rabi splitting energies are of great potential in future technologies such as quantum information processing. Here, atomically thin layers of transition metal dichalcogenides in close vicinity to metallic nanoparticles have recently been explored as excellent candidates for the observation of this coherent energy transfer from the exciton to its localized surface plasmon counterpart [1]. We here present first results of the interaction between surface plasmon polariton (SPP) waves induced in focused-ion beam written gratings in planar silver films with excitons from atomically-thin WS$_2$ flakes. By using confocal angle-resolved reflectance spectroscopy, the dispersion relation of the coupled system is mapped at room temperature. We observe a clear anti-crossing of the exciton and the SPP resonance with a normal mode splitting of up to 50meV. We take this splitting as a first signature for a strong coupling between the WS$_2$ exciton and the SPP wave in the silver grating [2].

[1] Schneider C. et al, Nature Comm. 9, 2695 (2018) [2] Vasa P, and C. Lienau, ACS Photonics 5, 2-23 (2018)

O 66.13 Wed 13:30 WIL B321

Substrate-dependent charge transfer mechanisms between monolayer MoS2 and molecular dopants — •Patrick Amsalem[1], Soohyung Park[1,2], Thorsten Schultz[1,3], Xiaomin Xu[1], Berthold Wegner[1,3], Areej Aljarb[4], Ali Han[4], Lain-Jong Li[4,5], Vincent C . Tung[4,6], and Norbert Koch[1,3] — [1]Humboldt-Universität zu Berlin, Institut für Physik & IRIS Adlershof, Berlin, Germany — [2]Korea Institute of Science and Technology (KIST), Seoul, South Korea — [3]Helmholtz-Zentrum für Materialien und Energie GmbH, Berlin, Germany — [4]King Abdullah University of Science and Technology, Thuwal, Saudi Arabia — [5]The University of New South Wales, Sydney, Australia — [6]Lawrence Berkeley National Lab, Berkeley, CA, USA

2D transition metal dichalcogenides monolayer films have recently gained enormous attention. Yet, to extend the range of applications of these emerging materials, tuning their Fermi level is of crucial importance. Here, we report on the adsorption of a strong p-type organic dopant, F6TCNNQ, as an efficient route for doping of MoS2 [1]. More specifically, we employ angle-resolved UV and X-ray photoelectron spectroscopy to reveal the charge transfer (CT) mechanisms taking place at a TMDC/organic interface as a function of the electrical properties of the employed supporting substrate, here sapphire, graphite and gold. The present findings can be exploited for the design of advanced hybrid heterostructures with tailored electronic properties. [1] S. Park et al., Communications Physics 2, 109 (2019).

O 67: Solid-Liquid Interfaces III: OER, ORR, CO2RR, etc.

Time: Wednesday 10:30–13:30 Location: WIL C107

Invited Talk O 67.1 Wed 10:30 WIL C107

The shiniest gold (111) surface — Weronica Linpe[1], Jonas Evertsson[1], Giuseppe Abbondanza[1], Alfred Larsson[1], Gary Harlow[1], Johan Zetterberg[2], Lisa Rämisch[2], Sebastian Pfaff[2], and •Edvin Lundgren[1] — [1]Division of Synchrotron Radiation Research, Lund University, Box 118, S-221 00, Sweden — [2]Division of Combustion Physics, Lund University, SE-22100 Lund, Sweden

We have studied in situ the development of the Au(111) surface during electrochemical Cyclic Voltammetry (CV) measurements using 2D Surface Optical Reflectance (SOR) and High Energy Surface X-Ray Diffraction (HESXRD) with high temporal resolution. We demonstrate that the famous Herring Bone (HB) reconstruction of Au(111) appears in HESXRD at voltages close to the hydrogen evolution reaction signature in the CV and is lifted close to the oxide formation signature. The 2D maximum SOR intensity is shown to coincide with the maximum of the HB intensity, demonstrating that the shiniest gold (111) surface is due to the presence of the HB. On the contrary, the crystal truncation rods exhibit a strong decrease in intensity in conjunction with the appearance of the HB reconstruction. The decrease in intensity of the CTRs can be attributed to the mixed fcc and hcp sites at the Au(111) surface in the HB structure.

O 67.2 Wed 11:00 WIL C107

ORR and OER on Ni-modified Co_3O_4(111) - a combined surface science and electrochemical model study for Zn-Air batteries — •Florian Buchner[1], Markus Eckardt[1,2], Timo Böhler[1], Jihyun Kim[1], Johannes Schnaidt[2], and R. Jürgen Behm[1,2] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, Helmholtzstr. 11, D-89081 Ulm, Germany

We report results of a combined surface science and electrochemistry study on the oxygen reduction and oxygen evolution reactions (ORR and OER) on structurally well-defined Ni-free and Ni-modified single crystalline Co_3O_4(111) thin films. These films, which serve as model for the air cathode in Zn-air batteries, were grown on a Ir(100)-(2x1)O surface under ultrahigh vacuum (UHV) conditions. Co_3O_4(111) and their Ni-modified derivatives were first characterized by X-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM) under UHV conditions. Post-deposition of Ni on a Co_3O_4(111) reveals a Ni^0 state in XPS, while simultaneous vapor deposition of Ni, Co and O_2 results in mixed metal oxides such as $Ni_xCo_{1-x}O$ or $Ni_xCo_{3-x}O_4$) (Ni^{2+} and Ni^{3+} states). STM images show extended flat island structures both for Co_3O_4(111) and mixed metal oxides, while post-deposited Ni forms clusters. The thin films revealed an up-shifted ORR onset for Co_3O_4 compared to pure Ni and Ir. Nickel doping improves the ORR current densities, while hardly influencing the ORR and OER onsets.

O 67.3 Wed 11:15 WIL C107

Ni-doped fe3o4(001) surface as simple model to understand oxygen evolution reaction — •Francesca Mirabella, Matthias Müllner, Florian Kraushofer, Michael Schmid, Gareth Parkinson, and Ulrike Diebold — Technische Universität Wien, Vienna, Austria

Electrochemical water splitting is an environmentally friendly technology to convert renewable energy into h2-fuels. Among the Earth-abundant first-row transition metal- based catalysts, mixed ni-fe oxides have shown promising performance for effective and low-cost catalysis of the oxygen evolution reaction (OER) in alkaline media. However, the synergistic role of fe and ni cations on the OER mechanism is yet unclear. The goal of this study is to develop a well-defined model system for understanding the OER and establishing the structure-reactivity relation on mixed fe/ni oxides. Reconstructed fe3o4(001) provides well-defined sites for the adsorption or incorporation of various metal atoms including ni. We combine UHV surface science techniques (LEED, XPS, ISS, STM) with exposure to ultrapure liquid water as well as cyclic voltammetry (CV) on UHV-prepared surfaces in alkaline media. When adding ni, we observed a significant improvement in the OER activity compared to the clean fe3o4 (001). An optimum fe:ni ratio of 1:9 is found, in good agreement with what was observed in powder catalysts. This observation makes our model system well suited to study the OER in alkaline media and gain further insight based on the high level of control of the surface and near-surface region, robustness and simplicity.

O 67.4 Wed 11:30 WIL C107

Stable and cost-efficient core-shell catalysts for the electrochemical oxygen evolution reaction–a first-principles approach — •Yonghyuk Lee, Christoph Scheurer, and Karsten Reuter — Technical University Munich, Germany

Most commercial oxygen evolution reaction (OER) catalysts in proton exchange membrane electrolyzers contain expensive IrO_2 due to its high catalytic activity and favorable stability in acidic electrolytes. Layer-coated IrO_2 on rutile TiO_2 has typically been utilized in order to reduce the price without sacrificing activity. However, thin IrO_2 films are not thermally stable on titania and a gradual dewetting of the film takes place.

In the present work, we use density-functional theory (DFT) calculations to explore alternative core-shell systems. We assess IrO_2 or RuO_2 thin films on lattice-matched rutile oxides as potentially highly active, relatively inexpensive, and long-term stable catalyst materials for water electrolysis. We calculate interface energy, interface formation energy, and the work of adhesion to quantify the stability of the oxide interfaces and compare to the dewetting behavior of IrO_2(110) films on TiO_2(110). *Ab initio* thermodynamics and the computational hydrogen electrode model are employed to determine relative stabilities of the core-shell systems compared to pure rutile catalysts at OER operating conditions [1]. Finally, we present thermodynamic reaction barriers for potential anodic OER pathways at surfaces of these core-shell materials and discuss design strategies for next-generation electrocatalysts. [1] D. Opalka *et al.*, ACS Catal. 9, 4944 (2019).

O 67.5 Wed 11:45 WIL C107

Effect of electric field on oxygen reduction kinetics at the Pt(111), Au(111) and Au(100) electrodes — •Sara Kelly[1], Charlotte Kirk[1], Karen Chan[2], and Jens Nørskov[2] — [1]SUNCAT Center for Interface Science and Catalysis, Department of Chemical Engineering, Stanford University, Stanford, California 94305, United States — [2]Department of Physics, Technical University of Denmark, Building 311, DK-2800 Lyngby, Denmark

Microkinetic modeling of the oxygen reduction reaction (ORR) has thus far failed to predict dependence of this reaction on pH on several important catalysts. In this work, we create a new microkinetic model for the ORR which incorporates field effects into the established computational hydrogen electrode (CHE) model. We find that field can significantly alter the binding energy of the $^*O_2$, $^*OOH$, and $^*H_2O_2$ adsorbates. By considering these effects, we find that we can accurately reproduce experimental polarization curves and rotating ring disk electrode (RRDE) currents on Pt(111), Au(111), and Au(100) electrodes, allowing us to predict both overall ORR activity and selectivity toward hydrogen peroxide. We then use these predictions to better understand activity and selectivity of ORR catalysts and how each of these depends on pH. We show that hydrogen peroxide selectivity depends mainly on the binding energy of $^*H_2O_2$ relative to that of $^*OOH$. Finally, we argue that considering field effects can expand the search for improved ORR catalysts by allowing us to deconvolute the activity dependence of catalysts on the standard hydrogen electrode (SHE) and the reversible hydrogen electrode (RHE).

O 67.6 Wed 12:00 WIL C107

DFT+U investigation of the OER activity at $LaCoO_3$(001) and (110) surfaces — •Achim Füngerlings, Hamidreza Hajiyani, and Rossitza Pentcheva — Department of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg

Using density functional theory calculations including an on-site Hubbard term we explore the oxygen evolution reaction at $LaCoO_3$ surfaces with different crystallographic orientations. For Co- and La-rich synthesis conditions respectively, the surface phase diagram is dominated by the (001) CoO_2- and LaO- termination over a wide range of oxygen partial pressures. The OER overpotential calculated from the binding energies of the adsorbed intermediates for a Co-reaction site at the

CoO_2-terminated (001) surface is 0.70V. To gain more insight, we analyze the changes of electronic structure during the reaction. Thereby, the cobalt's oxidation state, which is 3+ in the bulk structure and 2+ at the clean surface, becomes 3+ for an adsorbed OH-group and 4+ for the O intermediate. We furthermore explore the effect of A- and B-site substitution on the catalytic activity.

Support by the DFG within the CRC TRR 247, project B4, and a computational grant at the Leibniz-Rechenzentrum are gratefully acknowledged.

O 67.7 Wed 12:15 WIL C107

Improvement of OER performance by Fe and Ni doping at the Co_3O_4(001) surface — •Yuman Peng, Hamidreza Hajiyani, and Rossitza Pentcheva — Department of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg

Using density functional theory (DFT)+U method, we study the oxygen evolution reaction (OER) at the Co_3O_4(001) surface. The stability of different surface terminations as a function of oxygen partial pressure, as well as of pH and applied voltage (Pourbaix diagram) were investigated. The termination with octahedral Co and O ions is found to have the lowest overpotential of 0.46 V for an octahedral Co reaction site. Furthermore, we systematically investigated the effect of Fe and Ni doping on the overpotential. Our results indicate that Ni doping at octahedral site in the surface layer reduces the overpotential from 0.46 to 0.36 V and Fe doping at octahedral site at the tetrahedral Co termination reduces the overpotential from 0.63 to 0.37 V, with the octahedral Co site being the active site. The scaling relationship of ΔG_{*OOH} and ΔG_{*OH} binding energies is overall reproduced, the Ni-doped system lying close to the top of the volcano of the overpotentials versus (ΔG_{*O}-ΔG_{*OH}). Further insight was gained into the oxidation states of surface ions and in particular the Co active site during OER, by analyzing the magnetic and electronic properties. Support by the DFG, CRC TRR247, IMPRS-Surmat and a computational grant at the magnitUDE of the Center of Computer Science and Simulation are gratefully acknowledged.

O 67.8 Wed 12:30 WIL C107

Oxygen reduction by doped graphene in Li-air batteries — •Elmar Kataev[1], Daniil Itkis[2], Alina Belova[2], Carlos Escudero[3], Virginia Pérez-Dieste[3], Axel Knop-Gericke[4], and Lada Yashina[2] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Department of Chemistry, Moscow State University, Moscow, Russia — [3]ALBA Synchrotron Light Source , Barcelona, Spain — [4]Fritz-Haber Institute of the Max Planck Society, Berlin, Germany

Oxygen reduction reaction (ORR) plays a key role in lithium-air batteries (LABs) that attract great attention thanks to their high theoretical specific energy. Because of high surface area and electric conductivity, various carbons are often materials of choice for applications as the LAB cathode. Unfortunately, the practical applications of LAB batteries are impeded by poor rechargeability, associated with ORR side reactions. Recently it was shown that doping of carbon materials could change its catalytic activity and potentially reduce reactivity towards ORR products. However, the mechanisms of doped-carbon reactivity in LAB are still unclear. Here we report a direct photoemission study of ORR pathway on pure, nitrogen-, boron- and oxygen-doped graphene. We designed the electrochemical cell with two-layer graphene transferred on glass-ceramics electrolyte to avoid side reactions of ORR products with liquid electrolyte. Combining operando photoemission data with in situ observation of superoxide anion attack on graphene in model chemical systems, we reveal the impact of impurities in carbon on its reactivity in ORR.

O 67.9 Wed 12:45 WIL C107

Electroreduction of water on Mo_2C film electrodes affected by the presence of CO_2 — •Eva-Maria Wernig, Christoph Griesser, Daniel Winkler, Niusha Shakibi Nia, and Julia Kunze-Liebhäuser — Institute of Physical Chemistry, University of Innsbruck, 6020 Innsbruck, Austria

The materials class of transition metal carbides (TMCs) has gained importance among electrocatalysts for reduction processes such as the hydrogen evolution reaction (HER) and the CO_2 reduction reaction (CO_2RR). For a comprehensive understanding of the electrocatalytic properties of Mo_2C towards the HER under CO2RR conditions in aqueous electrolytes, the present study merges materials science and interface analytics with electrochemistry. We report on the synthesis of Mo_2C films using direct carburization of polycrystalline Mo substrates through carbothermal conversion. Cyclic voltammetry, complemented by rotating ring disc electrode (RRDE) measurements, was used to investigate the electrocatalytic activity of Mo_2C films towards the HER in the absence and presence of CO_2, while changes of the chemical composition at the surface were analyzed with ex-situ emersion X-ray photoelectron spectroscopy (XPS). In-situ infrared spectroscopy (SNIFTIRS) enabled the determination of reaction intermediates at the solid/liquid interface. Product analysis was accomplished with differential electrochemical mass spectrometry (DEMS) to monitor the formation of gaseous products such as hydrogen. The activity of Mo_2C film electrodes towards the HER was found to be significantly enhanced in the presence of CO_2.

O 67.10 Wed 13:00 WIL C107

In Operando Spectroscopy of CO_2 Reduction Reactions at Pt/Ionic Liquid Interfaces — •Andre Kemna, Björn Ratschmeier, and Björn Braunschweig — Institute of Physical Chemistry, WWU Münster, 48149 Münster, Germany

CO_2 reduction reactions (CO_2RR) at Pt(poly)/[BMIM][BF_4] interfaces were studied with cyclic voltammetry and in operando with IR absorption (IRAS) as well as sum frequency generation (SFG) spectroscopy to get mechanistic insights into CO_2RR. IRAS revealed a vibrational band centered at 1670 cm^{-1} at an onset potential of -0.65V vs SHE. We attribute the latter to the carbonyl stretching mode of an imidazolium carboxylic acid, which is generated via a carbene intermediate, for which we also present spectroscopic evidence. Via SFG spectroscopy we demonstrates that CO is formed in addition to [BMIM]-COOH on the Pt catalyst surface, at an onset potentials of -1.05 V. We therefore assume that the [BMIM]-COOH species is one reactive intermediate that results in low overpotentials for CO_2RRs. The [BMIM]-COOH species can be further catalyzed to formic acid during an anodic potential sweep. At an electrode potential of 1.6 V, a vibrational band at 1750 cm^{-1} arises in the IR spectra and is accompanied by a decrease of the imidazolium carboxylate band. We tentatively assign the former vibrational modes to C=O vibrations of formic acid. This indicates that electrocatalysis of CO_2 to formic acid may be possible in a two-step reaction process.

A. Kemna, N. García Rey, B. Braunschweig, *ACS Catal.* **2019**, *9*, *7*, 6284-6292.

O 67.11 Wed 13:15 WIL C107

A refined view on broken scaling relations for electrochemical CO_2 reduction on transition metal carbides — •Haobo Li and Karsten Reuter — Chair for Theoretical Chemistry, TU Munich, Germany

The electrochemical reduction of CO_2 (CO2RR) is a promising approach to generate chemical energy carriers from renewable electricity. Transition metal carbides (TMCs) are a promising non-noble material class to catalyze this reaction, with e.g. Mo_2C recently reported to convert CO_2 into CH_4 at low overpotentials [1]. Here, we further assess the proposition that this performance results from a break of scaling relations known to limit CO2RR on transition metals (TMs) and their alloys [2]. Using density-functional theory, we systematically compute the adsorption energies of key reaction intermediates at multiple adsorption sites offered at low-index surfaces of molybdenum carbides of varying stoichiometry. The obtained data base provides a refined view, with certain scaling relations indeed broken, but others maintained. We can rationalize these findings by the simultaneous presence of metal and carbon active sites at the surface of TMC catalysts and the concomitant stabilization of varying adsorption modes. With this understanding we revisit mechanistic CO2RR models established for TMs and explore routes to optimize CO2RR for TMCs.

[1] S.K. Kim *et al.*, ACS Catal. 6, 2003 (2016).

[2] R. Michalsky *et al.*, J. Phys. Chem. C 118, 13026 (2014).

O 68: PhD Focus Session: Symposium on "Magnetism – A Potential Platform for Big Data?" (joint session MA/AKjDPG/O)

As the title of a recent nature editorial article "Big data needs a hardware revolution" points out, new technologies and hardware architectures are necessary in order to cope with the ever increasing amount of information. Google's AlphaGo's success apprised of the potential of parallel computing, yet energy efficiency is a major challenge. Hardware developers came up with mimicking the human brain as the most efficient processor, leading to the field of neuromorphic computing. An immense amount of research is deployed in different fields to screen for fast, low energy consuming and scalable solutions. This focus session is meant to give insight into the current state-of-the-art computing together with its challenges as an introduction. Two major approaches to implement new computation technologies using magnetism, namely, neuromorphic computing based on spintronics, and wave-based computing using magnonics will be presented. A fourth talk, covering the prevailing use of magnetic tape for Big Data storage will give insight into the magnetic backbone of the largest information repositories.

Organizers: Mauricio Bejarano and Tobias Hula (Helmholtz-Zentrum Dresden Rossendorf), Luis Flacke and Lukas Liensberger (Walther-Meissner Institute and TU Munich)

Time: Wednesday 15:00–17:15 Location: HSZ 04

Invited Talk O 68.1 Wed 15:00 HSZ 04
Data Storage and Processing in the Cognitive Era — •Giovanni Cherubini — IBM Research - Zurich

In this talk, I will present the emerging vision of cognitive data systems. A data system comprises physical devices that provide means to acquire, store and modify data for analytics and communications tasks, with the goal of obtaining high-value information. With the need to deal with exponentially growing amounts of data, however, the system size and complexity present major challenges for data storage and processing. In addition, with the approaching end of Moore's law, there is a dire need to significantly improve the efficiency of data systems in terms of cost and energy. To address these challenges, cognitive data systems will require novel learning algorithms and computing paradigms. The talk will be divided into two parts, focusing on data storage and processing aspects. First, I will present advanced technologies for big data storage systems, with focus on magnetic tape drives of future generations, targeting areal densities of several hundred gigabits per square inch on a flexible medium. Next, I will introduce in-memory computing techniques and devices that are well suited for novel computing systems, which are based on non-von Neumann architectures and aim at achieving the efficiency of the human brain.

Invited Talk O 68.2 Wed 15:30 HSZ 04
Brain-inspired approaches and ultrafast magnetism for Green ICT — •Theo Rasing — Radboud University, Institute for Molecules and Materials, Heijendaalseweg 135, 6525AJ Nijmegen, the Netherlands

The explosive growth of digital data use and storage has led to an enormous rise in global energy consumption of Information and Communication Technology (ICT), which already stands at 7% of the world electricity consumption. New ICT technologies, such as Artificial Intelligence push this exponentially increasing energy requirement even more, though the underlying hardware paradigm is utterly inefficient: tasks like pattern recognition can be performed by the human brain with only 20W, while conventional (super)computers require 10 MW. Therefore, the development of radically new physical principles that combine energy-efficiency with high speeds and high densities is crucial for a sustainable future. One of those is the use of non-thermodynamic routes that promises orders of magnitude faster and more energy efficient manipulation of bits. Another one is neuromorphic computing, that is inspired by the notion that our brain uses a million times less energy than a supercomputer while, at least for some tasks, it even outperforms the latter. In this talk, I will discuss the state of the art in ultrafast manipulation of magnetic bits and present some first results to implement brain-inspired computing concepts in magnetic materials that operate close to these ultimate limits.

15 min. break.

Invited Talk O 68.3 Wed 16:15 HSZ 04
How good are spin waves for data processing? — •Andrii Chumak — Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria — Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany

Over the last decade, spin waves and their quanta magnons attract attention as data carriers in novel types of data processing units instead of electrons. Among the advantages proposed by spin waves, one can name added value given by the phase of the wave, pronounced nonlinear phenomena, scalability down to nm sizes, GHz to THz frequency range as well as low-loss information transport [1].

Recently, significant progress in the miniaturization of magnonic elements down to 50 nm took place [2, 3]. Moreover, a spin-wave directional coupler was investigated numerically [4] and realized experimentally on the nano-scale [5]. This is a universal unit allowing for the processing of analog RF and binary-coded digital information and is suitable for novel unconventional computing. E.g., the first integrated magnonic circuit in the form of half-adder was studied numerically [6].

Finally, now we are able to determine the parameters of future magnonic devices. The benchmarking of magnonic circuits with respect to 7 nm CMOS will be presented in the talk.

[1] A.V. Chumak, et al., Nat. Phys. 11, 453 (2015). [2] Q. Wang, B. Heinz, et al., Phys. Rev. Lett. 122, 247202 (2019). [3] B. Heinz, et al., arXiv: 1910.08801 (2019). [4] Q. Wang, P. Pirro, et al., Sci. Adv. 4, e1701517 (2018). [5] Q. Wang, M. Kewenig, et al., arXiv: 1902.02855 (2019). [6] Q. Wang, R. Verba, et al., arXiv: 1905.12353 (2019).

Invited Talk O 68.4 Wed 16:45 HSZ 04
Unconventional computing with stochastic magnetic tunnel junctions — •Alice Mizrahi[1,2,3,4], Tifenn Hirtzlin[2], Matthew Daniels[3,4], Nicolas Locatelli[2], Akio Fukushima[5], Hit Kubota[5], Shinsi Yuasa[5], MD Stiles[4], Julie Grollier[1], and Damien Querlioz[2] — [1]Unité Mixte de Physique CNRS, Thales, Univ. Paris-Sud, Université Paris-Saclay, 91767 Palaiseau, France — [2]Centre de Nanosciences et de Nanotechnologies, Univ. Paris-Sud, CNRS, Université Paris-Saclay, 91405, Orsay, France — [3]Maryland NanoCenter, University of Maryland, College Park, Maryland 20742, USA — [4]National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA — [5]Spintronics Research Center, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, 305-8568, Japan

Magnetic tunnel junctions are bi-stable nanodevices which magnetic state can be both read and written electrically. Their high endurance, reliability and CMOS-compatibility have made them flagship devices for novel forms of computing. While they are mostly used as non-volatile binary memories, they can be made unstable and thus behave as stochastic oscillators. Here, we show how stochastic magnetic tunnel junctions are promising elements for low energy implementations of unconventional computing. An analogy can be drawn between stochastic magnetic tunnel junctions and stochastic spiking neurons. We apply neuroscience computing paradigm to these devices and demonstrate that they can be the building blocks of low energy artificial neural networks capable of on-chip learning.

O 69: Tribology: Surfaces and Nanostructures (joint session O/CPP)

Time: Wednesday 15:00–16:00 Location: GER 37

O 69.1 Wed 15:00 GER 37

Effect of Environment on Microstructure Evolution and Frictional Behavior of Au-Ni Multilayers — •Ebru Cihan[1,2], Heike Störmer[3], Katherine Jungjohann[4], Nicolas Argibay[5], Michael Chandross[5], and Martin Dienwiebel[1,6] — [1]Institute for Applied Materials - Computational Materials Science (IAM-CMS), Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Institute of Applied Physics, Justus-Liebig University Giessen, 35392 Giessen, Germany — [3]Laboratory for Electron Microscopy (LEM), Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [4]Center for Integrated Nanotechnologies (CINT), Sandia National Laboratories, 87185 Albuquerque, NM, USA — [5]Material, Physical, and Chemical Sciences Center, Sandia National Laboratories, 87185 Albuquerque, NM, USA — [6]Fraunhofer Institute for Mechanics of Materials (IWM), MicroTribology Center μTC, 79108 Freiburg, Germany

We present results from a systematic investigation of environmental effects on microstructure and frictional behavior of Au-Ni multilayer films of varying interlayer spacing. Multilayer samples were initially analyzed under UHV and it was demonstrated that the interlayer spacing has a strong impact on friction due to the transition in the dominant deformation mechanism near the surface. A newly shear-induced phase, which can be interpreted as an AuNi alloy (60-65 at% Ni in Au) was observed in the tribolayer for thinner samples. Subsequently, experiments were performed in dry-nitrogen and higher friction forces were measured, leading to different microstructure evolution.

O 69.2 Wed 15:15 GER 37

Tuning the friction properties of reconstructed KBr on Ir(111) by intercalating a monolayer of graphene — Zhao Liu[1], Antoine Hinaut[1], Thilo Glatzel[1], Sebastian Scherb[1], Junyan Zhang[2], and •Ernst Meyer[1] — [1]Department of Physics, University of Basel, 4056 Basel, Switzerland — [2]State Key Laboratory of Solid Lubrication, Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, 730000 Lanzhou, People's Republic of China

The intercalation of graphene and other 2D materials is an effective approach to alter the structures and properties of the top conductive or insulated layers on metal surface [1]. In this work, the growth of KBr islands on Ir(111) is characterized via non-contact atomic force microscopy and friction force microscopy measurement at room temperature in ultrahigh vacuum. We observed the formation of KBr monolayer with highly corrugated superstructure. These superstructures are due to the adaptation of the KBr atoms to the substrate lattice resulting from a tiny misfit of the KBr islands lattice. The superstructure presents a higher friction force of KBr/Ir(111) compared to the bulk KBr(001) as well [2]. We also show the possibility to tune the friction properties of KBr by intercalating a graphene monolayer. Obviously, the reduced friction force is accompanied by the vanishing of the KBr superstructure, with the observation of the common cubic configuration. It gives another view to increase the critical normal load to maintain the superlubric state at the nano scale.

[1] M. Andersen, et al, Phys. Rev. B, 90 (2014) 155428. [2] C. Wieferink, et al, Phys. Rev. B, 83 (2011) 235328.

O 69.3 Wed 15:30 GER 37

Stick-slip and surface rippling in plastic and abrasive wear on the nanoscale — •Enrico Gnecco[1], Jana Hennig[1], and Juan Mazo[2] — [1]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Jena, Germany — [2]Department of Condensed Matter Physics, University of Zaragoza, Zaragoza, Spain

The formation of regular surface structures as a result of plastic and abrasive wear processes is a general but scarcely understood phenomenon. Here we will discuss this topic with the examples of polymer [1] and silica glass surfaces [2] scratched by silicon and diamond nano- and microtips respectively. In spite of the different nature of the nanoscopic wear mechanisms, quasi-periodic ripple patterns are formed in both cases. The physical interpretation of the observed structures relies on the time evolution of the friction forces acting in the stick-slip motion of the tip, which is simultaneously indented and elastically pulled along the surfaces in order to scratch them. The geometric shapes of the surface structures as well as their dependence on the scan velocity are consequently reproduced by solving the corresponding equations of motion of the tips in an evolving energy landscape.

[1] J.J. Mazo et al., Phys. Rev. Lett. 122 (2019) 256101 [2] E. Gnecco et al., Phys. Rev. Materials 2 (2018) 115601

O 69.4 Wed 15:45 GER 37

Temperature Scaling of Contact Aging Rates on Amorphous Silica Surfaces — Matthias Vorholzer[1], J. Guilherme Vilhena[2], Ruben Perez[3], Enrico Gnecco[4], •Dirk Dietzel[1], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig-Universität Giessen, 35392 Giessen, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [4]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, 07742 Jena, Germany

Contact ageing is a fundamental aspect to understand dynamic sliding scenarios with alternating phases of halting and sliding. On the nanoscale, recent experiments showed, that ageing effects can be connected to the formation of interfacial bonds. In this work, we now analyze the temperature dependent bond formation dynamics of silica contacts by measuring the pre-rupture contact stiffness. Using this parameter instead of the seemingly more obvious choice of measuring static friction, we can eliminate all effects related to temperature dependent contact rupture. Our results show logarithmic contact ageing at all temperatures and reveal that the ageing can be described by a temperature dependent slope $\alpha(T) \propto T$, which is a characteristic fingerprint of thermal activation, anticipated both by analytical calculations and MD-simulation of the bond formation process.

O 70: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions IV (joint session O/CPP/DS/HL)

Time: Wednesday 15:00–17:30 Location: GER 38

Invited Talk O 70.1 Wed 15:00 GER 38

Electron-phonon interactions in realistic materials — •Fabio Caruso — Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Functional materials used in actual devices are typically doped, they operate at finite temperature, and they may be subject to perturbations such as, *e.g.*, external fields and light pulses. These aspects may alter profoundly the electron-phonon interaction (EPI), its influence on the electronic properties of solids, and even lead to the manifestation of novel emergent phenomena absent in perfect crystals.

We conducted a first-principles investigation of the EPI in functional materials at realistic operational conditions based on many-body perturbation theory. Our work reveals that: (i) n-type doping of polar oxides, such as EuO and TiO_2, allows one to trigger and control the formation of polarons (electrons dressed by a phonon cloud) [1]; (ii) in the record-breaking thermoelectric material SnSe, temperature may lead to a five-fold suppression of carrier lifetimes due to enhanced phonon emission [2]. Overall, the striking sensitivity to doping, temperature, and external fields, makes the EPI a powerful tool to tailor the opto-electronic properties of quantum materials. Possible strategies to extend the many-body theory of the EPI to the study of time-dependent phenomena will further be discussed [3].

[1] J. Riley, F. Caruso, C. Verdi, *et al.*, Nature Commun. **9** (1), 2305 (2018). [2] F. Caruso, M. Troppenz, S. Rigamonti, C. Draxl, Phys. Rev. B **99** (8), 081104 (2019). [3] F. Caruso, D. Novko, C. Draxl, arXiv:1909.06549v (2019).

O 70.2 Wed 15:30 GER 38

Fully Anharmonic, Non-Perturbative First-Principles Theory of Electronic-Vibrational Coupling in Solids — Marios Zacharias, Matthias Scheffler, and •Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

The coupling between nuclear vibrations and the electronic structure plays a pivotal role for many material properties, including optical absorption and electronic transport. In this regard, however, today's state-of-the-art methodologies rely on two approximations [1]: the harmonic (phonon) approximation for the nuclear motion and the linear response description of the electronic structure with respect to harmonic displacements. In this work, we overcome ***both*** these approximations by performing fully anharmonic *ab initio* molecular dynamics (*ai*MD) calculations and by accounting for the non-perturbative, self-consistent response of the wave functions along the *ai*MD trajectory. By this means, we obtain fully anharmonic, vibronically renormalized spectral functions, from which macroscopic material properties like temperature-dependent band gaps and electronic transport coefficients are obtained. We validate our approach using silicon as an example, for which the traditional electron-phonon coupling formalism is recovered. Using cubic $SrTiO_3$ as example, we further demonstrate that anharmonic electronic-vibrational coupling effects are not captured in traditional formalisms, but they play a decisive role here and in other complex materials like perovskites.

[1] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).

O 70.3 Wed 15:45 GER 38

Thermal conductivity of highly-doped Si: Role of electron-phonon and point-defect phonon scattering — •Bonny Dongre[1], Jesús Carrete[1], Shihao Wen[2], Jinlong Ma[2], Wu Li[2], Natalio Mingo[3], and Georg KH Madsen[1] — [1]Institute of Materials Chemistry, TU Wien, A-1060 Vienna, Austria. — [2]Institute for Advanced Study, Shenzhen University, Shenzhen 518060, China — [3]LITEN, CEA-Grenoble, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France.

Theoretical investigation of the thermal conductivity reduction in highly-doped Si is an area of active research. Recently, first-principles electron-phonon scattering was found to produce a significant reduction in the thermal conductivity of highly-doped Si. However, the study could not reproduce the experimental results.

In the present work, we calculate the first-principles phonon scattering rates by electrons and point defects, and use them to calculate the thermal conductivity of highly-P- and B-doped Si for a range of temperatures and concentrations. We find that the phonon scattering by electrons dominates at carrier concentrations below 10^{19} cm^{-3} and is enough to reproduce the experimental thermal conductivity reduction at all temperatures. However, at higher defect concentrations point-defect phonon scattering contributes substantially to the thermal conductivity reduction even at room temperature. With a combined treatment of the phonon scattering by electrons as well as phonons, an excellent agreement is obtained with the experimental values at all temperatures.

O 70.4 Wed 16:00 GER 38

Precise yet Fast High-Throughput Search for Thermal Insulators — •Florian Knoop, Thomas A.R. Purcell, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft

We present a systematic and numerically precise computational search for thermal insulators in material space performed with the *FHI-vibes* high-throughput framework [1]. *FHI-vibes* employs a robust metric that quantifies the degree of anharmonicity in the nuclear dynamics via the statistical comparison of first-principles forces with those forces that would act in the harmonic approximation. This enables us to efficiently scan over many materials, including complex oxides and chalcogenides as well as ternary structures like perovskites. By this means, we single out strongly anharmonic systems, for which we perform *ab initio* Green-Kubo simulations to assess their thermal conductivities, thereby naturally including all anharmonic effects [2]. Our strategy allows to avoid redundant calculations and to achieve a much higher quality of information than traditional high-thoughput studies. Besides validating the performed search and analyzing its results, we discuss how big-data analytics techniques can be utilized to further accelerate and guide this search.

[1] https://vibes.fhi-berlin.mpg.de

[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017)

O 70.5 Wed 16:15 GER 38

Ambivalent Impact of Electron-Phonon Interaction on Electronic and Transport Properties of Organic Semiconductors — •Frank Ortmann — Center for Advancing Electronics Dresden, Technische Universität Dresden, Germany

Vibrations are omnipresent in molecules and of great importance in Organic Semiconductors due to the softness of the materials and the strong electron-phonon coupling. One possibility to investigate this interaction is to study the low-energy edge of optical absorption spectra, which lacks an in-depth understanding for organic materials. We have recently observed a strong dependence of low-energy excitonic features on the molecular building blocks in organic films, which we associated to molecular flexibility and polaron deformation. We will discuss implications of low-frequency molecular vibrations on the polaronic and excitonic density of states in donor-acceptor mixtures featuring charge-transfer excitons. We will also discuss how a distinguished treatment of strong-coupling molecular vibrations of different energies leads to an improved description of charge carrier transport in organic materials.

O 70.6 Wed 16:30 GER 38

Quantum Nuclear Effects in Thermal Transport of Semiconductors and Insulators — •Hagen-Henrik Kowalski[1], Mariana Rossi[1,2], Matthias Scheffler[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]MPI for Structure and Dynamics of Matter, Hamburg, Germany

To date, the computation of thermal conductivities relies on either perturbation theory or (*ab initio*) molecular dynamics (MD) [1]. While perturbative approaches include quantum-nuclear effects (QNE), they typically neglect higher orders of anharmonicity. Conversely, classical MD includes all orders of anharmonicity, but neglects QNEs. To overcome these limitations, we have developed a formalism that accounts for ***both*** quantum-nuclear effects and all orders of anharmonicity. For this purpose, the nuclear dynamics are assessed via Thermostatted Ring Polymer MD (TRPMD) [2] and the thermal conductivity is obtained via the Green-Kubo formalism using a newly proposed TRPMD based heat-flux estimator. Using solid Argon and Silicon as model systems, we discuss the influence of QNEs on thermal transport by comparing velocity, energy, and heat-flux autocorrelation spectra. This allows to rationalize the impact of QNEs on vibrational frequencies, lifetimes, and on the thermal conductivity in different temperature regimes.

[1] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901, (2017).

[2] M. Rossi, M. Ceriotti, D. Manolopoulos, *J. Chem. Phys.* **140**, 234116 (2014).

O 70.7 Wed 16:45 GER 38

Speeding-up *ab initio* molecular dynamics with hybrid functionals using adaptively compressed exchange operator based multiple time stepping — •Sagarmoy Mandal and Nisanth N. Nair — Department of Chemistry, Indian Institute of Technology Kanpur, India

Ab initio molecular dynamics (AIMD) with hybrid density functionals and a plane wave basis is known to predict the structural and dynamical properties of condensed matter systems accurately. However, such hybrid functional based AIMD simulations are not routinely used due to the high computational cost associated with the application of the Hartree-Fock exchange operator. We propose a strategy [1] to combine the Adaptively Compressed Exchange (ACE) operator formulation [2] and a multiple time step integration scheme to reduce the computational cost significantly. We also show that computing the ACE operator with localized orbitals can further improve the computational efficiency. Finally, we use this method in combination with the Well-Sliced Metadynamics approach to compute the free energy barrier of chemical reactions in systems containing hundreds of atoms.

[1] S. Mandal, N.N. Nair, J. Chem. Phys. **151** (2019) 151102.

[2] Lin Lin, J. Chem. Theory Comput. **12** (2016) 2242.

O 70.8 Wed 17:00 GER 38

Calculation of current-induced heating and vibrational instabilities in single molecule circuits — Giuseppe Foti and •Hector Vazquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

Current-induced heating in molecular wires arises from the interaction between tunneling electrons and localized vibrations. Vibrational instabilities occur when excitation of molecular vibrations is not balanced by dissipation mechanisms, and can lead to the breakdown of the junction. In this talk I will address predictions for vibrational instabilities in single molecule junctions with separated unoccupied resonances. We use DFT-NEGF to study the electronic structure of the junction under an applied bias, while rates of absorption and emission of vibrations are calculated using kinetic equations [1,2]. We find and characterize several unstable modes. These results are then generalized using model calculations to generate a stability diagram of the junction under bias [3]. The talk will discuss the effect of a self-consistent treatment of electron-vibration interaction, and highlight the role played by the structure of the electron-vibration coupling matrix. Our work reveals the interplay of electronic structure and electron-vibration coupling in a broad class of molecular wires.

[1] J-T Lü, P. Hedegaard and M. Brandbyge, Phys. Rev. Lett. 107, 046801 (2011).

[2] G. Foti and H. Vázquez, J. Phys. Chem. C 121, 1082 (2017).

[3] G. Foti and H. Vázquez, J. Phys. Chem. Lett. 9, 2791 (2018).

O 70.9 Wed 17:15 GER 38

***Ab Initio* Green-Kubo Approach of Charge Transport in Crystalline Solids** — •Zhen-Kun Yuan, Marios Zacharias, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

State-of-the-art approaches for calculating the charge transport coefficients in crystalline materials rely on a harmonic description of the lattice vibrations and a perturbative treatment of electron-phonon couplings (EPCs) [1]. For materials featuring sizable anharmonic lattice vibrations and/or strong EPCs, such approaches are, however, not applicable. Here, we present an *ab initio* approach based on the Green-Kubo theory of linear response [2] that does neither rely on the harmonic approximation nor on a perturbative treatment of EPCs, thus overcoming these issues. The electrical conductivity is obtained from the time correlations of the electric charge flux, which is computed along fully anharmonic *ab initio* molecular dynamics trajectories. We demonstrate our approach by calculating the electrical conductivity of the harmonic material Si and the anharmonic $SrTiO_3$. We carefully check the convergence behavior of the calculated results with respect to supercell size and examine possible strategies to overcome finite-size effects [3].

[1] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).

[2] R. Kubo, M. Yokota, and S. Nakajima, *J. Phys. Soc. Jpn.* **12**, 1203 (1957).

[3] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).

O 71: Electronic Structure of Surfaces I

Time: Wednesday 15:00–17:30 Location: REC C 213

Invited Talk O 71.1 Wed 15:00 REC C 213

Detection of strong interaction between electrons and antiferromagnetic magnons in $Ba_{1-x}K_xMn_2As_2$ — Tianlun Yu[1], Rui Peng[1], Guanghan Cao[2], •Haichao Xu[1], and Donglai Feng[1] — [1]Laboratory of Advanced Materials, State Key Laboratory of Surface Physics, and Department of Physics, Fudan University, Shanghai 200438, People's Republic of China — [2]Department of Physics, Zhejiang University, Hangzhou 310027, People's Republic of China

The behavior of itinerant carriers under an antiferromagnetic background is critical for many novel physics. K-doped $BaMn_2As_2$ hosts an robust antiferromagnetic order and strong Mn local moments in its highly hole doped metallic state. Here we revealed the band structure by angle-resolved photoemission spectroscopy, and a kink in dispersion is observed at Fermi energy. The coupling constant from self-energy analysis reveales an extremely strong coupling between the itinerant holes and antiferromagnetic magnons. The evolution of the Fermi surface volume with the hole doping follows the Luttinger theory of a normal metal, which rules out a simple half-metal picture of the itinernt ferromagnetism. The large mass enhancement of the As 4p holes by the electron-magnon coupling may be responsible for the emergent itinereant ferromagnetism.

O 71.2 Wed 15:30 REC C 213

Computation of photoelectron matrix elements for angle-resolved photoemission spectroscopy from first principles — •Ji Hoon Ryoo[1,2,3] and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

Despite the ever-growing role of photoemission spectroscopy in investigating electronic structure of molecules, bulk crystals and their surfaces, calculation of photoemission intensities is, although possible, considered far more difficult than conventional calculations of electronic structures near the Fermi energy. The main reason for the difficulty lies in obtaining electronic structure at energies far higher than the vacuum level, and thus photoelectron states are often approximated as plane-wave-like states [1]. However, several calculations using the KKR method or the embedding method (e.g., Ref. 2 and 3, respectively) have shown that in many cases a more realistic description of photoelectron states beyond the plane-wave approximation is necessary for interpreting the results of spin- and angle-resolved photoemission experiments. We discuss a different method of computing photoemission matrix elements that incorporates final-state effects from first principles.

[1] Z.-H. Zhu et al., Phys. Rev. Lett. 110, 216401 (2013).

[2] J. Sánchez-Barriga et al., Phys. Rev. X 4, 011046 (2014).

[3] H. Bentmann et al., Phys. Rev. Lett. 119, 106401 (2017).

O 71.3 Wed 15:45 REC C 213

The one-step model of time-dependent photoemission combined with time-dependent density functional theory — •Jürgen Braun, Sergiy Mankovsky, and Hubert Ebert — Department Chemie, LMU München

Our fully relativistic one-step model approach to time-resolved photoemission aims at a quantitative description of time-dependent spectroscopic properties of specific solid systems under consideration [1]. The formalism allows for the inclusion of static correlation effects within the LSDA+DMFT approach as well as for the inclusion of a time-dependent potential $V(\mathbf{r},t)$, which in principle is available from TDDFT. We used the Elk code [2] to calculate spin- and time-dependent potentials and corresponding occupation numbers for ferromagnetic Fe and Co. These objects, which serve as input quantities for our spectroscopical analysis, represent the feed back of the system generated by a pump pulse. The calculations are compared to corresponding pump-probe experiments.

[1] J. Braun and H. Ebert, Relativistic theory of 2PPE from ferromagnetic materials, Phys. Rev. B **98**, 245142 (2018)

[2] Elk.sourceforge.net: K. Dewhurst, S. Sharma, L. Nordström, O. Granas, E.K.U. Gross et al. (2019)

O 71.4 Wed 16:00 REC C 213

Co on W(110): Spin-dependent interface effects in the electronic structure — •Marcel Holtmann[1], Pascal J. Grenz[1], Eike F. Schwier[2], Shiv Kumar[2], Koji Miyamoto[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster — [2]Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan

The surface of W(110) exhibits a topologically nontrivial Dirac-cone like state within a spin-orbit induced symmetry gap [1, 2]. When depositing ultrathin Fe films, the state was found to behave differently depending on the film thickness, allowing for manipulation of the "Dirac-fermion mass" via magnetic influence [3]. In order to systematically study the impact of the magnetic adsorbate material, we have investigated the influence of cobalt on the occupied band structure of W(110). In this talk, I will be presenting our results on the preparation of Co/W(110) as well as spin-resolved measurements of the occupied band structure. As in the case of Ni/W(110), we observed growth in the Nishiyama-Wassermann mode. No alteration of the dispersion behavior of the Dirac-cone like surface state was observed - the state gradually fades away with increasing film thickness. Close to the Fermi energy we detected Co-induced interface states, which show Rashba-type spin splitting for submonolayer cobalt coverages.

[1] K. Miyamoto *et al.*, Phys. Rev. Lett. **108**, 066808 (2012) [2] D.

Thonig *et al.*, Phys. Rev. B **94**, 155132 (2016) [3] K. Honma *et al.*, Phys. Rev. Lett. **115**, 266401 (2015)

O 71.5 Wed 16:15 REC C 213

Fermi Surface Tomography of Palladium via Momentum Microscopy

— •Xin Liang Tan[1], Kenta Hagiwara[1], Ying-Jiun Chen[1,2], Jakub Schusser[3], Vitaliy Feyer[1], Jan Minar[3], Claus M. Schneider[1,2], and Christian Tusche[1,2] — [1]Forschungszentrum Jülich, Peter Grünberg Institut, Jülich — [2]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [3]New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic

The Fermi surfaces, which describe all thermodynamical and transport quantities of solids, of transition metals are often failed to be modeled by one-electron mean-field theory due to strong correlations among the valence electrons. In addition, relativistic spin-orbit coupling pronounced in heavier elements lifts the degeneracy of the energy bands and further modifies the Fermi surface. Palladium, a 4d metal attributed to both significant spin-orbit coupling and electron correlations, is ideal for a systematic and fundamental study on the two fundamental physical phenomena and their interplay in electronic structure. In this talk, we will explore the experimentally determined electronic structure of palladium in four dimensional energy-momentum space ($E_{Binding}$,k_x,k_y,k_z) obtained via constant initial-state momentum microscopy. The complete 3D-Fermi surface of palladium and corresponding isoenergy surfaces at higher binding energies were tomographically mapped with an energy- and polarization-variable light source. Spin-orbit coupling and electron correlations in palladium will be presented in the context of energy-momentum relations across the Fermi surface and isoenergy surfaces.

O 71.6 Wed 16:30 REC C 213

Orbital imaging: Sparsity-driven phase retrieval of angular-resolved photoemission spectroscopy data

— •Matthijs Jansen[1], Marius Keunecke[1], Marten Düvel[1], Christina Möller[1], David Schmitt[1], Wiebke Bennecke[1], Jasmin Kappert[1], Daniel Steil[1], Russell Luke[2], Sabine Steil[1], and Stefan Mathias[1] — [1]1st Physical Institute, University of Göttingen, Göttingen — [2]Institute for Numerical and Applied Mathematics, University of Göttingen, Göttingen

In recent years, iterative phase retrieval of angle-resolved photoemission spectroscopy (ARPES) has attracted interest as a method to visualize molecular orbitals in molecule-metal interfaces. This method, dubbed *orbital imaging*, relies on prior knowledge of the investigated orbital. So far, successful orbital imaging has been based on the support constraint, for which the shape of the orbital must be known.

We will present a sparsity-driven approach to phase retrieval, which uses only the number of non-zero pixels in the orbital. This sparsity constraint is easy to determine and independent of the orbital shape. Additionally, we include symmetry in the phase retrieval approach. We apply the resulting phase retrieval algorithms successfully to both simulated and experimental ARPES data, acquired using a so-called *momentum microscope*, which uses time-of-flight-based detection to measure the full momentum and energy-dependent spectrum in a single measurement. This enables us to image multiple molecular orbitals simultaneously. We conclude that sparsity-driven phase retrieval requires less prior knowledge to achieve good orbital imaging results.

O 71.7 Wed 16:45 REC C 213

Hard X-ray Valence-Band Mapping and Photoelectron Diffraction on InGaMnAs Thin Films

— •K. Medjanik[1], A. Winkelmann[2], O. Yastrubchak[3], J. Sadowski[4,5], L. Gluba[6,7], D. Vasilyev[1], S. Babenkov[1], S. Chernov[1], O. Fedchenko[1], H.J. Elmers[1], and G. Schönhense[1] — [1]JGU, Inst. für Physik, Mainz — [2]AGH Univ. of Science and Technology, Krakow, Poland — [3]Inst. of Semiconductor Physics, Kyiv, Ukraine — [4]Inst. of Physics, Warszawa, Poland — [5]Linnaeus Univ., Kalmar, Sweden — [6]Inst. of Agrophysics, Lublin, Poland — [7]Inst. of Physics, Lublin, Poland

The interplay of electronic and geometric structure is one of the key issues of materials research. We present results for the prototypical ferromagnetic semiconductor InGaMnAs (3% In, 2.5% and 5% Mn), recorded at photon energies between 3 and 5 keV at the new beamline P22 at PETRA III (Hamburg) by Time-of-Flight Momentum Microscopy [1]. In the non-centrosymmetric GaAs crystal structure, element-specific hXPD clearly reveals site-specific Ga and As diffraction patterns which are rotated by 90° at identical kinetic energies. The Mn-atoms show diffractograms, which are characteristic for the Ga-sites, as expected for substitutional Mn in GaAs [2]. Sharp valence-band k-patterns show that with increasing Mn-doping the splitting of the p1/2-derived band from the heavy- and light-hole p3/2-bands increases. In addition, the Fermi energy decreases i.e. with increased Mn content the frontier bands are less filled.

[1] K. Medjanik et al., J. of Synchr. Radiation 26, 1996 (2019). [2] T. Dietl & H. Ohno, Rev. Mod. Phys. 86, 187 (2014).

O 71.8 Wed 17:00 REC C 213

Surface electronic structure of Te on Ag(111) and Cu(111)

— •Begmuhammet Geldiyev, Jonas Hauner, Janek Rieger, M. Alexander Schneider, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The unoccupied and occupied surface electronic structure of Te on Ag(111) and Cu(111) was studied by bichromatic two-photon photoemission (2PPE) and laser-based one-photon photoemission (1PPE). For 1/3 monolayer of Te a $(\sqrt{3} \times \sqrt{3})R30^\circ$ superstructure forms on Ag(111) in contrast to the $(2\sqrt{3} \times \sqrt{3})R30^\circ$ structure on Cu(111) with a doubled unit cell. For both surfaces two occupied bands are found by 1PPE and one unoccupied surface band by 2PPE. For Te/Cu(111) the higher-lying occupied band is split into two bands for the inequivalent directions of the doubled unit cell. All bands on Cu(111) are shifted up in energy compared to Ag(111) in agreement with density-functional-theory calculations. The orbital character of the electronic bands is probed by polarization-dependent measurements in normal emission. On Te/Ag(111) time-resolved 2PPE measurements yield a lifetime of ≈ 31 fs for the unoccupied state located ≈ 0.53 eV above the Fermi level, which has an electron-like dispersion. For the analogous surface state on Cu(111) at ≈ 1.43 eV no measureable lifetime was found.

O 71.9 Wed 17:15 REC C 213

Double photoemission spectroscopy of $SrTiO_3$(001) using a high-order harmonics light source

— •Robin Kamrla[1], Cheng-Tien Chiang[1], Andreas Trützschler[1], Michael Huth[2], Frank Oliver Schumann[2], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

Photoelectron spectroscopy (PES) has provided deep insights into the electronic structure of solids. However, correlation effects can only be addressed indirectly. To observe such phenomena directly, double photoemission (DPE) spectroscopy is able to detect pairs of correlated photoelectrons that are emitted upon absorption of a single photon [1]. In this contribution we present PES and DPE data for $SrTiO_3$(001), obtained by a laboratory high-order harmonic (HHG) light source at $h\nu = 25.2$ and 32.4 eV operating at MHz repetition rates. Well-ordered $SrTiO_3$(001) surfaces have been prepared by annealing at 770 K in an oxygen atmosphere of $5 \cdot 10^{-6}$ mbar. PES confirms a TiO_2 terminated surface and reveals a binding energy of the O_{2p} state of 3.2 eV. In DPE we find an onset for emission of correlated photoelectrons at a pair binding energy of 7.5 eV, independent of the individual electron energies. The DPE data will be compared to data for NiO and CoO surfaces, as well as for Ag(001) [2], indicating the presence of a strong electron-electron interaction in $SrTiO_3$.

[1] J. Berakdar et al., Phys. Rev. Lett. **81** (1998)
[2] A. Trützschler et al., Phys. Rev. Lett. **118** (2017)

O 72: Scanning Probe Techniques I: STM-ESR and Method Development (joint session O/CPP)

Time: Wednesday 15:00–17:30 Location: TRE Ma

O 72.1 Wed 15:00 TRE Ma

Dynamics in spin excitation spectroscopy measurements — •Luigi Malavolti[1,2], Max Hänze[1,2], Gregory McMurtrie[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany. — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany.

Spin excitation spectroscopy has proven to be an essential tool for the investigation of magnetic phenomena at the atomic scale [1] forming the basis for RF-STM investigation of both electron spin resonance and spin dynamics [2]. However, certain spin dynamic phenomena can also be transduced directly via standard dIdV(V) measurements [3]. Here, the contribution of spin dynamic effects to static spectroscopy measurements is presented using a combined theoretical and experimental approach. Understanding these phenomena allows the behavior of spin systems with long-lived excitations to be anticipated, offering a fast and reliable way to access spin dynamics with standard STM techniques. [1] R. Wiesendanger, Rev. Mod. Phys. 81, 1495 (2009) [2] Loth S., Science, 329, 1628, (2010) [3] Rolf-Pissarczyk S., PRL, 119, 217201, (2017)

O 72.2 Wed 15:15 TRE Ma

Electron paramagnetic resonance of single Ti and Fe atoms with an out-of-plane magnetic field probed by STM — •Tom S. Seifert[1], Stepan Kovarik[1], Dominik Juraschek[1,2], Nicola A. Spaldin[1], Sebastian Stepanow[1], and Pietro Gambardella[1] — [1]ETH Zurich, Switzerland — [2]Harvard University, USA

Combining the sub-atomic resolution of scanning tunneling microscopy (STM) with the spectral resolution of electron-paramagnetic resonance (EPR) allows for sensitive probing magnetic interactions of single atoms on a surface [1]. However, the experimental requirements for driving the EPR transitions are still under debate [2,3]. In-depth understanding of what drives these spin rotations is mandatory to explore novel material systems and optimize the sensitivity of this technique. Here, we acquire EPR spectra of single Fe and hydrogenated Ti atoms on bilayer MgO on Ag using a radio frequency (RF) antenna close to the STM junction with a magnetic field applied perpendicular to the surface [4]. We investigate in a systematic way the impact of RF excitation strength and tunneling parameters on the EPR signal with emphasis on the electric and magnetic fields present at the tunnel junction. This analysis is supported by density functional calculations of the electronic and phononic density of states of the probed systems.

[1] S. Baumann et al., Science **350** (2015) [2] K. Yang, et al., PRL **122** (2019) [3] P. Willke et al., Nano Lett. **19** (2019) [4] T. S. Seifert et al., ArXiv 1908.03379 (2019)

O 72.3 Wed 15:30 TRE Ma

Electron spin resonance of an individual atom at mK temperature in a vector magnetic field — •Manuel Steinbrecher[1], Werner v. Weerdenburg[1], Jan W. Gerritsen[1], Niels v. Mullekom[1], Fabian D. Natterer[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, The Netherlands — [2]Department of Physics, University of Zurich, CH-8057 Zurich, Switzerland

It was recently shown that electron spin resonance (ESR) can be combined with spin-resolved scanning tunneling microscopy (STM) to quantify the resonant excitations of individual 3d transition metal atoms [1]. The combination of atomic-resolution and ultra-high energy resolution, compared to standard scanning tunneling spectroscopy, has e.g. enabled quantification of the hyperfine coupling of individual atoms at temperatures near 1K [2]. Nevertheless, probing small absolute energy scales down to MHz frequencies requires the implementation of this method at much lower temperature. We will present ESR performed in a home-made dilution refrigerator (T = 30mK) based spin-polarized STM including a vector magnet [3]. The ESR was recorded on individual atoms on a thin insulating film of MgO over a whole frequency range from several hundred MHz to tens of GHz. A vector magnetic field was applied and allowed ESR experiments in different crystallographic directions.

[1] S. Baumann *et al.*, Science **350**, 417 (2015)
[2] P. Willke *et al.*, Science **362**, 336 (2018)
[4] H. v. Allwörden *et al.*, RSI **89**, 033902 (2018)

O 72.4 Wed 15:45 TRE Ma

Electron spin resonance in scanning tunneling microscopy — •Andreas Heinrich — Center for Quantum Nanoscience, Seoul, Korea

The scanning tunneling microscope is an amazing 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 several microvolt energy resolution. In this talk we will apply these techniques to the investigation of the quantum spin properties of magnetic atoms sitting on thin insulating films. We will explore the superposition of quantum states which is inherent to spin resonance techniques. About 5 years ago it was demonstrated that electric field driven electron spin resonance (ESR) can be combined with STM on single Fe atoms on MgO (Science 2015). This technique combines the power of STM of atomic-scale spectroscopy with the unprecedented energy resolution of spin resonance techniques, which is about 10,000 times better than normal spectroscopy. We will give an update on recent advances in our team including pulsed ESR on Ti atoms on MgO (Science 2019).

O 72.5 Wed 16:00 TRE Ma

Transfer Function Compensation for High Frequency Radiation into an STM Tunnel Junction — •Maximilian Uhl, Piotr Kot, Robert Drost, and Christian R. Ast — Max-Planck-Institut für Festkörperforschung, Stuttgart

Creating constant amplitude radiation of varying frequencies in the tunnel junction of a scanning tunneling microscope is an important condition for probing the interaction of matter and electromagnetic waves at the nanoscale, such as for electron paramagnetic resonance [1]. The transfer function describes the transmission of an AC signal to the tunnel juntion and depends highly non-linearly on the frequency. A known transfer function can be compensated by a frequency dependent signal power. Reaching non-zero constant amplitudes at frequencies > 40 GHz has remained a challenge. Our setup makes this possible for frequencies up to 90 GHz. So far, transfer functions have been measured by plasmonic light emission [2] and rectification at current-voltage non-linearities [3]. Here, a new technique based on the Tien-Gordon equation [4] is demonstrated. It allows to probe even small AC voltages in the μV range, requiring only a single measurement point per frequency. For that, we use the coherence peak of a superconductor-insulator-superconductor junction. Generally, the technique can also be used with other peak types in the current-voltage derivative.

[1] S. Baumann et al.: Science **350** (6259), 417 (2015)
[2] C. Grosse et al.: Appl. Phys. Lett. **103**, 183108 (2013)
[3] W. Paul et al.: Rev. Sci. Instrum. **87**, 074703 (2016)
[4] G. Falci, V. Bubanja, G. Schön: Z. Phys. B **85**, 451 (1991)

O 72.6 Wed 16:15 TRE Ma

Hyperfine fields of magnetic adatoms on ultrathin insulating films — •Sufyan Shehada, Manuel dos Santos Dias, Filipe Souza Mendes Guimarães, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany

Individual nuclear spin states can have a very long lifetime and could in principle be used as qubits. A promising step in this direction was the recent detection of the hyperfine interaction between the atomic nucleus and the surrounding electrons for single Fe and Ti adatoms on MgO/Ag(001) [1]. Here, we report on systematic first-principles calculations of the hyperfine fields of magnetic transition metal adatoms (from Ti to Cu) placed on different ultrathin insulators, such as MgO, NaCl, CuN and hBN. We analyze the trends and the dependence of the computed hyperfine fields on the filling of the magnetic d-orbitals of the adatom and on the type and strength of the bonding with the substrate, and what is the impact of an underlying metallic surface. We also identify promising candidates for future experimental investigation with scanning probe techniques.

This work was supported by the Palestinian-German Science Bridge BMBF program and the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme

(ERC-consolidator Grant No. 681405-DYNASORE).

[1] P. Willke *et al.*, Science **362**, 336–339 (2018)

O 72.7 Wed 16:30 TRE Ma

Mapping the perturbation potential of metallic and dipolar tips in tunneling spectroscopy on $\mathbf{MoS_2}$ — •Christian Lotze, Nils Krane, Gaël Reecht, Nils Bogdanoff, and Katharina J. Franke — Freie Universität Berlin, Germany

Single layer molybdenum disulfide (MoS_2) features a direct band gap and strong spin-splitting of the valence band at the K-point, which make it an interesting material for optoelectronic applications.

We grow a single layer of MoS_2 epitaxially on a Au(111) surface, adopting a recipe from [1], and employ its decoupling properties for high resolution scanning tunneling spectroscopy of single molecules [2]. Because of the band gap and small electron-phonon coupling strength of MoS_2, it is possible to resolve spectral features down to few meV. Differential conductance spectra of 2,5-bis(3-dodecylthiophen-2-yl)thieno[3,2-b]thiophene (BTTT) molecules exhibit a multitude of sharp characteristic peaks, originating from vibronic states. Indeed, these allow even for an identification of different rotamers [2].

Here, we make use of these vibronic fingerprints to investigate the influence of the tip potential on the apparently shifted molecular states along the extended molecular backbone of BTTT. Our analysis further allows us to distinguish between the inhomogeneous shape of the bias potential in the junction and possible intrinsic tip dipoles [3].

[1] Sørensen, *et al.*, Langmuir, 31, 35, 9700 (2015)
[2] Krane, *et al.*, ACS Nano, 12, 11, 11698 (2018)
[3] Krane, *et al.*, Phys. Rev. B, 100, 035410 (2019)

O 72.8 Wed 16:45 TRE Ma

Fast quasiparticle interference mapping through traveling salesperson and sparse sampling optimization — •Jens Oppliger and Fabian D. Natterer — Department of Physics, University of Zurich, Switzerland

STM investigations are slow and render complex measurement tasks, such as QPI mapping, impractical. Conventionally, QPI patterns are composed from a Fourier-transform of hundreds of thousands of point-spectra that encode LDOS modulations from which the scattering space is inferred. Yet, despite this measurement complexity, we rely heavily on QPI since it provides insight into materials that are experimentally inaccessible to ARPES. Surprisingly, QPI patterns contain only little information, despite their origin from many data-points. Since sparsity is one key-ingredient for compressive sensing, we use it here to fundamentally speed-up QPI mapping [1]. In view of the incoherent measurements required for CS, we sparsely sample LDOS at randomly selected locations using constant and varying probability density. To that end, we move the STM-tip according to a traveling salesperson and ultimately achieve a 5-50 times faster QPI mapping.
[1] J. Oppliger and F.D. Natterer, arXiv 1908.01903

O 72.9 Wed 17:00 TRE Ma

Development of a Variable-Temperature High-Speed Scanning Tunneling Microscope — •Zechao Yang, Leonard Gura, Jens Hartmann, Heinz Junkes, William Kirstädter, Patrik Marschalik, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Scanning probe microscopy allows for resolving the atomic structure of crystalline and vitreous thin oxide films on metal substrates. For understanding the structural transition of these films as a function of temperature in real space and at real time, we developed a variable-temperature high-speed scanning tunneling microscope (STM).

The experimental setup consists of a two-chamber ultra-high vaccum (UHV) system including a preparation and a main chamber. The preparation chamber is equipped with standard preparation tools for sample cleaning and film growth. The main chamber hosts the STM that is located within a continuous flow cryostat for counter-cooling during high-temperature measurements. The microscope body is compact, rigid, and highly symmetric to ensure vibrational stability and low thermal drift. We designed a scanner made of two independent tube piezos for slow and fast scanning, respectively. Here we have decided to implement non-conventional spiral geometries for high-speed scanning. A Versa Module Eurocard bus system enables the fast scan control and is implemented in the EPICS software framework.

With sprial scans, we atomically resolved diffusion processes within an O(2x2) coverage on Ru(0001) and achieved a time resolution of 25 milliseconds per frame.

O 72.10 Wed 17:15 TRE Ma

Integrated Electrodes in H:Si(001) for Scanning Gate Microscopy — •Matthias Koch, Alex Kölker, Leonid Shupletsov, Takashi Kumagai, and Martin Wolf — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Single atoms or molecules can not only be characterized but also manipulated by exploiting the incredible high spatial resolution of the scanning tunneling microscopy. However, often the electrical characterization is limited by the experimental setup which consists of only two electrodes (tip and sample). Although multi-tip setups or scanning gate microscopes exist their operation is often demanding [1].

Here, we demostrate a sample system, compatible to most commercial low-temperature SPMs, equipped with multiple integrated electrodes. These in-plane electrodes, which are in close proximity to the surface, act as drain or gate contacts. We realize the *m-large electrodes by ultra-shallow ion-implantation in an otherwise highly resistive silicon crystal [2]. Notably, even after high-temperature treatment to prepare atomically flat silicon, the electrodes behave ohmic. The optimal distance between two electrodes is determined by in-situ transport measurements. Furthermore, the applicability of our sample system is demonstrated by first gating experiments. In future it will be used to study lateral nano-circuits in-operando with the SPM tip as a mobile electrode.

[1] B. Voigtländer et. Al, Rev. Sci. Instrum. 89, 101101 (2018)
[2] A.N. Ramanayaka et. al Scientific Reports 8, 1 (2018)

O 73: Organic Molecules on Inorganic Substrates V: Adsorption, Growth and Networks

Time: Wednesday 15:00–18:15 Location: TRE Phy

O 73.1 Wed 15:00 TRE Phy

Comparison of the adsorptions of ethanol and azobenzene molecules on single-layer hexagonal boron nitride on Rh(111) — •Krisztián Palotás[1,2,3], Arnold Farkas[3,4], Ádám Szitás[3], Dániel Jurdi[3], Richárd Gubó[3,4], Tibor Pásztor[3], László Óvári[3,4], János Kiss[3], András Berkó[3], and Zoltán Kónya[3] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]Wigner Research Center for Physics, Budapest, Hungary — [3]University of Szeged, Szeged, Hungary — [4]ELI-ALPS, Szeged, Hungary

The nanomesh structure of single-layer hexagonal boron nitride (hBN) on various metal surfaces can be used as a nanotemplate for molecular adsorption. Possible applications can be molecular electronics, heterogeneous catalysis, sensing, or light harvesting. We investigate the adsorption properties of ethanol and azobenzene molecules on the hBN/Rh(111) surface by density functional theory calculations and experimental methods. We find high selectivity of the nanomesh structure for the azobenzene adsorption, but no selectivity for the ethanol adsorption. The latter finding is in line with experimental observations of a very weak interaction between ethanol and the hBN/Rh(111) substrate. Finally, we analyze the trans- and cis-azobenzene adsorption and azobenzene-azobenzene interactions in great details by using theoretical means. These results contribute to the understanding of the behavior of photo-switching molecules on nanotemplated surfaces.

O 73.2 Wed 15:15 TRE Phy

Boron-doping Induced States in Single Graphene Nanoribbons Probed in Transport Measurements — •Niklas Friedrich[1], Pedro Brandimarte[2], Jingcheng Li[1], Thomas Frederiksen[2], Aran Garcia-Lekue[2], Daniel Sánchez-Portal[3], and J.I. Pascual[1] — [1]CIC nanoGUNE, San Sebastian (Spain) — [2]Donostia International Physics Center, San Sebastian (Spain) — [3]Centro de Física de Materiales, San Sebastian (Spain)

Bottom-up synthesized graphene nanoribbons (GNRs) are a versatile playground for engineering electronic properties of low-dimensional systems. Numerous predictions state that certain GNR shapes carry zero energy states hosting an even number of electrons. Despite their large potential for spintronics, the synthesis and observation of magnetism in graphene-based structures is so far very limited.

Here, we show that a spin-polarized state can be induced in 7-armchair GNRs by substitutional Boron-doping of two central Carbon atoms. Electronic transport measurements through a B-doped GNR suspended between the Au(111) substrate and the tip of scanning tunnelling microscope reveal a zero-bias Kondo resonance, attributed to the induced spin-polarization. Density functional theory simulations confirm an emerging spin-polarization in the GNR upon detachment of the dopant from the surface.

Simulations also reveal strong kinetic exchange interactions between doping sites within the same GNR, which modifies the net spin-polarization of the ribbon. Our experimental transport results confirm the presence of such a non-conventional spin texture.

Invited Talk O 73.3 Wed 15:30 TRE Phy

1.*Real-space investigation of the influence of polar species on ice structure — •Karina Morgenstern — Physikalische Chemie I, Ruhr-Universität Bochum, Germany

The interaction of water with solid surfaces is crucial in several scientific disciplines as diverse as environmental science, solvation science, biophysics, and astrochemistry. In these disciplines, there are several major water ice-related challenges that require a molecular-level understanding and description of water. In particular atmospheric chemistry, where most reactions in the atmosphere proceed on ice-covered nanoparticles poses a large variety of unanswered questions with respect to ice surfaces. Thereby, natural water was and is never as pure as distilled water, but contains air, salts, dust, organics, bacteria and so forth. Appropriate answers of relevance to real systems thus require a fundamental understanding of the structure of ice, not only in its purest, but in particular in its more realistic contaminated state. We explore how contaminants, in particular organic molecules and cations, alter the structure of ices on the (111) faces of the coin metals using low-temperature scanning tunneling microscopy. The systems discussed in this talk are azobenzene [1,2] and carbene [3] as prototypes for polar molecules and lithium and cesium ions as prototypes for cations. Moreover, we will present an example, how the structure of ice influences the reactivity of a photo-induced reaction [4].

[1] J. Am. Chem. Soc. 136, 13341 (2014); [2] Angew. Chem. Int. Ed. 57, 1266-1270 (2018); [3] Angew. Chem. Int. Ed. 57, 16334-16338 (2018); [4] Phys. Rev. Lett. 121, 206001 (2018)

O 73.4 Wed 16:00 TRE Phy

STM Investigation on Structural Transformation of Terphenylthiol Self-Assembled Monolayers Induced by Electron Irradiation — •Patrick Stohmann, Sascha Koch, Yang Yang, Christopher David Kaiser, Xianghui Zhang, and Armin Gölzhäuser — Physics of Supramolecular Systems and Surfaces, Bielefeld University, 33615 Bielefeld, Germany

Carbon Nanomembranes (CNMs) are two-dimensional sheets with tailored physical and chemical properties. They are prepared via electron irradiation induced cross-linking of aromatic self-assembled monolayers (SAMs). However, the molecular structure of CNMs and the underlying mechanisms of the cross-linking process are not fully understood. Here, the structural transformation of a pristine p-terphenylthiol (TPT) SAM on Au(111) was studied with a scanning tunneling microscope (STM) combined with a scanning electron microscope (SEM). STM images of the initial steps of irradiation exhibit depressive spots in the SAM, which is analogous to nucleation sites and could be correlated with radical chain reactions connecting up to 40 molecules. The chain reactions could be initiated by 6 eV (secondary) electron attachment and potentially terminated by steric hindrance. The electron irradiation was carried out by employing a low-energy flood gun emitting 50 eV electrons for a comparative study.

O 73.5 Wed 16:15 TRE Phy

Solvation of Large Organic Molecules in Two Dimensions - Imaging Single Cage Precursor Molecules in Chloroform Supported on Ag(111) — •Marvin Quack[1], Karina Morgenstern[1], Haeri Lee[2], and Guido Clever[2] — [1]Physical Chemistry I, Ruhr-University of Bochum, Germany — [2]Chair for Bioinorganic Chemistry, TU Dortmund, Germany

Exploring the solvation of molecules is of utmost importance for the basic understanding of chemical processes, since the interaction of solvent and solute determines reaction pathways as well as the structure of the solute. However, the investigation of solvated molecules in the liquid phase is restricted to averaging methods or theory due to the dynamic nature of solvation processes. In order to overcome this problem, we present the formation of a two dimensional solvent layer supported on a metal substrate, enabling us to study the structure of solvated molecules in real space by the means of low-temperature scanning tunneling microscopy (STM). To understand the interaction of single molecules with its solvent, we coadsorbed the bidentate ligand molecule $C_{75}H_{51}N_3O$ and chloroform on a Ag(111) single crystal surface by the means of atomic layer injection, followed by cooling to 5 K. The STM results reveal the molecule in three different conformations embedded within the 2D chloroform layer. In addition, the structure of the solvent layer is disturbed compared to the ordered structure of pure chloroform on Ag(111). The significance of these results with regard to solvation will be discussed in this contribution.

O 73.6 Wed 16:30 TRE Phy

Pentamers-like molecules forming a self-assembled monolayer onto a FCC(111) surface: a theoretical study — •Eduardo Cisternas[1,2], Gonzalo dos Santos[3], Marcos Flores[2,4], Eugenio Vogel[1,5], and Antonio Ramírez-Pastor[6] — [1]Universidad de La Frontera, Temuco, Chile — [2]Millenium Nucleus MultiMat — [3]Universidad de Mendoza, CONICET Mendoza, Argentina — [4]Universidad de Chile, Santiago, Chile — [5]Center for the Development of Nanoscience and Nanotechnology (CEDENNA), Santiago, Chile — [6]Universidad Nacional de San Luis, CONICET San Luis, Argentina

In the aim to understand the formation of a self-assembled monolayer when 2-thiophene molecules are adsorbed on a Au(111) surface, we studied the deposition of rigid straight pentamers onto a FCC(111) surface. Thus, by combining density functional theory calculations and Monte Carlo simulations we have found that for a certain value of the chemical potential there exists an isotropic-nematic phase transition which can explain the formation of a self-assembled monolayer. An order parameter is defined to characterize the transition which presents a step-like behavior at a critical chemical potential value. The possible nature of the nematic transition is discussed as future work by means of statistical physics techniques.

O 73.7 Wed 16:45 TRE Phy

Polymorphism of 6,13-Pentacenequinone on Ag(111) in the monolayer regime — •Jari Domke, Falko Sojka, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Pentacene and its derivatives have been studied extensively and with great interest in the last decades due to their potential and actual application in organic electronics. For devices utilizing those molecules an understanding of the layer growth on a distinct substrate is of fundamental importance, as this can be strongly affected by introducing functional groups – for example – to promote hydrogen bonds.

We structurally investigated 6,13-pentacenequinone (P2O) on Ag(111) in monolayer and sub-monolayer regimes using distortion-corrected low-energy electron diffraction (LEED) and low-temperature scanning tunneling microscopy (STM). Accordingly, several coverage-dependent structures were found, most of them exhibiting an on-line epitaxy. Additionally, a phase consisting of many line-shaped nano domains was observed for annealed samples in STM, yielding a consistent model for LEED patterns that would otherwise suggest a commensurate structure incompatible with the molecular size of P2O.

O 73.8 Wed 17:00 TRE Phy

Self-assembly, metalation and oxidation of a novel macrocyclic compound on Ag(111) — •Felix Haag[1], Peter Deimel[1], Raphael Lauenstein[2], Manuel Kaspar[2], Johannes Barth[1], Corinna Hess[2], and Francesco Allegretti[1] — [1]Physics Department E20, Technical University Munich, Germany — [2]Chemistry Department, Technical University Munich, Germany

We report the first experimental study of the adsorption of the free-base macrocyclic biquinazoline (H-mabiq) on a model solid surface. This tetraaza-macrocycle offers two potential coordination sites combined with multi-electron transfer capacity - properties reaching beyond the well-studied surface-confined metallo-porphyrins and -phthalocyanine systems. Those coordination sites can be occupied by different metal atoms, rendering adsorbed mabiq complexes promising candidates for photocatalytic applications as well as epoxidation reactions.

Here, we report on the bonding and self-assembly of H-mabiq on Ag(111) by using X-ray photoelectron spectroscopy (XPS), low-energy electron diffraction (LEED) and temperature programmed desorption (TPD). We confirm the molecular integrity and establish protocols for well-ordered single layers and controlled metalation with Co atoms. A number of long-range ordered structures are identified, depending critically on molecular and metal coverage. Furthermore, reversible cycling between different phases is observed by tuning the H-mabiq surface density and the temperature. Finally, the interaction of adsorbed H-Mabiq and Co-mabiq with dioxygen is compared.

O 73.9 Wed 17:15 TRE Phy

2D molecular Self-assembly of C8-BTBT on metallic surfaces — •Sebastian Becker[1,2], Lu Lyu[1], Sina Mousavion[1], Maniraj Mahalingam[1], Benjamin Stadtmüller[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Department of Chemistry, University of Kaiserslautern, Erwin-Schrödinger-Str. 52, 67663 Kaiserslautern, Germany

Owing to a unique high mobility, [1]Benzothieno[3,2-b]benzothiophene (BTBT) based organic semiconductors (OSCs) have an enormous potential for photonic and spintronic applications. Here we systematically investigate the self-assembly of 2,7-Dioctyl-BTBT (C8-BTBT) molecules on Cu(111), Cu(001) and Co/Cu(001) surfaces. In the first monolayer, C8-BTBT molecules adopt a flat lying geometry on these surfaces due to dominant molecule-metal interactions. Depending on sample temperature, various C8-BTBT phases with different unit cells are found on Cu(111), in which the molecular C8-arms rotate into different orientations. On the more reactive surface of a Co thin film on Cu(100), a chemical desulfurization is observed in the first layer of C8-BTBT in contrast to the adsorption of C8-BTBT directly on Cu(001). The desulfurization reaction blocks the electron transfer across the interface. Our findings will provide new insight into the structural and electronic properties of BTBT-derivatives on metallic surfaces

O 73.10 Wed 17:30 TRE Phy

Adsorption Behaviour of Benzohydroxamic Acid on TiO_2(110) — •Julia Köbl, Elmar Kataev, Daniel Wechsler, Lisa-Marie Augustin, Hans-Peter Steinrück, and Ole Lytken — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058

We are aiming for a deeper understanding of basic interactions between organic molecules and oxide surfaces, as these interfaces are apparent in many electronic devices, such as dye-sensitized solar cells and organic field effect transistors. Thus, we studied the adsorption properties of the model system benzohydroxamic acid on rutile TiO_2 (110)-(1x1) as a function of coverage and temperature. This molecule is an interesting candidate for anchoring larger organic molecules like porphyrins on oxide surfaces. Using Synchrotron Radiation Photoelectron Spectroscopy (SRPES), we studied the bonding mechanism and thermal stability of benzohydroxamic acid, which was deposited by evaporation. From SRPES, we can identify different species in the N 1s spectra. The results are compared to our previous studies on phosphonic acid. Supported by the DFG through FOR 1878 (funCOS).

O 73.11 Wed 17:45 TRE Phy

Molecular arrangement discloses intermolecular interactions: The case of 1D structure formed by 3-hydroxybenzoic acid on calcite(10.4) — •Maximilian Vogtland[1], Christoph Schiel[2], Jonas Staude[1], Julia Neff[1], Hagen Söngen[1], Philipp Maass[2], Ralf Bechstein[1], and Angelika Kühnle[1] — [1]Universität Bielefeld, Deutschland — [2]Universität Osnabrück, Deutschland

Molecular self-assembly constitutes a convenient way to create molecular structures at surfaces. In the past, the focus of controlling the structure has been on attractive interactions, while repulsive interactions have been explored only rarely. Our group has investigated the self-assembly of benzoic acid derivatives with dynamic atomic force microscopy (AFM) at room temperature on calcite (10.4). Here, we focus on 3-hydroxybenzoic acid (3-HBA) that forms a 1D (striped) structure. The obtained next-neighbour stripe distance distributions differ substantially from what is expected for randomly placed, non-interacting stripes. These distance distributions have been explained by a long-range repulsion of adsorption induced dipoles. On the other hand, the stripe length distribution is a result of short-range attractive and long-range repulsive forces. We show how to extract the strength of repulsive and attractive interactions between the 3-HBA molecules by combining the information from length and distance distributions. In the future, we want to compare with other 1D structures, e.g., 3-aminobenzoic acid on calcite(10.4). We believe that tuning repulsive interactions is a powerful tool to influence molecular structure formation on bulk insulator surfaces.

O 73.12 Wed 18:00 TRE Phy

Multi-method study of trans-DBPen on coinage metal (111)-surfaces — •Felix Otto, Maximilian Schaal, Tobias Huempfner, Falko Sojka, Marco Gruenewald, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Several polycyclic aromatic hydrocarbons (PAHs) become superconducting after the intercalation of alkali metal atoms. The number of promising candidates has increased in the last few years. Among them, $K_{3.45}$1,2:8,9-dibenzopentacene (trans-DBPen, $C_{30}H_{18}$) is the one with the highest critical temperature reported so far. Nevertheless, the microscopic mechanisms of superconductivity in K-doped PAHs are still under debate. One open question is, for example, the effect of structural order in bulk materials as well as two-dimensional layers.

Our work deals with the growth of trans-DBPen on Ag(111), Au(111), and Cu(111) in the monolayer (ML) regime. The self-assembled thin films were prepared using organic molecular beam epitaxy. The structure was characterized by means of low energy electron diffraction (LEED). In the sub-ML range, we observe a 2D gas-like behavior, whereas the first MLs on the different substrates are characterized by highly ordered structures. Photoelectron spectroscopy (PES) including photoelectron momentum maps (PMMs) was used to study the interaction of the molecules with the substrate as well as the influence of the second ML on the electronic structure. The investigated systems exhibit notable differences according to the different interaction strengths with the substrate.

O 74: Nanostructured Surfaces and Thin Films I: Synthesis and Properties (joint session O/CPP)

Time: Wednesday 15:00–17:30 Location: WIL B321

O 74.1 Wed 15:00 WIL B321

Imaging the phase transition in thin film VO_2 microstructures — •Jan O. Schunck[1,2], Florian Döring[3], Benedikt Rösner[3], Jens Buck[4], Sanjoy Mahatha[1], Moritz Hoesch[1], Christian Schüssler-Langeheine[5], Adrian Petraru[6], Hermann Kohlstedt[6], Kai Rossnagel[1,4], Christian David[3], and Martin Beye[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg — [2]Physics Department, Universität Hamburg — [3]Paul Scherrer Institut, Villigen-PSI, Switzerland — [4]Institut für Experimentelle und Angewandte Physik, CAU Kiel — [5]Helmholtz-Zentrum Berlin — [6]Nanoelektronik, Techn. Fakultät, CAU Kiel

Vanadium dioxide (VO_2) is an intruiging compound, since upon heating it exhibits an insulator-to-metal transition (IMT) at a critical temperature T_c of around 340 K, which is characterised by a decrease in resistivity of several orders of magnitude. On a microscopic level, the phase transition is accompanied by a rearrangement of the crystal structure as well as electronic bands around the Fermi level and proceeds in a percolative manner, meaning that both phases coexist over a temperature range of several K around T_c.

Here, we present results of an experiment which combines X-ray spectroscopic methods for electronic structure analysis with imaging capabilities of a few micrometers spatial resolution. Studying electronic structure changes during the thermally driven IMT in a pulsed laser deposition-grown and microstructured VO_2 thin film, shows that T_c differs by around 2 K between the edges and centres of VO_2 squares with an edge length of 30 μm.

O 74.2 Wed 15:15 WIL B321

investigation of Fe(CO)5 as precursor for gas-assisted electron beam lithography techniques on cobalt oxide surfaces

— •Elif Bilgilisoy[1], Christian Preischl[1], Rachel Thorman[2], Howard Fairbrother[2], and Hubertus Marbach[1] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen, Germany — [2]Department of Chemistry, Johns Hopkins University, Baltimore, Maryland/USA.

Electron Beam Induced Deposition (EBID) is a gas-assisted direct write electron-lithography fabrication technique in which structures from certain precursor molecules are deposited. A second technique is Electron Beam Induced Surface Activation (EBISA). In EBISA, a focused electron beam is used to locally modify the substrate such that it becomes active towards the decomposition of subsequently dosed precursor molecules [1]. Both approaches were conducted with Fe(CO)5 on a Co3O4/Ir(100) surface. We will present first successful results on a clean Co3O4 surface with Fe(CO)5 for EBID and EBISA. To achieve a deeper understanding of the EBID process, corresponding surface science experiments were conducted, in which the dynamics and behavior upon low energetic electron[2] and ion beam irradiation of thin Fe(CO)5 layers at liquid nitrogen temperatures were investigated using x-ray photoelectron spectroscopy (XPS) under UHV. We will compare the corresponding results and discuss the reaction mechanisms of Fe(CO)5. [1] H. Marbach, Appl. Phys. A 117 (2014) 987 [2] S. G. Rosenberg, et al., J. Phys. Chem. C, 117 (2013)16053

O 74.3 Wed 15:30 WIL B321

Interaction of topological boundary states in graphene nanoribbon heterojunctions — •Qiang Sun[1], Oliver Gröning[1], Xuelin Yao[2], Akimitsu Narita[2], Klaus Müllen[2], Pascal Ruffieux[1], and Roman Fasel[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, nanotech@surfaces Labora-tory, 8600 Dübendorf, Switzerland — [2]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Graphene nanoribbons (GNRs), narrow stripes of graphene, are promising candidates for future elec-tronic applications due to their widely adjustable electronic properties. The precise control of their atomic structure, including their termini, edges and width, allow for the realization of specific electronic quantum phases. For example, GNRs with chiral edges or cove edges have been predicted to host spin-polarized edge states. And recently, topological electronic quantum phases have been predicted and realized in the junctions between GNR segments belonging to different topological classes. Here, I will show the synthesis and characterization of width-modulated GNRs that host topological junction states. By investigating such GNRs as a function of the number of periodically aligned junction states along the GNR axis, we follow the evolution of the new electronic bands formed by the finite overlap between the junction states. Furthermore, we investigate the interaction between boundary states in topological heterojunctions, revealing an interaction-induced energy splitting that decays exponentially with their relative separation.

O 74.4 Wed 15:45 WIL B321

Determination of Carbon Nanomembrane Diffusion Coefficients via radioactive tracer experiments — Raphael Dalpke[1], Anna Dreyer[2], •Riko Korzetz[1], André Beyer[1], Karl-Josef Dietz[2], and Armin Gölzhäuser[1] — [1]Faculty of Physics, Bielefeld University — [2]Faculty of Biology, Bielefeld University

In recent years, 2D materials have gained a lot of attention as highly efficient filter materials. One class of materials are carbon nanomembranes (CNM), which are fabricated by self-assembly of organic precursors onto metal substrates and subsequent cross-linking by electron irradiation. They can be released from their original substrate and transferred onto arbitrary supports. Specifically, CNMs made from terphenylthiol (TPT) exhibit a very high selectivity towards water in combination with an outstanding permeance [1].

Here, we present new permeation measurements of TPT-CNMs utilizing radioactively marked water as well as carbonate and phosphate ions. We show that water and carbonate can pass through while phosphate ions are completely blocked by the CNM. The resulting diffusion coefficients in combination with recent findings indicate that the permeation across the membrane primarily occurs by transport of neutral species. This implies a fast transport of CO_2 in aqueous solution, while dry TPT-CNMs are not permeable to CO_2, which suggests a facilitated transport in the presence of water.

[1] Yang *et.al., ACS Nano* **2018** 12(5), 4695-4701

O 74.5 Wed 16:00 WIL B321

The electronic structure of atomically-precise graphene nano-ribbons investigated by photoemission tomography — Lukas Reicht[1], Xiaosheng Yang[2,3], Larissa Egger[1], Philipp Hurdax[1], Francois C. Bocquet[2,3], Georg Koller[1], Petra Tegeder[4], Alexander Gottwald[5], Mathias Richter[5], Michael G. Ramsey[1], F. Stefan Tautz[2,3], Serguei Soubatch[2,3], and •Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany. — [3]Jülich Aachen Research Alliance (JARA), Germany — [4]Physikalisch-Chemisches Institut, Universität Heidelberg, Germany. — [5]Physikalisch-Technische Bundesanstalt (PTB), Germany.

In this contribution we investigate the electronic structure of armchair graphene nanoribbons (AGNRs) by means of angle-resolved photoemission spectroscopy and density functional calculations. Specifically, using an orientated AGNRs with a width of 7 carbon atoms adsorbed on a stepped Au surface, we demonstrate how photoemission tomography can be used to shed light on the electronic structure of its frontier valence bands. We present a series of constant binding energy momentum maps which allow us to identify all relevant valence (sub)-bands of this graphene nanoribbon. By comparing theoretical results for free-standing and adsorbed ribbons, we investigate the degree of molecule-substrate hybridization and inter-ribbon interactions thereby demonstrating that photoemission tomography proves to be a powerful technique to study the electronic structure of such quantum confined 1D systems.

O 74.6 Wed 16:15 WIL B321

Tuning electronic transport of 1D coordination polymers by the choice of the transition metal: Fe, Co and Ni — •Aleš Cahlík[1], Christian Wäckerlin[1], Santhini Vijai Meena[1], Oleksander Stetsovych[1], Jesus Mendieta[1], Pingo Mutombo[1], Simon Pascal[2], Olivier Siri[2], and Pavel Jelínek[1] — [1]Institute of Physics, Czech Academy of Sciences, v.v.i., Czech Republic, — [2]Aix Marseille Université, CNRS, Marseille, France,

The choice of transition metal atom in organometallic complexes can significantly influence their electronic and spintronic properties. Here, we study the electronic transport through 1D coordination polymers contacted by the tip of a scanning probe microscope (SPM). The polymers are synthesized in-situ by co-deposition of Fe, Co or Ni atoms and the quinonediimine (2,5-diamino-1,4-benzoquinone-diimine) ligand onto Au(111). The combination of STM and nc-AFM allows for simultaneous measurement of the current, conductance and force gradient as a function of bias voltage and lifting height. We observe a distinct bandgap opening behavior depending on the incorporated metal element. In addition, we show the possibility to modulate the conductance of these wires between highly conductive and non-conductive by increased bias voltage or upon light illumination.

O 74.7 Wed 16:30 WIL B321

Nitrogen Doped Carbon Nanofiber Composites as Anode for Sodium-Ion Batteries — •Mo Sha, Long Liu, Huaping Zhao, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Recently, sodium-ion batteries (SIBs) have attracted increasing attention as an important supplement or alternative to lithium ion batteries (LIBs) due to the abundance of sodium resources and its much lower cost. A critical issue and great challenge in current battery research for the extensive application of SIBs is the development of earth-abundant and high-performance electrode materials. In various studies of these electrode materials, carbon nanofibers have been identified as promising anodes for SIBs, because of the low cost and environment friendly features. In this study, nitrogen-doped carbon nanofiber (NCNFs) have been synthesized by an electrostatic spinning technique and used as anodes for SIBs. The corresponding specific capacity can reach about 175 mA h g-1 at 0.1C after 100 cycles. The results demonstrate that this NCNFs composite is a promising anode material with good reversible capacity and cycling performance for SIBs.

O 74.8 Wed 16:45 WIL B321

Ultra Large Lifting Installations (ULLIS) on HOPG — •Tristan J. Keller, Georgiy Poluektov, Anna Jochemich, Anna Krönert, Stefan-Sven Jester, and Sigurd Höger — Kekulé-Institut für Organische Chemie und Biochemie, Bonn, Deutschland

Self-assembled monolayers at the solid/liquid interface on graphite (HOPG) are investigated by scanning tunneling microscopy (STM). Recently, we reported *i*-gonal arylene-alkynylene macrocycles ($i =$

3,4,5,6) that form tiling patterns that correspond to the macrocycle shapes and the interdigitation of adjunct -$OC_{16}H_{33}$ side chains.[1]

Here, we present a novel approach for supramolecular surface patterning incorporating a tetraphenylmethane building block into a shape-persistent macrocycle in order to address the volume phase above the substrate. We observe monolayers with lattice constants in the range of 10 nm that are independent of the exact substitution of the pillar unit (e.g. propargylic alcohol, or fullerene). In addition, we present cocrystals of these triangular species and a molecular hexagon. The research aims at a detailed understanding on how functional groups that point into the third dimension can be incorporated in appropriate systems.

[1] S.-S. Jester, E. Sigmund, S. Höger, *J. Am. Chem. Soc.* **2011**, *133*, 29, 11062-11065.

O 74.9 Wed 17:00 WIL B321

Atomic-scale mechanical evidence of surface-catalyzed gold-carbon covalent bonding — •Benjamin Lowe, Jack Hellerstedt, Dhaneesh Kumar, and Agustin Schiffrin — School of Physics and Astronomy, Monash University, Clayton VIC 3800 Australia

Surface-confined self-assembly is a versatile method for creating and tuning the properties of low-dimensional nanostructures. Here we study the results of gold atoms and dicyanoanthracene (DCA) molecules deposited on Ag(111) in ultrahigh vacuum, characterized at 5K using combined scanning tunneling and non-contact atomic force microscopies (STM/nc-AFM). We found that the two-dimensional metal-organic self-assembly was composed of close-packed DCA-Au-DCA units, in which a single Au atom binds covalently to a carbon atom at the anthracene ends. This conclusion is based on submolecular resolution ncAFM imaging achieved with a CO-functionalized probe, as well as STM manipulation demonstrating the robustness of these DCA-Au-DCA units. Further experiments performed on an atomically thin insulator (hexagonal boron nitride) suggest the covalent DCA-Au-DCA bonding is catalyzed by the Ag surface. We expect these findings to inform the pursuit of metal-organic frameworks predicted to host topological electronic properties [1].

[1] Zhang, L. Z. et. al. Nano Letters (2016). 10.1021/acs.nanolett.6b00110.

O 74.10 Wed 17:15 WIL B321

Methyl and Vinyl Functional Groups in On-Surface Synthesis — •Marco Di Giovannantonio[1], José I. Urgel[1], Shantanu Mishra[1], Kristjan Eimre[1], Aliaksandr V. Yakutovich[1], Carlo A. Pignedoli[1], Pascal Ruffieux[1], Uliana Beser[2], Qiang Chen[2], Zijie Qiu[2], Akimitsu Narita[2], Klaus Müllen[2], and Roman Fasel[1,3] — [1]Empa - Swiss Federal Laboratories for Materials Science and Technology, nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland — [2]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [3]Department of Chemistry and Biochemistry, University of Bern, 3012 Bern, Switzerland

On-surface synthesis has opened pathways to molecular nanostructures that have been inaccessible so far. Here, we demonstrate the successful use of methyl and vinyl groups to achieve one-dimensional (1D) polymers composed of repeat units with specific ring topologies.

Methyl groups are proven to undergo an oxidative cyclization to the neighboring phenyl, forming five-membered rings and affording unprotected indenofluorene isomers, some of which exhibit high radical character. Vinyl groups enable the formation of additional six-membered rings, affording benzo[k]tetraphene units after a stable intermediate with CH2 groups protruding out of five-membered rings.

The structure and electronic properties of the obtained polymers have been characterized by STM, nc-AFM, and STS, and supported by theoretical calculations. The observed reaction steps and products extend the knowledge of on-surface reactions to fine tune architectures and functionalities.

O 75: Metal Substrates: Growth Studies

Time: Wednesday 15:00–17:00 Location: WIL C107

O 75.1 Wed 15:00 WIL C107

Growth studies of the potential Rashba surface alloy Tl on Ag(111) — •Patrick Härtl and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

It is well known, that surface alloys of Ag(111) with heavy post-transition metals, such as the group V element Bi or the group IV element Pb, i.e., $BiAg_2$ [1] or $PbAg_2$ [2], respectively, exhibit a giant spin–orbit coupling resulting in Rashba spin-split surface states. Looking in the periodic system it can be speculated whether surface alloying of Ag with the group III element thallium (Tl) results in a comparable electronic structure. As a first step towards this goal we have studied the growth of Tl on Ag(111) by low-energy electron diffraction (LEED), Auger electron spectroscopy (AES), and scanning tunneling microscopy (STM). LEED reveals a $(\sqrt{3} \times \sqrt{3})$Tl/Ag(111)$R30^\circ$ structure at submonolayer coverage and additional $(4\sqrt{3} \times 4\sqrt{3})$ spots for thicker films. The intensity and sharpness of the $(\sqrt{3} \times \sqrt{3})$ is used to identify optimal growth conditions. The LEED results are compared to real space data by making use of Fourier transformed STM images. STM data obtained on Tl films with a thickness of several atomic layers still show a pronounced moiré pattern, thereby indicating a sizable rotation of the Tl lattice with respect to the underlying Ag(111) substrate. The results will be discussed by comparison with Bi and Pb films.

[1] L. El-Kareh *et al.*, Phys. Rev. Lett. **110**, 176803 (2013).
[2] L. El-Kareh *et al.*, New Jour. Phys. **16**, 045017 (2014).

O 75.2 Wed 15:15 WIL C107

Submonolayer growth of Te on Cu(111) — •Tilman Kisslinger, Andreas Raabgrund, Maximilian Ammon, M. Alexander Schneider, and Lutz Hammer — Lehrstuhl für Festkörperphysik, Universität Erlangen–Nürnberg, D–91058 Erlangen, Germany

Tellurium (Te) based alloys play an important role in metallurgy, thermoelectricity and photovoltaics [1]. Thus, an accurate knowledge of the crystallographic surface structure and elemental composition of such systems is the first step to any understanding of their diverse physical properties. We studied the adsorption of Te on Cu(111) for submonolayer coverages with quantitative low-energy-electron diffraction (LEED), scanning tunneling microscopy (STM) and density-functional theory (DFT).

Below Θ =1/12 ML we find Te atoms to form a disordered structure. Above this threshold a $(2\sqrt{3} \times \sqrt{3})R30^\circ$ structure evolves that is fully developed at a coverage of 1/3 ML. STM shows a well-ordered surface phase that is solved by our LEED-analysis (Δ E = 8.7 keV, R = 0.127) to consist of Te_2Cu_2 chains in hcp-sites of the first substrate layer in perfect agreement with the structure calculated by DFT. Furthermore, we show that the finding of a $(\sqrt{3} \times \sqrt{3})R30^\circ$ structure at similar coverages reported in [2] is the consequence of an adsorbate induced phase transition as observed e.g. for H_2 or CO.

[1]: Ibers J., Nat. Chem. **1**, 508 (2009)
[2]: Lahti et al., Surf. Sci. **622**, 35 (2014)

O 75.3 Wed 15:30 WIL C107

STM investigations of Bi thin films on oxidized and clean Nb(110) — •Robin Boshuis, Artem B. Odobesko, Johannes Jung, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Motivated by the still ongoing quest for topological superconductivity, the proximity coupling of strongly spin-orbit–coupled Bi films with superconducting substrates gained wide interest. In this context a precise control of the surface termination via the epitaxial relationship at the interface between the superconductor and the Bi film may crucially influence the electronic structure.

We perform STM and STS investigations to study the growth of Bi thin films on Nb(110). We find that the surface structure of Bi crucially depends on the surface quality of the niobium substrate. While Bi grows in a hexagonal (111) structure on the oxygen-reconstructed surface of Nb(110), deposition on the clean Nb surface results in a Bi(110) surface with a rectangular atomic lattice. The different expitaxial relationships of Bi on clean and oxygen-reconstructed Nb(110) offer a versatile platform to investigate strongly spin-orbit–coupled superconductors and their interaction with magnetic nanostructures towards topological superconductivity.

O 75.4 Wed 15:45 WIL C107

Investigation of the lithium fluoride growth on the silver (100) surface — •Vladyslav Romankov and Jan Dreiser — Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Lithium fluoride (LiF) has been shown to be an interesting material for spintronic applications [1], and it is a potential candidate for decoupling single-molecule magnets (SMMs) from metallic substrates, which helps to enhance their magnetic stability [2]. To understand the growth of LiF on Ag, we have investigated samples of up to a few nominal monolayers deposited in ultra-high vacuum from an effusion cell onto the Ag(100) surface held at room temperature. Our study combines scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and polarized X-ray absorption spectroscopy (XAS).

The XAS results show that the fluorine local environment of the samples is virtually identical to the one in bulk LiF, while the appearance of the linear dichroism is consistent with a small tetragonal distortion, arising from the LiF-substrate interaction. STM and LEED reveal that LiF forms islands with a dendritic shape, whose branches extend along the <010> directions of the Ag(100) plane. We also observe an inhomogeneous vertical growth of the dendrites with increasing amount of deposited material. By deposition onto the hot Ag(100) substrate, we expect to obtain flat, two-dimensional islands, which are suitable for decoupling of SMMs.

References: [1] - A. J. Drew et al., Nature Materials, **8**, 109, (2009); [2] - C. Wäckerlin et al., Advanced Materials, **28**, 5142, (2016).

O 75.5 Wed 16:00 WIL C107

Investigation of the stability of bimetallic surface alloys: A kinetic Monte Carlo study — •David Mahlberg and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

Bimetallic surfaces are attractive substrates for catalytic purposes, due to the possibility to tailor their structure and hence, their stability and reactivity on an atomic scale. This offers great potential, e.g., with respect to rational catalyst design. However, operation conditions are often extreme in terms of temperature and pressure. Therefore, it is necessary to have detailed knowledge about the properties and stability of surface alloys when composition and/or temperature is modified. In our work, we use first principles-based kinetic Monte-Carlo (kMC) simulations to analyse AgPd/Pd(111), PtRu/Ru(0001), and InCu/Cu(100) bimetallic surface alloys.

We have studied the stability of these surface alloys by monitoring the changes that occur via vacancy diffusion. In order to simulate vacancy diffusion, first-principles electronic structure calculations are used to derive the energy barriers that enter kMC simulations. Thus, the structure formation of surface alloys on macroscopic time scales and mesoscopic length scales as a function of composition and temperature can be monitored for varying concentrations of the alloyed metal, respectively. The energy barriers and diffusion behaviour are analysed in terms of the interaction between constituents that change with the particular local arrangements.

O 75.6 Wed 16:15 WIL C107

Comparative investigation of strain induced effects in Dy-Ag and Dy-Cu surface alloys — •Sina Mousavion, Johannes Seidel, Lu Lyu, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, Erwin Schroedinger Straße 46, 67663 Kaiserslautern, Germany

Intermetallic compound systems such as surface alloys offer the intriguing possibility to tailor the structural and electronic and ferromagnetic properties [1 ,2] in low dimensions. Here we focus on surface alloys formed between the lanthanide atoms and fcc(111) noble metal surfaces. These types of surface alloys are particularly interesting since their intermetallic structure is typically dominated complex Moiré pattern. We combine LEED and STM to determine the surface structure of two distinctive surface alloys: a Dy-Ag and a Dy-Cu surface alloy. Both reveal the formation of different incommensurate superstructures along with different Moiré patterns. We correlate these different Moiré patterns of to strain effects induced by the different lattice constant of the substrates. We propose that the surface strain in these surface alloys can have significantly influences of the magnetic order of lanthanide-noble metal surface alloys which has been reported for low sample temperature. [1] Nano Lett., 16, 4230*4235 (2016) [2] Phys. Rev. B 88, 125405 (2013)

O 75.7 Wed 16:30 WIL C107

Epitaxy on (quasi-)liquid surfaces: A new paradigm for 2D materials growth? — •Dominik Steiner, Thomas Mairegger, and Erminald Bertel — Physikalische Chemie, Universität Innsbruck, Österreich

Lattice matching is usually an important consideration when choosing templates for epitaxial growth. Recently, Lee et al. achieved large-scale single-domain growth of hexagonal Boron Nitride (h-BN) on a liquid gold surface[1]. We obtained excellent single-domain growth of h-BN on Pt(110), despite the vastly different symmetries of D_{3h} versus C_{2v}. We observed a transition from growth conditions yielding a strongly perturbed multi-domain film on a rough substrate to single-domain growth on large terraces at a critical temperature of ~1100 K[2].

Intensity analysis of low-energy electron diffraction spots shows the hallmarks of a true phase transition suggesting a relation to the deconstruction or the roughening temperature of the clean Pt(110) surface[3]. Paradoxically, smooth, nearly perfect film growth is obtained only above the roughening temperature. The observations raise questions about the role of lattice matching in 2D crystal growth. Apparently, a high surface atom mobility of the template at growth conditions is superior to precise lattice matching in promoting 2D epitaxial growth.

[1] Lee, J.S. et al., Science **362** , 817(2018).

[2] Steiner, D., Mittendorfer, F., Bertel, E., ACS Nano **13** , 7083(2019).

[3] Krzyzowski, M. A. et al., Phys. Rev. B **50** , 18505(1994).

O 75.8 Wed 16:45 WIL C107

Reaction of Na/Br-carbenoid on NaBr surface investigated by scanning tunneling microscopy — •abhijit bera[1], katharina dilchert[2], viktoria däschlein gessner[2], and karina morgenstern[1] — [1]Ruhr-Universität Bochum, Chair of Physical Chemistry I, Bochum, Germany — [2]Ruhr-Universität Bochum, Chair of Inorganic Chemistry II, Bochum, Germany

Understanding of active radicals is important as they are short-lived intermediates in almost all chemical reactions, but because of their limited life-time, there is very little fundamental knowledge about it. For investigating radicals on surface science approach, we have grown sodium bromide (NaBr) layers on Ag(111) at room temperature and investigated layer formation, atomic resolution, defects and a moiré pattern by scanning tunneling microscopy. We employ this spacer layer to analyse a carbenoid compound, which is a reactive intermediate of many reactions. Recently metal halide (M/X) carbenoids attracted interest of many chemists due to their strong electrophilic character. However, the major concern is the stability because of their tendency of M-X eliminations. In solutions, it is possible to stabilize the carbenoid by addition of metal salt. We have deposited the Na/Br carbenoid with the type of [Ph2P(S)]2CMX on Ag(111) and also on the NaBr surface at 100-110 K and imaged at 120-140 K.We found that this compound tends to dissociate on Ag(111) surface and lose its character. But on the NaBr surface it is uniformly distributed and keeps its shape intact, which strongly suggests that,Na/Br-carbenoid makes coordination with NaBr salt.

O 76: Plasmonics and Nanooptics V: Tunable Structures and Nanoparticles (joint session O/CPP)

Time: Wednesday 15:30–18:15 Location: WIL A317

O 76.1 Wed 15:30 WIL A317

Thermally regulated smart mid-infrared modulators enabled by phase-change materials and phase-transition materials — Xinrui Lyu[1], Andreas Hessler[1], Xiao Wang[2], Alfred Ludwig[2], Matthias Wuttig[1], and •Thomas Taubner[1] — [1]Institute of Physics (IA), RWTH Aachen University — [2]Institute for Materials, Ruhr-University Bochum

Phase-change materials (PCMs) and phase-transition materials (PTMs) both show a large contrast in their optical properties upon switching, enabling compact optical components with diverse functionalities like sensing, thermal imaging and data recording. However, their switching properties differ significantly, i.e., non-volatile for PCMs while volatile for PTMs. For the first time, we combined PCMs, $Ge_3Sb_2Te_3$ (GST) or $In_3Sb_1Te_2$ (IST), with the PTM VO_2 as active layers in the design of the smart mid-infrared modulators with switchable absorption, reflection, and transmission. The VO_2 is employed as a dynamic mirror, switching between transmission (semiconducting VO_2) and absorption modes (metallic VO_2) with continuously tuned amplitudes up to 90%. Meanwhile, the PCMs on top of the VO_2 are used either for continuously shifting the absorption peak (up to 1.8 μm) by switching GST or for switching between reflection (R=0.85) and absorption modes (A=0.99) by switching IST. Merging the concepts of static (PCMs) and dynamic (PTMs) thermal modulation, the presented combination of non-volatile PCMs and volatile PTMs empowers new generation optical components like dynamic thermal imaging and optical switches.

O 76.2 Wed 15:45 WIL A317

Programmable Phase-Change Plasmonics with $In_3Sb_1Te_2$ — •Andreas Hessler[1], Sophia Wahl[1], Till Leuteritz[2], Matthias Wuttig[1], Stefan Linden[2], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen — [2]Physikalisches Institut, University of Bonn

The high optical contrast of non-volatile phase-change materials (PCMs) between their switchable amorphous and crystalline structural phases enables exciting nanophotonic functionalities [1,2]. So far, the employed PCMs mostly have dielectric optical properties in both phases. Now, we introduce the next-generation PCM $In_3Sb_1Te_2$ (IST) for reconfigurable nanophotonics. In contrast to the commonly used PCMs, its optical properties change from dielectric to metallic upon crystallization in the whole infrared spectral range. We show how resonant metallic nanostructures can be directly written and erased in an IST thin film by a pulsed switching laser, enabling direct and reconfigurable lithography. With this new technology, we demonstrate striking resonance shifts of plasmonic nanoantennas of more than 4 μm, a programmable mid-infrared perfect absorber with nearly 90% absorptance as well as screening and nanoscale "soldering" of metallic nanoantennas. Our novel concepts of programmable phase-change plasmonics could enable inexpensive fabrication and improved designs of programmable plasmonic devices for infrared optics, sensing and telecommunications.

[1] M. Wuttig et al., *Nature Photonics* **11**, 465-476 (2017)
[2] F. Ding et al., *Advanced Optical Materials* **7**, 1801709 (2019)

O 76.3 Wed 16:00 WIL A317

Tunable Heterostructure Polaritonic Cavity — •Mohsen Janipour[1], Matthias Hensen[2], and Walter Pfeiffer[3] — [1]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, Bielefeld 33615, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, Bielefeld 33615, Germany

Realizing and designing of tunable cavities at the infrared frequencies is crucial for achieving novel integrated photonic circuits. In the infrared regime, semiconductors like GaAs can support the excitation of surface phonon polaritons in the Reststrahlen band with the ability to tune through carrier concentration. In this study, we explore a novel heterostructure cavity composed of a hollow circular hole drilled in an Ag film which is stacked on a GaAs substrate. We show that this cavity can support two types of resonant modes consisting of circular cavity resonant modes and the surface modes due to the excitation of polaritonic modes in the Reststrahlen band. We indicate that the polaritonic modes can be tuned through controlling the distribution of the substrate*s carriers in the Reststrahlen band.

O 76.4 Wed 16:15 WIL A317

Silicon Metasurfaces for Nonlinear Holography and Wavefront Control — •Bernhard Reineke[1], Basudeb Sain[1], Ruizhe Zhao[2], Luca Carletti[3], Bingyi Liu[4], Lingling Huang[2], Costantino De Angelis[5], and Thomas Zentgraf[1] — [1]Department of Physics, Paderborn University, Warburger Straße 100, D-33098 Paderborn, Germany — [2]School of Optics and Photonics, Beijing Institute of Technology, Beijing 100081, China — [3]Department of Information Engineering, University of Padova, 35131 Padova, Italy — [4]Institute of Modern Optics, Department of Physics, Harbin Institute of Technology, Harbin 150001, China — [5]Department of Information Engineering, University of Brescia, 25123 Brescia, ItalyNational Institute of Optics (INO), CNR, 25123 Brescia, Italy

Metasurfaces based on dielectric nanostructures are an ideal platform for nonlinear optical experiments (such as third-harmonic generation). They provide high damage thresholds and strong nonlinear responses; Therefore, many works show progress dielectric metasurfaces with high nonlinear conversion efficiency. However, in achieving nonlinear wavefront control, less progress has been made. Therefore, we show the nonlinear wavefront control for the third-harmonic generation with a silicon metasurface. We choose a geometric phase approach to encode phase gradients and holographic images on a dielectric metasurface. In our experiment, we demonstrate the wavefront control and the multiplexed reconstruction of holograms at the third-harmonic wavelength. Our approach provides a simple principle for designing metasurfaces for nonlinear optical applications with dielectric building blocks.

O 76.5 Wed 16:30 WIL A317

Polarization-selective orbital angular momentum multiplexed meta-hologram — •Basudeb Sain[1], Hongqiang Zhou[2], Yongtian Wang[2], Christian Schlickriede[1], Lingling Huang[2], and Thomas Zentgraf[1] — [1]Department of Physics, Paderborn University, Warburger Straße 100, 33098 Paderborn, Germany — [2]School of Optics and Photonics, Beijing Institute of Technology, Beijing, 100081, China

Metasurface holography has the advantage of realizing complex wavefront modulation together with the progressive technique of computer-generated holographic imaging. Despite of having the well-known light parameters, like amplitude, phase, polarization and frequency, the orbital angular momentum (OAM) of a beam can be regarded as another important degree of freedom. Utilizing the orthogonality between different OAM modes and the OAM conservation law, here, we demonstrate orbital angular momentum multiplexed polarization-encrypted holography using a birefringent metasurface. The polarization selectivity of such metasurface relies on the birefringent response of the incident light. The holographic information can only be reconstructed with exact topological charge and a specific polarization state, providing an unprecedented advantage for holographic encryption. By using an incident beam with different topological charges as erasers, we mimic a super-resolution case for the reconstructed image, in analogy to the well-known stimulated emission depletion (STED) technique in microscopy. Such technique can open new avenues for beam shaping, optical camouflage, data storage, and dynamic displays.

O 76.6 Wed 16:45 WIL A317

Mode conversion in tilted plasmonic nanocones confirmed by second harmonic imaging — Christoph Dreser[1], Dominik A. Gollmer[1], Godofredo Bautista[2], Xiaorun Zang[2], Dieter P. Kern[1], Martti Kauranen[2], and •Monika Fleischer[1] — [1]Institute for Applied Physics and Center LISA+, Eberhard Karls University of Tübingen, Germany — [2]Laboratory of Photonics, Tampere University, Finland

Plasmonic nanocones offer strong, highly localized near-fields at the cone apex that can be utilized for applications in microscopy and sensing. However, for an efficient excitation of the tip mode the electric field vector of the exciting electromagnetic wave needs to have a significant component parallel to the vertical axis. To enable the excitation of the tip mode under vertical illumination, two processes for the nanofabrication of tilted gold nanocones with defined tip displacements are presented. The asymmetric geometry supports the transformation of an in-plane electric far-field to an out-of-plane plasmonic excitation. Extinction spectra and corresponding simulations will be shown, in which cones with different tilting angles are illuminated under various illumination angles. The tip excitation is confirmed by the nonlinear optical properties of the nanocones observed in second harmonic generation scanning microscopy with cylindrical vector beams.

[C. Dreser et al., Nanoscale 11, 5429 (2019)]

O 76.7 Wed 17:00 WIL A317

Hydrogen Sensing with Palladium-based Perfect Absorber under variable ambient pressures — •Ramon Walter[1], Florian Stern[1], Ediz Herkert[1,2], Tobias Pohl[1], and Harald Giessen[1] — [1]University of Stuttgart, Germany — [2]ICFO - The Institute of Photonic Sciences, Castelldefels (Barcelona), Spain

The increasing C02-content makes it necessary to replace the fossil energy carrier by alternative climate-neutral energy sources. Hydrogen has the potential to be one of this new energy sources. However, this gas has a high potential risk when mixed with oxygen. A reliable and sensitive sensor is needed to reduce this risk and safe lives.

Previous works showed that palladium is an ideal material for such a sensor. Nanoparticles made out of palladium will change under hydrogen pressure their lattice constant and consequently their dielectric properties. This will have a measurable influence of their optical properties depending on the hydrogen content in the lattice.

In this work, we investigate the potential of such palladium based perfect absorber devices as hydrogen sensor under different variable ambient pressures, which is required for a number of technically relevant applications. We believe that this should extend the range of possible applications without increasing a potential risk, as the sensor works pure optical and is completely separated by any kind of evaluation electronics. Furthermore, means to shield the sensor from contamination with other gases and the consequences for our sensing geometry are discussed.

O 76.8 Wed 17:15 WIL A317

Colloidal quantum dots coupled to electrically connected optical antennas — •Patrick Pertsch, René Kullock, Monika Emmerling, and Bert Hecht — NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany

Semiconductor quantum dots (QDs) attract a lot of interest due to their tunable light emission, high efficiency and single-photon characteristics. Combining them with optical antennas can not only lead to strong coupling [1] but also to enhanced and directional emission. To achieve that the QDs have to be positioned accurately within the antenna which, in the past, has been realized by complex and time consuming processes [2,3].

Here we report on a much simpler process, utilizing dielectrophoresis, to load the gap of electrically connected antennas with colloidal QDs. The QDs are positioned accurately inside the 30-nm gaps of the antennas, show strong photoluminescence and are promising for electro-optical applications. The reported method allows the preparation of QD-antenna systems within a few minutes.

[1] H. Groß et al., Science Advances 4, eaar4906 (2018)
[2] A. G. Curto et al., Science 329, 930-933 (2010)
[3] E. Tranvouez et al., Nanotechnology 20, 165304 (2009)

O 76.9 Wed 17:30 WIL A317

Plasmonic K-Au nanoparticles from helium droplet synthesis — •Roman Messner[1], Daniel Knez[2], Ferdinand Hofer[2], Wolfgang Ernst[1], and Florian Lackner[1] — [1]Technische Universität Graz, Institut für Experimentalphysik, 8010-A — [2]Technische Universität Graz, Institut für Elektronenmikroskopie und Nanoanalytik, 8010-A

We report on experiments on K-Au nanoparticles produced under UHV conditions by synthesis in helium nanodroplets. The particles are fabricated by coagulation of metal atoms after pickup by the cold droplets. The employed experimental techniques encompass in-situ spectroscopy as well as ex-situ investigations via transmission electron microscopy (TEM). Plain K clusters solvated in helium droplets exhibit a strong resonance at about 600 nm. The position of the resonance, thereby, depends on the K partial pressure in the pickup region, i.e. the size of the nanoparticles. After adding a gold shell-layer to the potassium particles, a blue shift of the resonance is observed, towards the well-known localized plasmon resonance of plain Au nanoparticles. An important aspect of our current research is to test the possibility of passivating the highly reactive K clusters with a Au shell, which would allow for the preparation of K-Au nanoparticle decorated substrates that can be investigated outside the UHV. First TEM investigations show promising results, opening up new perspectives for the production of novel material combinations for plasmonics with helium droplet based nanoparticle synthesis.

O 76.10 Wed 17:45 WIL A317

Synthesis of plasmonic Ag@ZnO core@shell nanoparticles inside superfluid helium droplets — •Alexander Schiffmann[1], Thomas Jauk[1], Daniel Knez[2], Harald Fitzek[2], Ferdinand Hofer[2], Florian Lackner[1], and Wolfgang E. Ernst[1] — [1]Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria — [2]Institute of Electron Microscopy and Nanoanalysis & Graz Centre for Electron Microscopy, Graz University of Technology, Steyrergasse 17, A-8010 Graz, Austria

Plasmonic Ag@ZnO core@shell nanoparticles in the sub 10 nm size regime have been synthesized in a unique way by employing the helium nanodroplet approach. A peculiarity of this low temperature technique, where the particles are formed within a superfluid helium environment, is the complete absence of solvents and surfactants. Scanning transmission electron microscopy (STEM) and energy dispersive X-ray spectroscopy (EDS) give insight into the composition and structure of the particles, revealing a very uniform thickness and shape of the ZnO shells surrounding the Ag cores. The oxidation state of the shell was investigated by ultraviolet photoelectron spectroscopy (UPS). Photoelectron spectra of Ag@ZnO, ZnO, and Ag nanoparticles have been recorded by two-photon photoelectron (2PPE) spectroscopy. The employed laser with a photon energy of 3 eV is resonant to the localized surface plasmon in Ag. In the case of Ag and Ag@ZnO an excitation of this plasmon gives rise to an increased yield of electrons with high kinetic energy.

O 76.11 Wed 18:00 WIL A317

Helium Droplet Mediated Synthesis of Rhodamine B Functionalized Au Nanoparticles — Roman Messner[1], Harald Fitzek[2], Wolfgang E. Ernst[1], and •Florian Lackner[1] — [1]Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [2]Institute of Electron Microscopy and Nanoanalysis & Graz Centre for Electron Microscopy, Graz University of Technology, Steyrergasse 17, 8010 Graz, Austria

Helium nanodroplets provide a new route for the synthesis of plasmonic nanoparticles. [1] Metal atoms are picked up by the droplets and agglomerate to particles, subsequent deposition on surfaces allows for the fabrication of plasmonic nanoparticle films without any solvents or surfactants. We show that the approach can also be used to produce complexes consisting of a plasmonic nanoparticle surrounded by a shell of molecules on the example of Au particles and rhodamine B. Surface enhanced Raman spectroscopy (SERS) indicates that the formed complexes stay intact after deposition. Our current efforts are geared towards the study of interactions between plasmon oscillations in the metal particles and the attached molecules. Therefore, experiments are carried out in-situ, while the particles are solvated in the helium droplets, employing laser induced fluorescence spectroscopy. The rhodamine B dye molecules are excited by a 532 nm laser, the detected fluorescence signal is found to be strongly quenched as soon as Au nanoparticles are added to the helium droplet.

[1]...Eur. Phys. J. D, 73 (5), 104 (2019)

O 77: Poster Session - 2D Materials: Stacking and Heterostructures

Time: Wednesday 18:15–20:00 Location: P2/EG

O 77.1 Wed 18:15 P2/EG

Electronic transport in graphene on monolayer hexagonal boron nitride on the local scale — •Benno Harling, Anna Sinterhauf, and Martin Wenderoth — IV. Physikalisches Institut, Universität Göttingen, Germany

The promising electronic transport properties of the first true two-dimensional material graphene are known to be strongly affected by interactions with the substrate below the graphene sheet. One method currently being considered to reduce this influence is the use of suitable dielectric substrates such as boron nitride.
Here, we use the AFM-based method of Kelvin probe force microscopy with additionally applied in-plane bias voltage [1] to investigate the local electronic transport properties of the commercially available van-der-Waals-system monolayer graphene on monolayer hexagonal boron nitride on SiO_2 under ambient conditions. Our measurements reveal a highly inhomogeneous transport behavior. We find a strongly locally varying potential gradient as well as local voltage drops. These local voltage drops depend on the direction of the current flow through the sample and on the current density. The asymmetric behavior of the device under current flow reversal is additionally observed in macroscopic measurements. Furthermore, we find a dependence of the sheet resistance on temperature and propose a model based on a resistor network consisting of ohmic resistors and diodes, with which it is possible to describe large parts of the experimental findings. Financial support by the DFG through project We 1889/13-1 is gratefully acknowledged.
[1] Willke et al., Carbon 102, 470-476 (2016)

O 77.2 Wed 18:15 P2/EG

Substrate dependent energy level alignment at a hybrid transition metal dichalcogenide monolayer/molecular semiconductor interface — •Jie Ma[1,2], Patrick Amesalem[1], Xiaomin Xu[3], Thorssten Schultz[1,2], Dongguen Shin[1,2], and Norbert Koch[1,2] — [1]Institut für Physik & IRIS Adlershof, Humboldt Universität zu Berlin, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Germany — [3]Tsinghua-Berkeley Shenzhen Institute (TBSI), China

Combining transition metal dichalcogenides (TMDCs) and molecular semiconductors (MSCs) is an attractive route for forming van der Waals heterostructures[1] with novel (opto-)electronic properties. Such properties are expected to strongly depend on the energy level alignment at the corresponding interfaces, which may also be influenced by the employed supporting substrate[2]. In particular, a detailed microscopic understanding of the impact of the substrate electrical properties on the energy level alignment at TMDC/MSC interfaces is still lacking. Here, we determined by angle-resolved ultraviolet and X-ray photoelectron spectroscopy the electronic band line-up at a WS2/C60 interface supported by either an insulating or a semi-metallic substrate. These insights can be useful for future design of functional heterostructures with tailored (opto-)electronic properties based on the combination of 2D and molecular semiconductor materials.

[1] D. Jariwala. et al. Nano Lett. 16, 497-503 (2016).
[2] P. Soohyung. et al. Commun Phys. 2 (2019) 109.

O 77.3 Wed 18:15 P2/EG

Air tightness of hBN encapsulation and its impact on Raman spectroscopy of sensitive van der Waals materials — •Lorenz Bauriedl[1], Johannes Holler[1], Tobias Korn[2], Andrea Seitz[1], Furkan Özyigit[1], Michaela Eichinger[1], Christian Schüller[1], Kenji Watanabe[3], Takashi Taniguchi[3], Christoph Strunk[1], and Nicola Paradiso[1] — [1]University of Regensburg — [2]University of Rostock — [3]National Institute for Materials Science, Tsukuba

In this work, we study the air-tightness of hBN encapsulation of devices based on sensitive 2D materials, as e.g. $NbSe_2$. hBN encapsulation is the most common passivation method for a wide range of 2D material-based devices. We use Raman spectroscopy to monitor the photo-oxidation induced by intense illumination as a function of time for several encapsulation layouts. We demonstrated that full encapsulation in hBN effectively provides a long term protection against oxidation for samples kept in ambient conditions. The same does not hold for half encapsulated devices, i.e. with hBN applied only on the top. In this latter case, we observe a slow but relentless diffusion of oxygen in between the hBN layer and the SiO_2 substrate.

O 77.4 Wed 18:15 P2/EG

Raman Spectroscopy of layered magnetic systems — •Mainak Palit, Anudeepa Ghosh, and Subhadeep Datta — School of Physical Sciences, Indian Association for the Cultivation of Science, Kolkata, India

Metal phosphorus trichalcogenides (MPX3) have emerged as an exciting class of layered magnetic 2D materials for future spintronics. Retaining long range magnetic ordering even in the exfoliated few layers is the hallmark of 2D magnetism. Raman spectroscopy can be an effective probe to identify low-energy phonon modes and possible spin-phonon coupling in reduced dimension from bulk crystal. In this study, temperature dependent Raman Spectra of exfoliated iron phosporous trichalcogenides (FePS3) flakes reveal a distinct shift of the large wave number phonon peaks towards higher wavenumber as temperarure decreases. A clear deviation from standard anharmonic behavior below characteristic Néel temperature (TN) is also observed. Other low wave number symmetry modes exhibit temperature dependent non-anharmonic self-energy as a function of layer thickness below TN, related to the strong spin-lattice interaction due to short-range magnetic order. Energies and symmetries of the observed Raman-active modes are in agreement with DFT calculations. Below TN low wave number broad mode in the paramagnetic state(T>TN) splits into multiple distinct modes and evolve further into a possible magnon mode. We believe these results will pave way for possible spintronic applications exploiting magnons.

O 77.5 Wed 18:15 P2/EG

Towards high mobility graphene field effect transistors with ultraclean exposed surface ensuring scanning probe compatibility — •Rosen Sofroniev, Yanting Liu, Tjorven Johnsen, Sayanti Samaddar, and Markus Morgenstern — II. Institute of Physics B, RWTH Aachen University and JARA-FIT, Otto-Blumenthal-Str., 52074 Aachen, Germany

Providing large, clean surfaces of gated graphene and other 2D materials is the key challenge for investigating them by Scanning tunnelling spectroscopy (STS). Most of the fabrication processes that have resulted in exceptionally high mobility devices yet, have targeted transport measurements such that the 2D material is encapsulated or the surface cleanliness is not ensured. In this work, we assemble boron nitride/graphene stacks with a graphite back-gate on SiO2/Si substrate, with all contacts realized prior to the graphene transfer i.e. we transfer the graphene as the last step over a centrally placed graphite (gate)/hBN stack and two neighbouring contacted graphite flakes on either side that would serve as source and drain electrode. The final PMMA based dry transfer, ensures clean surfaces free of any resist and the possibility of parallel probing by STS and electronic transport at low temperature. In future application, this technique would allow transfer of air sensitive 2D material inside argon glove boxes.

O 77.6 Wed 18:15 P2/EG

A setup for time-resolved second-harmonic imaging microscopy to study charge-transfer processes in 2D heterostructures at cryogenic temperature. — •Marleen Axt, Ulrich Höfer, and Gerson Mette — Fachbereich Physik, Philipps Universität Marburg, Germany

Two dimensional materials like transition metal dichalcogenides (TMDC) have attracted tremendous interest in designing optoelectronic devices. Of special interest are vertically stacked 2D Van-der-Waals heterostructures and their charge-transfer processes including the formation of strongly bonded interlayer excitons. However charge transfer at atomically sharp interfaces has been found to be extremely rapid, occuring on a femtosecond time scale and therefore is rarely observed.

Here, we present an experimental setup to study ultrafast charge-transfer dynamics at cryogenic temperatures with time-resolved second-harmonic imaging microscopy. Symmetry-based nonlinear optical properties of 2D materials are used to determine the crystallographic orientation of individual layers. Pump-probe experiments are performed using a new laser system providing ultrashort laser pulses (< 30 fs) with tunable energies for both, pump and probe laser pulses. With high temporal and spatial resolution we investigate TMDC-monolayers and heterostructures including temperature-dependent measurements for systematic studies.

O 77.7 Wed 18:15 P2/EG

Growth and Characterization of van-der-Waals heterostructures prepared from modulated elemental precursors — •Fabian Göhler[1], Erik C. Hadland[2], Marisa Choffel[2], Aalaa Osman[1], Constance Schmidt[1], Dietrich R.T. Zahn[1], Florian Speck[1], David C. Johnson[2], and Thomas Seyller[1] — [1]Chemitz University of Technology, 09126 Chemnitz, Germany — [2]University of Oregon, Eugene, OR 97403, United States

Modulated elemental reactants (MER) offer a new avenue to synthesize a virtually unlimited number of previously unknown heterostructures. In this two step synthesis, an amorphous precursor is first deposited by sequential physical vapor deposition. By precisely calibrating the thicknesses and layering sequence of the constituents to mimic the targeted structure, it is possible to crystallize the precursor into a layered thin film via annealing in inert atmosphere. Due to the structuring of the precursor on an atomic level, the necessary energy input as well as layer intermixing during crystallization is reduced, enabling the synthesis of metastable structures with arbitrary complexity. [1] Recently, we were able to push the MER synthesis towards the two-dimensional limit by preparing a one monolayer thick, nanocrystalline layer of $MoSe_2$ on a substrate of epitaxial graphene on SiC. [2] Building on these results, we are now exploring the incorporation of different types of bismuth selenide layers into the heterostructure to tune the electronic and structural properties of the $MoSe_2$.

[1] Westover et al., *J. Solid State Chem.* **236**, 173 (2016).

[2] Göhler et al., *Phys. Stat. Sol. B* **256**, 1800283 (2018).

O 77.8 Wed 18:15 P2/EG

Probing two-dimensional magnets with single spin magnetometer — •Qi-Chao Sun[1], Tiancheng Song[2], Rainer Stöhr[1], Xiaodong Xu[2], and Jörg Wrachtrup[1,3] — [1]3. Physikalisches Institut, Universität Stuttgart, Stuttgart 70569, Germany — [2]Department of Physics, University of Washington, Seattle, Washington 98195, USA — [3]Max Planck Institute for Solid State Research, Stuttgart 70569, Germany

The two-dimensional (2D) magnets, which show novel phenomena due to the reduced dimensionality, open up opportunities to understand the magnetic properties in materials as well as design new spintronic devices. Here, we report our recent measurement on the atomically thin chromium trihalides materials by using a cryogenic scanning magnetometer based on a single nitrogen-vacancy (NV) center in a diamond tip. By quantitatively measuring the stray magnetic field of the material, we reconstructed the magnetization with a spatial resolution of ~80 nm, which is consistent with the previously reported value. Moreover, the scanning NV magnetometer is also capable of detecting the AC magnetic field generated by spin fluctuation and spin-wave, paving a new way of studying the 2D magnets.

O 78: Poster Session - Focus Session: Functional Molecules at Surfaces - Motion and Intramolecular Processes

Time: Wednesday 18:15–20:00 Location: P2/EG

O 78.1 Wed 18:15 P2/EG

The influence of the screening towards the properties of phthalocyanine monolayer structures — •T.T.Nhung Nguyen, T.N.H. Nguyen, T. Sollfrank, and C. Tegenkamp — TU Chemnitz, Germany

Proximity effects due to molecular monolayers on two-dimensional materials, e.g. on epitaxial graphene, is a promising approach to modify the properties of the delocalized charge carriers. Thereby, long-range dispersing forces between the molecules and of the molecular film with the substrate provide a high degree of flexibility to realize various phases. Moreover, the concomitant screening of the substrate adds a further degree of freedom to alter the properties of the molecular film. Using STM/STS, we investigated the electronic properties of shuttlecock-like PbPc and planar magnetic MnPc on epitaxial graphene on SiC(0001) and compared with results on highly oriented pyrolytic graphite (HOPG). The incommensurate ratio of the graphene lattice with the molecular size fosters the growth of densely packed and chiral PbPc monolayers, with similar lattice parameters on monolayer graphene (MLG) and quasi-free monolayer graphene (QFMLG). The pronounced difference of the electronic structure is related to the different dielectric screening. On contrast, magnetic MnPc on MLG shows zig-zag like structures coexisting with a square unit cell, seen for PbPc. Such effects were not found for Pc/HOPG despite the same surface structure of graphene and graphite. Apparently, the dielectric screening of the 2D and 3D versions of the C-sp2 allotrope is different and modifies the molecular interaction scheme.

O 78.2 Wed 18:15 P2/EG

Fast one-dimensional motion of single molecules on a metal surface — •Donato Civita, Grant J. Simpson, and Leonhard Grill — Department of Physical Chemistry, University of Graz, Austria

Molecular motion on crystalline surfaces is of great importance to understand fundamental physical and chemical properties as well as in the field of heterogeneous catalysis. We studied the lateral motion of molecules over a Ag(111) surface by scanning tunnelling microscopy (STM). Single molecules are observed in a stable adsorption orientation, but by manipulating the molecules with the STM tip they can be reoriented into an orientation where they move much more easily. This behaviour will be discussed in terms of incommensurability, which creates a low diffusion barrier, and molecule composition as we have compared different molecules. It turns out that the implementation of halogen atoms surprisingly does not alter the effect of the fast motion, but increases the adsorption energy and stability of the molecule in one orientation and consequently the one-dimensionality of the motion.

O 78.3 Wed 18:15 P2/EG

Covalent-Coupling Reaction of Aromatic Aldehyde on Ag(111) — •Nan Cao, Maryam Ebrahimi, Alexander Riss, Aleksandr Baklanov, Knud Seufert, Eduardo Corral Rascon, Willi Auwärter, and Johannes V. Barth — Physics Department E20, Technical University of Munich, D-85748 Garching, Germany

Surface-confined reactions offer a promising pathway for the controlled synthesis of two-dimensional (2D) molecular networks. The 2D structures can be further characterized at an atomic scale resolution using scanning probe microscopy techniques. Within the last decade, many organic reactions have been investigated on metal single crystal surfaces, for examples, Ullmann-coupling, Glaser-coupling, and Schiff-base condensation. Here, we report on a new coupling reaction of aromatic aldehyde molecules on Ag(111) under ultrahigh vacuum conditions. The deposition of aldehyde reactants on Ag(111), following a post-annealing treatment, resulted in the formation of an polymeric network. Our atomic force microscopy and scanning tunnelling microscopy data indicate the linkage of aldehyde groups in the periphery of the reactants. Furthermore, we propose a reaction pathway enriched from our complementary X-ray photoelectron spectroscopy and density functional theory calculations data. Our data suggest on an unprecedented on-surface reaction strategy for designing novel 2D polymers.

O 79: Poster Session - Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interaction

Time: Wednesday 18:15–20:00 Location: P2/EG

O 79.1 Wed 18:15 P2/EG

Photoexcited oxirane modelled by ab initio nonadiabatic molecular dynamics — •Marvin Krenz, Wolf Gero Schmidt, and Uwe Gerstmann — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn,Germany

Oxirane, C2H4O, is a prototypical model system to explore photoreactions [1] and theirtheoretical modelling [2]. In this study we explore the prowess of constrained density-functional theory (cDFT) for optically excited states [3] in conjunction with Tully's fewest switches surface hopping [4] in describing the dynamics of photoexcited oxirane. Using nonadiabatic molecular dynamics in the Libra-X implementation [5], we study the influence of the initial atomic temperature on the photoreactions of oxirane.

Different atomic temperatures are modelled by initial velocities as well as by using the Nosé-Hoover thermostat. The results are compared to experimental [1] and earlier theoretical findings [2]. It is found that the cDFT approach in conjunction with an a temperature description based on the initial atomic velocities well explains the measured data on the reaction path distribution, while the usage of the thermostat tends to slow down the reactions.

[1] M. I. Masahiro Kawasaki et. al., Chemical Physics (1973).

[2]U. R. C. F. Enrico Tapavicza et. al., Journal of Chemical Physics 129 (2008).

[3] T Frigge et al., Nature 544, 207 (2017).

[4] JC Tully, J. Chem. Phys 93, 1061 (1990).

[5] E Pradhan et al., J. Phys.: Condens. Matter 30, 484002 (2018).

O 79.2 Wed 18:15 P2/EG

Electronic and optical properties of $CoFe_2O_4$ and Co_3O_4 including many body effects — •Shohreh Rafiezadeh, Hamidreza Hajiyani, and Rossitza Pentcheva — Department of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg

Cobalt oxides such as $CoFe_2O_4$ play an important role as anode material for photocatalytic water splitting, necessitating detailed understanding of their optical properties. Here, we investigate the electronic and optical properties of $CoFe_2O_4$ and Co_3O_4 based on density functional theory (DFT) calculations. Previous experimental studies of $CoFe_2O_4$ have reported a wide range of values for both indirect and direct band gap between 0.9-1.5 eV and 2.0-2.76 eV, respectively. While DFT+U indicates a direct one (1.38 eV), an indirect band gap of 1.81 eV emerges when many body effects are included. Comparison of the real and imaginary part of the dielectric function within the independent-particle picture, G_0W_0 and by solving the Bethe-Salpeter equation (BSE) indicates the relevance of excitonic effects. Support by the German Science Foundation (DFG), CRC/TRR 247, project B04 and a computational grant at MagnitUDE are gratefully acknowledged.

O 79.3 Wed 18:15 P2/EG

Electron-phonon interaction in hybrid inorganic/organic systems: implementation within the LAPW formalism — •Ignacio Gonzalez Oliva, Fabio Caruso, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Electron-phonon interactions (EPI) are ubiquitous in condensed matter and manifest themselves in a wide range of physical phenomena, such as the temperature dependence of the electrical resistivity and the emergence of conventional superconductivity. While in the last decade computational tools to study EPI in crystalline solids from first principles have become accessible, their application to hybrid inorganic/organic systems (HIOS) and interfaces is still hindered by the high computational cost of EPI calculations. We are developing an effective first-principles approach to extend EPI calculations to HIOS. Considering the vibrational properties of the constituents, we include their effects in the electronic properties of the hybrid system. This approach is being implemented in the `exciting` code, a full-potential all-electron code based on the linearized augmented plane-wave plus local orbitals (LAPW + lo) method. We will present details on the implementation and first applications.

O 79.4 Wed 18:15 P2/EG

An efficient representation of the Kohn-Sham potential and its use in density functional calculations — •Rudolf Zeller — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In the standard numerical treatment, the main effort is directed at an efficient description of the density, usually by applying a judicious expansion in basis functions or a sophisticated choice of numerical grid points. The potential $V(\underline{r})$ is then represented by its matrix elements determined by the basis functions or grid points. In view of the computational cost, this number is reduced as much as possible, often by replacing the real potential with a pseudopotential.

In my presentation, instead, the emphasis is put on an efficient description of the potential in terms of spherical harmonics used to expand the potential at the nuclear sites. The potential is understood as an integral operator $V(\underline{r})\delta(\underline{r}-\underline{r}')$ approximated by $\delta(r-r')\sum_{lml'm'} Y_{lm}(\underline{r})Y_{l'm'}(\underline{r}')V_{lml'm'}(r)$ with a finite number of spherical harmonics. For such potentials the density can be evaluated practically exactly by a mathematically rigorous expression [1]. The calculated densities converge fast with increasing number of harmonics and excellent total energies are obtained at low computational cost.

[1] R. Zeller, J. Phys.: Condens. Matter 27, 306301 (2015).

O 79.5 Wed 18:15 P2/EG

Adaptive meshes for Brillouin zone integrations — •Patrick Dieu[1], Maria Troppenz[2], and Claudia Draxl[3] — [1]Humboldt Universität zu Berlin, Germany — [2]Humboldt Universität zu Berlin, Germany — [3]Humboldt Universität zu Berlin, Germany

Adaptive schemes for selecting k-points in the Brillouin zone allow for accurate and efficient calculations of integrals in electronic-structure theory. Such techniques generate dense samplings in regions with high relevance for the integrand while maintaining a coarse grid in other regions. We implement a scheme for k-mesh refinement in the density-functional-theory package exciting [1] for the main purpose of calculating transport coefficients with high efficiency. The transport coefficients are obtained by solving the linearized Boltzmann equation [2]. Our method devides the Brillouin zone in cuboidal blocks with the k-points as vertices. We investigate the performance of this approach with respect to several parameters, e.g. the initial k-grid and different termination criteria of the algorithm. Our adaptive scheme can also be used for a precise determination of the Fermi surface. Overall, we demonstrate that this adaptive scheme saves a significant amount of computational time in comparison to methods using equispaced k-grids.

[1] A. Gulans, et al., J. Phys.: Condens. Matter 26, 363202 (2014).

[2] B. R. Nag; Electron Transport in Compound Semiconductors, Springer, New York, pp. 171-229 (1980).

O 80: Poster Session - Graphene: Adsorption, Intercalation and Doping

Time: Wednesday 18:15–20:00 Location: P2/EG

O 80.1 Wed 18:15 P2/EG

Low-energy ion implantation of Cobalt in graphene investigated by scanning tunneling microscopy — •Anna Sinterhauf[1], Manuel Auge[2], Felix Junge[2], Philip Willke[3], Hans Hofsäss[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Universität Göttingen, Germany — [2]II. Physikalisches Institut, Universität Göttingen, Germany — [3]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Republic of Korea

To tailor the properties of a graphene sheet by band structure engi-

neering, the issue of doping is decisive to turn graphene into a true device material. For this purpose, a direct incorporation of foreign atoms into the graphene layer by low-energy ion beam implantation has shown to be a versatile method [1] as demonstrated for B and N. Here, we report on the successful implantation of Cobalt atoms into the graphene lattice achieved by low-energy Cobalt implantation at an ion energy of 20eV. After transfer through air, reinsertion into UHV and annealing at 400°C for 30 minutes, the structural and electronic properties of the ion implanted epitaxial graphene are investigated by scanning tunneling microscopy and spectroscopy (STS). Contrary to B and N [1], we find a negligible charge transfer from Co to graphene in agreement with theoretical considerations [2]. In addition, at the topographic position of the defects, STS reveals a pronounced peak in dI/dV-spectra at zero bias voltage. Financial support by the DFG through project We 1889/13-1 is gratefully acknowledged.
[1] P. Willke et al., Nano Lett. 15(8), 5110-5115, 2015
[2] E. J. G. Santos et al., Phys. Rev. B 81, 125433, 2010

O 80.2 Wed 18:15 P2/EG

Doping of ta-C by ultra-low energy implantation — •Felix Junge, Manuel Auge, and Hans Hofsäss — II. Institute of Physics, Georg-August-University Göttingen, 37077 Göttingen, Germany

Doping of graphene to change its electrical properties is highly desirable. To achieve this, we use a unique mass-selected ion beam deposition system, which makes it possible to work in an energy range of $10 < E < 600\,$eV for implantation and thus to implant into a 2D-lattice. In order to test the possible implantion in graphene with different elements, we perfomed ultra low-energy (10-25 eV) implantation in layers of tetrahedral amorphous carbon (ta-C) on silicon. Fluence and retention rate were measured after implantation with RBS using a 860 keV He^{2+}-beam and NRA to analyze the light elements using a 430 keV proton beam. With this setup a detection limit for e.g. boron of about $6 \cdot 10^{13}$ B/cm^2 in 1000 s could be achieved. Furthermore, the measurement results were compared with simulations done with SDTrimSP. Successful implantation was possible for e.g. He, B, N, Ne, P, Ar, Cr, Mn, Fe, Co, Se and Au.

Financial support by the DFG through project We1889/13-1 is gratefully acknowledged.

O 80.3 Wed 18:15 P2/EG

Structural and local electronic properties of clean and Li-intercalated graphene on SiC(0001) — •Maryam Omidian[1], Nicolas Néel[1], Eberhard Manske[2], Jörg Pezoldt[3], Yong Lei[1], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [2]Institut für Prozess- und Sensortechnik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [3]Institut für Mikro- und Nanoelektronik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

A low-temperature scanning tunneling microscope has been used to study the graphene-SiC(0001) interface before and after Li intercalation. For clean graphene, spectroscopy of the differential conductance corroborates previous theoretical findings for the interfacial electronic structure (M. Kajihara et al., Surf. Sci. 647, 39 (2016)). An unambiguous relation between the spectroscopic onset of the interface states with changes in STM images is presented. Li intercalation induces a shift of the Dirac point to lower energies and efficiently suppresses the interface states.

O 80.4 Wed 18:15 P2/EG

Intercalation of silver between graphene and silicon carbide studied by PEEM and AFM — •Philipp Weinert[1,2], Richard Hönig[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]TU Dortmund, Dortmund, Deutschland — [2]DELTA, Dortmund, Deutschland

Due to its outstanding electronic and mechanical properties graphene is of particular interest for many applications, for example as a new material in transistor applications, or constructing microscale structures.

In this study the intercalation of silver between one layer of graphene, the so called buffer layer, and the silicon carbide substrate is investigated. Other studies have shown, that covalent bounds between the silicon carbide and the buffer layer are released by intercalation, which leads to quasi free standing graphene.

To achieve the intercalation, samples have been coated with thin silver-films of different thicknesses. Subsequently, the samples were annealed to initiate the intercalation. In different steps of the annealing process, photoemission electron microscopy (PEEM) has been carried out to investigate the work function of the surface. This investigation has proven that silver intercalated underneath the buffer layer during the annealing. Furthermore, atomic force microscopy (AFM) has been carried out to investigate the topography of the samples after the intercalation. This study has shown that a small part of the silver does not intercalate, but forms islands on the surface.

O 80.5 Wed 18:15 P2/EG

Proximity superconductivity in hydrogen-intercalated graphene on $\boldsymbol{6H}$-SiC(0001) — •Tobias Birk[1], Fabian Paschke[1], Ulrich Starke[2], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

Here we investigate the superconducting proximity effect in hydrogen-intercalated graphene on $6H$-SiC(0001) by means of scanning tunneling microscopy and spectroscopy. We epitaxially grow Pb islands (width 10-50 nm, thickness 4-15 monolayers) on top of the quasi-free standing monolayer graphene. Low bias tunneling spectra measured at 1.8 K show a bulk-like BCS gap on top of the islands. The critical field of the Pb islands is found to strongly correlate with size and number of monolayers. The variations of the proximity-induced superconducting gap is measured on graphene in the vicinity of Pb islands, both as function of spatial position and magnetic field strength. Our study provides a foundation for realization of graphene-superconductor heterostructures on large-scale SiC(0001) wafers suitable for future technological applications.

O 80.6 Wed 18:15 P2/EG

Hydrogen treatment of bilayer graphene — •Claus F. P. Kastorp[1], Andrew M. Cassidy[1], Anders L. Jørgensen[2], Marta Scheffler[1], Paolo Lacovic[3], Silvano Lizzit[3], Liv Hornekaer[1], and Richard Balog[1] — [1]Dept. of Physics and Astronomy, Aarhus University, Aarhus, Denmark — [2]The Mads Clausen Institute, SDU NanoSYD, Sønderborg, Denmark — [3]Elettra Sincrotrone Trieste, Basovizza, Italy

In single layer graphene on Ir(111), hydrogenation causes a tunable band gap, [1]. Starting with bilayer graphene on Ir(111), one may produce diamane, a 2D equivalent of diamond [2], with the same approach.

I will present the results of STM and XPS measurements of MBE grown bilayer graphene on Ir(111) exposed to either excited H$_2$ molecules or hot atomic hydrogen under different conditions.

The processes leading to different hydrogenated structures will be investigated and explained.

[1] Balog, et al. Nature materials 9.4 (2010): 315.
[2] Leenaerts, et.al., Phys. Rev. B, 80.24 (2009): 245422.

O 81: Poster Session - New Methods: Theory

Time: Wednesday 18:15–20:00 Location: P2/EG

O 81.1 Wed 18:15 P2/EG

Specular-diffusive decomposition of the transmission function — Michael Czerner[1,2], Jonas F. Schäfer-Richarz[1,2], and •Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Zentrum für Materialforschung (LaMa), Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

A conscious design of electronic transport is crucial for all nanoelectronic devices. This necessitates a precise understanding of the behaviour of electrons as they traverse a device. To this end, $k_\parallel$-resolved transmission maps provide a valuable tool for relating the observed phenomena, such as tunnel magnetoresistance effects, to microscopic processes. A description by slabs of material with a 1×1-supercell is insufficient when imperfections within the device are to be described. Impurities, dislocations, skyrmions, and thermal disorder may modulate the transport properties of a nanoelectronic device. In essence, such imperfections break translational invariance. Because most such defects are localized, the transmission can be projected onto the perfectly ordered leads of the transport system. Thus, a transmission map $T(k_{\|}, k'_{\|})$ connecting Bloch states in the left and right lead can be recovered. This transmission map may be split into a specular part, which is $k_{\|}$ conserving, and a diffusive part, which allows scattering between $k_{\|}$-vectors of the leads. We implemented this decomposition of transmission maps in our Korringa-Kohn-Rostoker code. As a test case, we show the transmission through iron bulk, where either atomic positions or their magnetic moments were randomly displaced.

O 81.2 Wed 18:15 P2/EG

PyFLOSIC: Insights, developments and progress — •Sebastian Schwalbe[1], Jakob Kraus[1], Kai Trepte[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Germany — [2]Central Michigan University, USA

We present the current status as well as new developments within PyFLOSIC [1,2], an Open-Source implementation of the Fermi-Löwdin orbital self-interaction correction (FLO-SIC) [3,4] based on the highly modular and modern PySCF code infrastructure. FLO-SIC aims to counter the well-known self-interaction error (SIE) of density functional theory (DFT). Within PyFLOSIC, the FLO-SIC method can be applied to any functional implemented in the libxc library. The new implementation is written in the python programming language. The choice of python enables fast developments to implement numerical speed-ups, algorithmic advances as well as the extension of the FLO-SIC method to new research topics. Various results for extended molecules and preliminary results for solids are discussed in detail.

[1] S. Schwalbe et al., arXiv:1905.02631 (2019)
[2] S. Schwalbe et al., JCC, vol. 40, 2843 (2019)
[3] S. Schwalbe et al., JCC, vol. 39, 2463 (2018)
[4] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)

O 81.3 Wed 18:15 P2/EG

Fermi-orbital descriptors: Interpretation, generation and bond order — •Sebastian Schwalbe[1], Jakob Kraus[1], Kai Trepte[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Germany — [2]Central Michigan University, USA

Fermi-orbital descriptors (FODs) [1,2] are the core elements of the Fermi-Löwdin orbital self-interaction correction (FLO-SIC) method [3,4]. We provide an interpretation of these FODs and suggest that they carry chemical bonding information. A central result is that optimized FOD positions forming an electronic geometry are in correspondence with conceptional expectations from Linnett's double-quartet theory, an extension of Lewis' theory of bonding. In addition, the implementation and application of independent methods for the automatic generation of these chemically important descriptors are discussed.

[1] S. Schwalbe et al., JCC, vol. 40, 2843 (2019)
[2] S. Schwalbe et al., arXiv:1905.02631 (2019)
[3] S. Schwalbe et al., JCC, vol. 39, 2463 (2018)
[4] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)

O 82: Poster Session - Organic Molecules on Inorganic Substrates: Networks and Overlayers

Time: Wednesday 18:15–20:00 Location: P2/EG

O 82.1 Wed 18:15 P2/EG

Surface properties of en-APTAS SAMs on ZnO surfaces — •Nurhalis Majid[1,2], Gerhard Lilienkamp[1], and Winfried Daum[1] — [1]Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstraße 4, 38678 Clausthal-Zellerfeld, Germany — [2]Research Centre for Physics, LIPI, Kawasan Puspiptek, 15314 Tangerang Selatan, Indonesia

Surface functionalization of ZnO nanowires with N-[3-(trimetoxylsilyl) propyl]ethylenediamine (en-APTAS) self-assembled monolayers (SAMs) provides the base for an NO2 gas sensor with high sensitivity and selectivity [1]. For a better understanding of the attachment of en-APTAS to the ZnO substrate, a comparative AFM, AES and XPS study of the chemical functionalization of undoped Zn-polar ZnO(0001) and nonpolar ZnO(11-20) single crystal surfaces with en-APTAS SAMs has been carried out. Monolayer films are readily deposited on ZnO(0001) by dip coating, while complete monolayer wetting of ZnO(11-20) was not achieved so far. An anomaly of the SiLVV/SiKLL Auger line intensity ratio for the Si atoms of the adsorbed en-APTAS layer is observed on both substrates. Possible implications of this anomaly and of incomplete hydrolysis of en-APTAS for the molecular adsorption geometry are discussed.

[1] M. W. G. Hoffmann et al., Adv. Mater. 26, 8017 (2014)

N. Majid would like to thank the Ministry of Research, Technology and Higher Education of the Republic of Indonesia (RISTEKDIKTI) for the RISETPro Ph.D. scholarship and Indonesian-German Centre for Nano and Quantum Technologies (IG-Nano) for support.

O 82.2 Wed 18:15 P2/EG

Surface-templating effect in the self-assembly of carboxyl-functionalized bridged triphenylamine molecules — •Kevin Dhamo[1], Tobias Müller[1], Martin Gurrath[1], Jia Liu[2], Mirunalini Devarajulu[2], Sabine Maier[2], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Department of Physics, FAU Erlangen-Nürnberg

Since carboxyl groups form strong hydrogen bonds, one would expect that self-assembly of carboxyl-functionalized molecules is dominated by molecule–molecule interactions. However, in STM and AFM studies of carboxyl-substituted dimethylene-bridged triphenylamine (CDTPA) molecules the formation of very different networks was observed for Au(111), NaCl(001) and KBr(001) substrates. By using density-functional theory (DFT) calculations we analyze in detail the molecule–substrate and the molecule–molecule interactions for the different binding motifs. We show how site-specific interactions and enhanced van der Waals attraction between the molecules at denser packing stabilize alternative network structures depending on the lattice constant of the substrate. The possibility to tune self-assembly of organic molecules via the substrate lattice constant offers another degree of freedom for the rational design of functional molecular structures on surfaces.

O 83: Poster Session - Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy

Time: Wednesday 18:15–20:00 Location: P2/EG

O 83.1 Wed 18:15 P2/EG

Steps towards higher harmonics pump-probe spectroscopy — •Julian Obermeier, Thorsten Schumacher, and Markus Lippitz — University of Bayreuth, Germany

In the last decade the field of nonlinear plasmonics has been growing rapidly. Many fascinating experiments have shown the nonlinear emission of complex nanostructures, methods to enhance the emission and that the nonlinear near field of nanostructures can be shaped remotely. Yet, also some fundamental questions are still unanswered, for example, how nonlinear plasmonic effects are connected to the band structure and especially the electronic occupation function. A well known way to cause time-dependent modifications of both is intense pulsed optical pumping. Interband absorption followed by Auger recombination as well as rethermalized electron distributions both lead to a transiently drastically increased electron temperature.

Here we investigate the influence of hot electrons on the nonlinear optical response of plasmonic particles and structures. This will not only give us new insight in the nonlinear processes themselves but also allow us to deterministically alter them. We present our higher harmonics pump-probe setup and experimental results of pump induced changes in the third harmonic emission of plasmonic structures.

O 83.2 Wed 18:15 P2/EG

Measuring Hot-Electron Dynamics by Pump-Probe Spectroscopy — •Fabian Paul, Julian Obermeier, Christoph Schnupfhagen, Thorsten Schumacher, and Markus Lippitz — University of Bayreuth, Germany

After excitation of a plasmonic structure with an ultrashort laser puls an athermal occupation function of electrons is generated that rethermalizes to a Fermi-Dirac distribution within about 15 fs. During the next tens of femtoseconds the most energetic electrons relax due to Coulomb interactions between each other and at last on a scale of several picoseconds interacting with the lattice structure relax back to thermal equilibrium. Due to the enormous improvement of super continuum lasers and pulse shapers in the last years, it is possible to generate femtosecond laser pulses and shape them nearly unlimited, so that one can easily do pump-probe experiments.

With this techniques it is now possible to measure the decay of these high energetic electrons on ultrafast timescales. We are using in the first step plasmonic nano-structures to increase the signal. The results will improve our understanding of the microscopic origin of plasmonic nonlinearities.

O 83.3 Wed 18:15 P2/EG

Nanoparticle-on-mirror systems for strong coupling with emitters — •Christoph Schnupfhagn, Thorsten Schumacher, and Markus Lippitz — Experimental Physics III, University of Bayreuth, Germany

Plasmonic nanostructures allow to increase the interaction with light by resonant oscillations of the conduction electrons. Over the last years, the nanoparticle-on-mirror geometry has received increasing interest, where plasmonic nanoparticles are placed above a metallic substrate. If the gap size between particle and substrate is on the order of only a few nanometers, the systems couple and form a cavity mode. In the literature, mode volumes as small as $40\,\mathrm{nm}^3$ have been realized. When incorporating emitters into the gap, this allows for strong coupling between emitter and the plasmonic mode. Here, we will present results on the spectroscopy of colloidal gold nanoparticles on top of crystalline gold flakes. Furthermore, we will give an outlook how emitters could be positioned in the cavity.

O 83.4 Wed 18:15 P2/EG

Coupling single quantum dots to plasmonic waveguide structures — •Michael Seidel[1], Gerhard Schäfer[1], Peter Schnauber[2], Armando Rastelli[3], Stephan Reitzenstein[2], and Markus Lippitz[1] — [1]Experimental Physics III, University of Bayreuth, Bayreuth, Germany — [2]Institute of Solid State Physics, Technische Universität Berlin, Berlin, Germany — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University, Linz, Austria

Integrated plasmonic nanocircuits are highly promising building blocks for future quantum optical applications. In combination with self-assembled quantum dots as stable, bright and narrow-band single-photon sources, ultra-compact nanocircuits operating below the diffraction limit can be designed. A crucial aspect is the coupling of the quantum dot emission into plasmonic waveguide modes. In this work, we propose a plasmon–quantum dot hybrid structure which offers a highly efficient coupling scheme due to enhanced light-matter-interaction. We perform numerical simulations to optimize the coupling efficiency and show first experimental steps towards fabricating the proposed structure.

O 83.5 Wed 18:15 P2/EG

Step towards Two Dimensional Electronic Spectroscopy (2DES) of a single molecule using fluorescence based detection scheme — •Sanchayeeta Jana, Christoph Schnupfhagn, and Markus Lippitz — Experimental Physics III, University of Bayreuth, Bayreuth, Germany

2DES is an ultrafast spectroscopic technique which can give us the information about the couplings between the molecular energy levels due to the added dimensionality. This technique uses two replicas of an ultrashort laser pulse with controllable delay between them to excite the sample and a third pulse probes the excited sample after some time. But performing this kind of experiments on a single molecule is extremely difficult since the absorption cross section of a single molecule is much smaller than the probe volume resulting very low signal to background noise ratio. To overcome this, fluorescence based detection scheme can be used where fluorescence from the excited state is measured using an additional 4th pulse.

In this work, we describe the experimental challenges for such an experiment on a single molecule and propose the convenient procedure to overcome those.

O 83.6 Wed 18:15 P2/EG

Quantifying quantum dot fluorescence in the near-field — •Niklas Stenger, Thorsten Schumacher, Jonas Albert, and Markus Lippitz — University Bayreuth, Chair Experimental Physics III

The spatial resolution in the far field is limited by diffraction. To overcome this limitation, atomic force microscopy can be used. We present a powerful tool to investigate the light-matter interaction on the nanoscale: an AFM combined with a time-correlated single photon counting setup to measure fluorescence as well as the probe topography. The AFM tip used to investigate the tip-induced quenching of quantum dots in the near-field. The influence of factors like tip geometry, tip-probe distance and wavelength on the fluorescence signal will be presented.

O 83.7 Wed 18:15 P2/EG

Spatially-resolved hyper spectral single quantum dot strong coupling — •Benedikt Schurr, Daniel Friedrich, Heiko Gross, and Bert Hecht — NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany

Strong coupling single emitters and plasmonic nano resonators at ambient conditions opens new prospects for applications of quantum technologies. In the past decade multiple types of photonic cavities and emitters were investigated. [1] However only recently it became possible to directly tune the coupling strength by means of scanning probe technology. [2]

Here, we report a qualitative hyperspectral analysis of strong coupling between single colloidal CdSe quantum dots and plasmonic nanoresonators fabricated at a scanning probe tip. When using precise helium ion beam milling to achieve sub 10 nm light localization, we observe an increased Rabi splitting of up to 160 meV. The larger splitting in combination with high-resolution scanning allows us to record spatially resolved maps of the coupling strength between the emitter and the plasmonic resonator mode.

[1] O. Bitton et al., Nanophotonics 8 (4), 559-575 (2019)
[2] H. Gross et al., Sci. Adv. 4, eaar4906 (2018)

O 83.8 Wed 18:15 P2/EG

Massive parallel heterogeneous assembly of single-crystalline Ag and Au spheres — •Daniel Schletz[1], Johannes Schultz[2], Martin Mayer[1], Anja Maria Steiner[1], Axel Lubk[2], Tobias König[1], and Andreas Fery[3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Germany — [3]Department of Physical Chemistry of Polymeric Materials TU Dresden, Germany

In pursuit of new optical properties, different materials and particle morphologies have been investigated in detail. Combining multiple of these building block types promises novel properties with respect to the single use thereof. Due to the nature of combinatorics, introducing more than a single building block leads to an exponential increase in parameter space, unable to be explored by established linearly scaling fabrication methods.

In an innovative approach, heterogeneous single particle lines of single-crystalline Ag and Au spheres are manufactured in a massive parallel approach by stochastic confinement assembly. By assembling billions of particles in one step, millions of combinations are generated. These ensembles are then studied in detail by electron energy loss spectroscopy (EELS) to reveal their plasmonic properties and to gain insight into heterogeneous coupling efficiencies.

O 83.9 Wed 18:15 P2/EG

Nano-scale Analysis of Surface Phonon Polaritons in $SrTiO_3$ using a scattering-type Scanning Near-field Optical Microscope — •Daniel Wendland[1], Julian Barnett[1], Marc Rose[2], Felix Gunkel[2], Regina Dittmann[2], and Thomas Taubner[1] — [1]Institute of Physics (IA) RWTH Aachen — [2]Peter Grünberg Institut, Forschungszentrum Jülich GmbH

Metasurfaces can arbitrarily manipulate light through resonant structures. Many metasurfaces are based on plasmonic materials, but phonon-based metasurfaces are on the rise, benefiting from the excitation of Surface Phonon Polaritons (SPhP) which can offer low losses and high propagation lengths [1]. $SrTiO_3$ (STO) could be an interesting candidate, because it supports strong phonon modes in its undoped state as well as nonvolatile resistive switching, which gives control over the local doping level. This switching process is reversible and could allow rewritable metasurfaces. To estimate the viability for SPhP-based resonator metasurfaces, we will investigate the SPhP behaviour in STO for different resonator geometries and doping levels. The latter allows us to gain a better understanding of plasmon-phonon-coupling [2], which is fundamental for this type of resonators. Here Scattering-type Scanning Near-field Optical Microscopy is applied to obtain nanoscale IR spectra and images. Using these results, we aim to predict the behaviour of STO resonator arrays and the viability of resistive switching for phonon-based metasurfaces.
[1] J. D. Caldwell et al., Nanophotonics, 4, 44 (2015)
[2] M. Lewin et al., Adv. Funct. Mater. 28, 1802834 (2018).

O 83.10 Wed 18:15 P2/EG

Towards Plasmonic Transistors - Plasmon damping on J-aggregated Squaraine dye coated gold films — •Christoph Bennenhei[1], Moritz Gittinger[1], Sven Stephan[1], Jennifer Zablicki[2], Arne Lützen[2], Manuela Schiek[1], Christoph Lienau[1], and Martin Silies[1] — [1]Carl von Ossietzky Universität Oldenburg — [2]Rheinische Friedrich-Wilhelms-Universität Bonn

Surface plasmon polaritons (SPPs) generated in metallic waveguides provide the possibility to manipulate light below the diffraction limit and are hence a first building block towards all-optical switching on the nanoscale. For ultrafast all-optical switching, coupling of the SPP modes to highly nonlinear excitonic materials [1] is necessary. We present J-aggregated squaraine dye (SQ) thin films as a promising candidate, since it shows a broad spectral resonance tunable by a thermal annealing process [2]. Here, we investigate power-dependent photobleaching of 10nm spin-coated ProSQ-C16 films in a confocal reflection spectroscopy setup, in a second step, we study the damping of the SPP modes propagating along the metal-SQ film interface by measuring the amount of light that outcoupled from pairs of grating couplers with varying distances. We find a significantly reduced decay length of the SPP for the SQ-metal interface around the excitonic resonance compared to an air-metal interface. High oscillator strength and photostability of SQ motivate future investigations of both optical pumping to invert damping rates as well as coherent energy transfer between SQ and SPPs. [1] P. Vasa, et al., Nature Photonics, 7 (2), pp 128-132 (2013) [2] M. Schulz, et al, Nat Commun 9, 2413 (2018)

O 83.11 Wed 18:15 P2/EG

Plasmoemission from a Plasmonic Nanofocus — •Jan-Henrik Herrig, Pascal Dreher, David Janoschka, Ping Zhou, Michael Horn-von Hoegen, and Frank Meyer zu Heringdorf — Faculty of Physics, University of Duisburg-Essen, Germany

Nonlinear photoemission from metal surfaces can be manipulated by strong plasmonic fields that are present during the emission process. Electron emission exclusively from such strong plasmonic fields (plasmoemission) can be distinguished from photoemission by spatio-temporal separation [1]. Obtaining the necessary field intensities requires efficient excitation of strong plasmonic fields.

We employed amplified laser pulses to excite surface plasmon polaritons in Archimedean spirals [2], which transiently form a diffraction-limited nanofocus if illuminated by circularly polarized light of the appropriate handedness. Plasmonic field intensities on the order of 10^{13} W/cm^2 were obtained at the Au(111) surface. The energetic distribution of the emitted electrons reveals the interaction with the plasmonic field.

[1] Podbiel *et al.*, Nano Letters 2017, 17(11): 6569-6574.
[2] Spektor *et al.*, Science 2017, 355(6330): 1187-1191.

O 83.12 Wed 18:15 P2/EG

Far-infrared sum-frequency generation wide-field microscopy — •Richarda Niemann, Riko Kiessling, Christopher Winta, Sören Wasserroth, Yujin Tong, Martin Wolf, and Alexander Paarmann — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Super-resolution microscopy typically makes use of nonlinear-optical effects, such as multi-photon absorption or stimulated emission depletion microscopy, to overcome the diffraction limit of optical beams. In the infrared spectral range, infrared-visible sum-frequency generation (SFG) can provide vibrational contrast with a spatial resolution ultimately limited by the visible SFG wavelength [1]. In particular for far-infrared SFG, this would enable imaging resolution well below $\lambda_{IR}/100$.

As a proof-of-concept, we recently demonstrated SFG microscopy beyond infrared wavelength of 10 μm for surface phonon polariton resonance imaging [2], using a scanning-focus method. In the current work, we introduce our new approach of SFG wide-field microscopy [1]. Specifically for high-intensity, low-repetition rate lasers, the usage of wide-field nonlinear imaging efficiently avoids otherwise ubiquitous sample damage problems. Here, the laser focal size is adapted to the field-of-view of the imaging system, reducing the laser fluence without deteriorating the microscopes resolution [1].

[1] Hoffmann et al.,Rev. Sci. Instrum, 3221 (2002)
[2] Kiessling et al., ACS Photonics, (2019)

O 83.13 Wed 18:15 P2/EG

Coupling of quantum emitters to localized photonic modes in disordered structures — •Patrick Folge, Mohsen JaniPour, Ruben Pompe, Felix Fenner, and Walter Pfeiffer — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

We investigate the coupling between quantum emitters to localized photonic modes in disordered dielectric waveguide structures. Localization of electromagnetic fields facilitates enhanced light matter interaction as it is commonly used in photonic crystal cavities. Periodic placement of holes in a two-dimensional waveguide forms photonic crystals with photonic band gaps that enable the formation of defect induces localized modes. Here we focus on disordered placement of these holes in a dielectric waveguide to achieve localization. Therefore we perform FDTD field simulations to calculate the Purcell factor, which can quantifies the light matter interaction. And we investigate the spectral features of the modes in the disordered structures. Thereby we find Purcell factors up to 25.

O 83.14 Wed 18:15 P2/EG

Low temperature scanning tunneling microscope light emission. — Liv Hornekaer and •Richard Balog — Aarhus University, Aarhus, Denmark

I will present modifications implemented in a Createc type low temperature scanning tunneling microscope (LT-STM) situated at iNano, Aarhus University, Denmark, expanding the capabilities of the setup towards tip-induced light emission experiments. Here, the light generated by tunneling electrons is collected by optics located nearby the STM head and then spectrally resolved and detected by a high efficiency LN2 cooled detector. The overall light detection system is optimized for the VIS-NIR range (400 nm - 1000 nm). The design and preliminary STM-light emission experiments on an Au(111) substrate and graphene covered SiC (0001) will be presented, demonstrating the full potential of the setup to reveal complex opto-electronic properties of the samples.

O 84: Poster Session - Solid-Liquid Interfaces: Reactions and Electrochemisty

Time: Wednesday 18:15–20:00 Location: P2/EG

O 84.1 Wed 18:15 P2/EG

Water-Based Electrolytes and Porous Tungsten Oxide in Electrochromic Cells — •Florian Eberheim, Thi Hai Quyen Nguyen, and Derck Schlettwein — Justus Liebig University Gießen, Institute of Applied Physics

Sputter-deposited tungsten oxide (WO_3) is commercially applied in light-managing devices (smart windows). The aim of this work consists in the preparation of porous WO_3 films and in the measurement of their electrochromic characteristics in contact to aqueous $LiCl$, $NaCl$, KCl and H_2SO_4 as alternatives to the established Li^+-containing organic electrolytes. The films were prepared by spin-coating a precursor solution with $poly(ethylene\ glycole)(PEG)$ of different molecular weight as additives and subsequent heating on a hot-plate at 250°C. Amorphous WO_3 was formed, shown by SEM and EDX. The transparent films were characterized by cyclic voltammetry and chronoamperometry while optical transmission was simultaneously monitored. It was shown that the films prepared with PEG as additive showed improved contrast of transmission compared to films prepared without additives. The water-based electrolytes led to the same blue coloration as the films in contact to Li^+. Electrolytes with protons as ions reached the best coloration characteristics, but led to faster degradation of the films. It was shown in this study that porous WO_3 films reversibly switch their optical transmission by intercalation of ions from water-based electrolytes. Such combinations could be a healthy and inexpensive alternative to the established state-of-the art.

O 84.2 Wed 18:15 P2/EG

Ab-initio studies of surface interactions on chevrel and spinel phases — •Katharina Helmbrecht — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

Due to substantial supply risks and safety issues associated with Li-ion batteries, there is a need for the development of post lithium batteries employing more abundant battery chemistries. However, this requires to identify new materials for electrodes and electrolytes. We will present first-principles electronic structure calculations based on density functional theory (DFT) to determine the most stable surface configuration of the chevrel phase ($\mathrm{Mo_6S_8}$) which is regarded as a promising electrode material for Mg-ion batteries.

In order to estimate the Mg ion mobility in the chevrel phase, Mg bulk diffusion barriers were determined. Furthermore, the adsorption and intercalation of aluminum chlorides were studied, since aluminum is often used as a 'collector' for the chloride ions left on the surface after magnesium intercalation. In addition, a magnesium-lithium hybrid battery model was investigated by comparing the intercalation of lithium chloride and magnesium chloride into the chevrel phase. In order to model the electrode-electrolyte interface, the interaction of an organo-aluminum electrolyte proposed by Aurbach et al.[1] was determined, which also allows addressing desolvation processes and first steps of the formation of the solid electrolyte interphase (SEI). The results will be compared to corresponding studies for the spinel phase ($\mathrm{Mg(SSc_2)_2}$).

[1] D.Aurbach et al., Nature **407**, 724-727 (2000).

O 84.3 Wed 18:15 P2/EG

Exploiting TEMPOL as redox mediator in water-based DSSCs — •Roberto Fantin, Andreas Ringleb, Raffael Ruess, Daniel Holzhacker, and Derck Schlettwein — Justus Liebig University Gießen, Institute of Applied Physics

In recent years, water-based dye-sensitized solar cells (DSSCs) emerged as a valid alternative to traditional organic solvent-based DSSCs, to improve stability and environmental compatibility, and reduce overall costs. Thus, all the other components of the device should be tailored to water. In this work, an aqueous solution of $4-hydroxy-2,2,6,6-tetramethylpiperidinyloxyl$ ($TEMPOL$) was investigated as a study case in combination with photoanodes made of TiO_2 nanoparticles sensitized by a commercial dye, $Y123$. The multiple interactions occurring between electrolyte, photoanode, and cathode are highlighted. $TEMPOL$ is a hydrophilic derivative of $TEMPO$, which is already known as a redox shuttle due to the fast and reversible charge-transfer kinetics. The interactions between $TEMPOL$ and common additives in DSSCs such as $1-methylbenzimidazole$ and $4-tert-butylpyridine$, needed to slow down recombination processes at the anode, dramatically change the reaction mechanism at the counter electrode (CE). Pt and $PEDOT$ were tested on the CE to improve the reduction of $TEMPOL^+$. Both types of CE were modified with an ionomer ($Nafion$) in an attempt to accumulate $TEMPOL^+$. Full DSSCs were characterized by I-V curves and electrochemical impedance spectroscopy (EIS), while the CEs were separately studied by cyclic voltammetry (CV) in a symmetrical two electrode setup.

O 84.4 Wed 18:15 P2/EG

Assembly and Characterization of Aqueous Dye-sensitized Solar Cells with Organic Nitroxides as Redox-mediators — •Daniel Holzhacker, Raffael Ruess, and Derck Schlettwein — Justus Liebig University Gießen, Institute of Applied Physics

Dye-sensitized solar cells (DSSCs) present a possible low-cost technology for the conversion of sunlight into electrical energy. The most efficient DSSCs are based on organic *cobalt* (II/III)-complexes in organic solvents, i.e. acetonitrile. Due to environmental reasons it is attractive to avoid the organic solvents. In view of the damage caused by water contamination in organic electrolytes, replacing acetonitrile by water seems to be a big challenge in DSSC research. Following tests on one or two components, complete aqueous DSSCs were assembled. Using cyclic voltammetry (CV) the diffusion coefficient and the redox-potential of the organic nitroxides in water were determined. For the investigation of the energy levels of the adsorbed dyes, CV and UV/vis-spectroscopy were performed. The cells were based on thin ($2-3\ \mu$m) screen-printed and annealed *titania* films, sensitized with different organic dyes ($D51$, $D35$ or $Y123$) overnight. J-V-curves and transient photocurrents of the different types of cells were measured. Power conversion efficiencies up to 4.4 %, which are among the highest reached for aqueous DSSCs so far, could be achieved using the molecule $TEMPO$ as redox-mediator. Its derivates $AZADO$ and $TEMPOL$ showed great potential in photocurrent and open circuit voltage but a limitation in the fill factor indicates the need for further investigations.

O 84.5 Wed 18:15 P2/EG

Characterization of Microelectrodes for Scanning Electrochemical Microscopy — •Leon Rosenbecker, Raffael Ruess, and Derck Schlettwein — Justus Liebig University Gießen, Institute of Applied Physics

Scanning electrochemical microscopy (SECM) can be used to investigate the dye regeneration process of dye-sensitized solar cells (DSSCs).[1] In the present work, we studied the performance and stability of different catalytic layers for the microelectrodes. The electrodes have been structured using photolithography on a polyethylene terephthalate (PET) substrate coated with indium tin oxide (ITO). However, as shown by cyclic voltammetry (CV), ITO does not provide sufficiently fast electrode kinetics. Therefore, PEDOT and gold have been coated onto the ITO microelectrodes. Sputtered gold has proven to be a suitable layer since it has shown high catalytic activity and high stability. Gold coated microelectrodes have then been used for SECM measurements in feedback mode using an actuator to press the microelectrodes against an insulator. A decrease in steady state current has been measured. However, the measured decrease is lower than expected. This is due to an imprecise landing of the microelectrode on the substrate. Presently, we are working on a more precise arrangement and progress will be discussed.

[1]. R. Ruess, S. Scarabino, A. Ringleb, K. Nonomura, N. Vlachopoulos, A. Hagfeldt, G. Wittstock, D. Schlettwein, *Phys.Chem.Chem.Phys.*, 2019, **21**, 13047-13057.

O 84.6 Wed 18:15 P2/EG

Effects of $\mathbf{H_2O}$ on $\mathbf{CO_2}$ Electroreduction Reactions at Platinum/Imidazolium Based Ionic Liquid Interfaces — •Björn Ratschmeier, Andre Kemna, and Björn Braunschweig — Institute of Physical Chemistry, Münster, Germany

$\mathrm{CO_2}$ reduction reactions ($\mathrm{CO_2RR}$), which are interesting for power-to-x applications, have been studied on polycrystalline Pt electrodes in the following room-temperature ionic liquids (RTIL): [EMIM][DCA], [EMIM][$\mathrm{BF_4}$] and [OMIM][$\mathrm{BF_4}$]. Because water can play an important role as cosolvent and coreactant, we have addressed $\mathrm{CO_2RR}$ as a function of water concentration. Cyclic voltammetry (CV) indicates a strong rise of activity for CO_2RR when the water concentration was increased. In order to provide molecular-level details, we have additionally applied *in operando* IR Absorption spectroscopy (IRAS) to reveal reaction products in the bulk electrolyte and *in situ* vibrational sum-frequency generation (SFG) to address surface-adsorbed species. From IRAS, we show that the formation of a imidazolium-COOH intermediate takes place at electrode potentials of -0.9 V vs SHE when the water concentration was as low as 31 mM, but is shifted to lower overpotentials at 1 M H_2O for all studied ionic liquids. In addition, SFG spectroscopy provides clear evidence for the formation of CO on Pt atop surface sites, which was used to determine the onset potential for the formation of CO. While in [OMIM][BF_4] no CO is formed even at very low potentials of -1.5 V, a significant decrease of the onset potential for CO formation with increasing water concentration is seen for the other RTIL.

O 84.7 Wed 18:15 P2/EG

Sum-Frequency Generation Spectroscopy of Water at [EMIM][BF_4]/Platinum Electrolyte/Electrode interfaces — •Andre Kemna and Björn Braunschweig — Institute of Physical Chemistry, WWU Münster, 48149 Münster, Germany

In room-temperature ionic liquids (RTIL), the presence of water can heavily influence reactions at the electrode/electrolyte interface. In case of CO_2 reduction reactions, water influences the catalysis of CO_2 substantially. In order to gain a detailed molecular-level understanding, in situ studies of the interfacial water structure as a function of electrode potential are desirable. Using vibrational sum-frequency generation (SFG), we have now revealed the presence and structure of water at platinum interfaces in contact with a RTIL and as a function of electrode potential. At the [EMIM][BF_4]/Pt interface, the addition of water leads first to negligible O-H contributions to the SFG spectra at open circuit potentials, but to broad bands at 3200 and 3450 cm^{-1} when the potential control is established. These bands are attributable to O-H stretching bands from hydrogen bonded interfacial molecules. Because the SFG intensity of the O-H bands increases during a cathodic sweep of the electrode potential, we propose that the interfacial layer of [EMIM][BF_4] in contact with a Pt electrode can be enriched with water molecules at low electrode potentials. In order to investigate the interaction of water at RTIL interfaces in more detail, we have applied SFG to the liquid/gas interface as an easily accessible model system. Here we demonstrate that the enrichment of water at RTIL interfaces strongly depends on the chemical identity of the cation.

O 84.8 Wed 18:15 P2/EG

Analysis of the electrochemical properties of $Li(Ni_{1/3}Co_{1/3}Mn_{1/3})O_{2-\delta}$ (NCM) thin film model cathodes — •Julius K. Dinter, Hendrik Hemmelmann, and Matthias T. Elm — Center for Materials Research, Gießen, Germany

Lithium ion batteries often suffer from capacity fading due to undesired side reaction occurring at the cathode surface. To get a deeper understanding of these side reactions, 2D model system are necessary. For this purpose, thin film NCM thin films were prepared via spin coating and annealing at high temperatures. A homogenous distribution of Ni, Co and Mn could be confirmed by EDX and SIMS measurements. The structural characteristics were analysed using Raman spectroscopy and XRD. Electrochemical properties were measured via cyclovoltammetrie and cyclopotentiometrie, confirming structural changes of the surface and an increase of the cell resistance, which indicates the formation of an solid electrolyte interface (SEI). Furthermore, the thin films were coated with Al_2O_3 using atomic layer deposition (ALD). Due to the coating of the NCM-thin film the long-term cycling stability could be improved and surface reactions were suppressed.

O 84.9 Wed 18:15 P2/EG

Characterization of the surface properties of coated and uncoated Ni-rich NCM cathodes by conductive atomic force microscopy — •Miguel Wiche, Rajendra S. Negi, and Matthias T. Elm — Center for Materials Research, Gießen, Germany

One possibility to improve the cell performance of Lithium-ion batteries is coating of the cathode with a protective layer. The protective layer is typically an electronically insulating oxide, which suppresses side reactions at the electrode-electrolyte interface. However, a detailed understanding of the beneficial effect of the coating is still missing. Here, we present the coating of Ni-rich $Li(Ni,Mn,Co)O_2$ (NCM) powder with Al_2O_3 using an atomic-layer-deposition like solution based wet-chemical process. Energy dispersive X-ray spectroscopy images confirm a homogeneous Al_2O_3 coating on the NCM particles. From the powders cathodes were prepared using binder and carbon as conductive additive. C-Rate and cycling tests indicate an improved electrochemical performance in comparison to cells with cathodes prepared from uncoated NCM powder. The surface of the cathodes of coated and uncoated NCM particles were investigated by conductive atomic force microscopy before and after cycling.

O 84.10 Wed 18:15 P2/EG

Surface plasmon resonance spectroscopy for surface reactions in aggressive organic solvents — •Adrian Joe Urban[1], Daniel Nürenberg[1], Deb Kumar Bhowmick[2], and Helmut Zacharias[1] — [1]Center for Soft Nanoscience, Busso-Peus-Straße 10, Münster — [2]Faculty of Chemistry, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel

Surface plasmon resonance (SPR) spectrometry in the Kretschmann configuration is a well established method to probe the gold-liquid interface. Commercially available devices typically work with aquaeous solutions as the liquid phase while devices for more challenging solvents are rare. We have constructed an SPR spectrometer suitable for aggressive organic solvents and air-sensitive reagents in order to investigate the self-assembly of catalytically active, gold-based systems in organic solution. As a proof of concept, we have studied the self-assembly kinetics of alkanethiole monolayers on a gold-surface. In these experiments, we obtained angle resolutions of up to $\Delta\theta = 0.01°$, corresponding to $\Delta n \leq 10^{-3}$. Formation of the monolayers was complete after fifteen minutes.

O 84.11 Wed 18:15 P2/EG

In situ X-ray studies of electrodeposition at electrolyte-liquid metal interface — •Andrea Sartori[1], Olaf Magnussen[1,2], and Bridget Murphy[1,2] — [1]University of Kiel — [2]Ruprecht Haensel Laboratory, Kiel

We investigate nucleation and growth by in situ x-ray reflectivity and diffraction at liquid-liquid interfaces, focusing on Hg as liquid metal substrate in an electrochemical environment. By changing the electrolyte concentration, species and potential we can control the deposition mechanism. Liquid electrodes provide a stresses and defects-free template for nucleation and growth and ensure high mobility of reagent and products leading to high quality crystals. In previous studies of electrolyte containing NaF+NaBr+PbBr2 the growth of a monolayer followed by 3D nanocrystal formation of PbBrF was observed. In the current experiments electrolytes were employed, which contain only a single halide aniona species, namely NaBr+PbBr2, NaCl+PbCl2 NaF+PbF2. Growth of Pb halide compounds is initiated by changing the potential from the amalgamation region, where the Pb2+ ions dissolve in the Hg, to a more positive potential, where the lead ions are deamalgamated. In all cases, a defined ultrathin adlayers are formed, followed by quasi-epitaxial growth of Pb-halides bulk crystals. These observations indicate that this growth behaviour is a general phenomenon.It may be explained by considering that for a potential positive of the amalgamation potential, the halide ions adsorb onto the Hg surface. When the Pb2+ is released from the Hg bulk, they coadsorbe on top of the halide adsorbate, resulting in adlayer formation.

O 84.12 Wed 18:15 P2/EG

Magnesium intercalation in layered MoS_2 - Fast kinetics by Mg^{2+} complexation with DME ligands and MoS_2 phase transition upon intercalation — Zhenyou Li[1,2], Xiaoke Mu[2], Zhirong Zhao-Karger[1,2], •Thomas Diemant[3], R. Jürgen Behm[1,3], Christian Kübel[1,2,4], and Max Fichtner[1,2] — [1]Helmholtz Institute Ulm (HIU), Helmholtzstr. 11, D-89081 Ulm, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany — [3]Institute of Surface Chemistry and Catalysis, Ulm University, Albert-Einstein-Allee 47, D-89081 Ulm, Germany — [4]Karlsruhe Nano Micro Facility, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany

Rechargeable magnesium batteries are one of the most promising candidates for next-generation battery technology. Despite recent significant progress, it remains a challenge to overcome the sluggish kinetics caused by the strong interaction between double charged Mg^{2+} ions and the intercalation host. Herein, we report that fast intercalation kinetics in layered MoS_2 can be achieved when using solvated $Mg(DME)_x{}^{2+}$. The high charge density of Mg^{2+} is mitigated by DME complexation, reducing the trapping force of the cathode lattice to the Mg^{2+} cations. We also studied the intercalation process by various spectroscopic and microscopic methods and found a phase transition of the MoS_2 host from the semi-conductive 2H to the metallic 1T phase upon intercalation.

O 84.13 Wed 18:15 P2/EG

DFT study of the effect of Br co-adsorbates on the adsorption energy and diffusion energy barrier of S ad-atoms on Ag(100) — •Sönke Buttenschön and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Halides affect adsorption and diffusion of ad-atoms on coinage metal surfaces (see the work of O. Magnussen and his group, e.g. Ref. [1]). We have carried through density-functional total-energy calculations using the code PWscf and PWneb from the Quantum Espresso package [2] to quantify the effect of a single or few Br co-adsorbates on the adsorption energy and diffusion energy barrier of a sulfur ad-atom on the Ag(100) surface. We find a repulsive S–Br interaction, which amounts to a decrease of the absolute value of the sulfur adsorption energy by about 0.06 eV if S and Br occupy next-nearest neighbor positions on the p(1×1) substrate lattice. The repulsion decreases rapidly with separation. The S–Br interaction is compared with a superposition of the interaction energies of individual S–Br pairs. The energy of the transition state for sulfur surface diffusion varies less. We discuss the correlation with the adsorption energies of the respective initial and final S-adsorption configurations.

[1] B. Rahn, O. M. Magnussen, ChemElectroChem **5**, 3073 (2018).

[2] P. Giannozzi *et al.*, J. Phys. Condens. Matter **21**, 395502 (2009), *ibid.* **29**, 465901 (2017).

O 84.14 Wed 18:15 P2/EG

Au (111)-water interface under external electric fields: An ab initio molecular dynamics study — •Azade YazdanYar, Yuki Nagat, and Katrin Domke — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Metal-water interfaces are present in many experimental settings and are of great relevance to various fields of study including electrochemistry. Therefore, a thorough understanding of water structure on the surface is essential and yet missing for many systems. Due to the exceptional properties of water and its complex behavior, computational methods can be great assets in providing unique insights to the metal-water interfaces, which may not be easily accessible via experiment.

Here, we study the Au (111)-water interface in the presence of an electric field using ab initio molecular dynamics simulations. The effect of the presence of the electric field and its strength on the interfacial water is studied. To be able to distinguish the effect of hydrogen bonding on the extent of re-orientation of water molecules due to the applied electric field, we compare the system containing a single water molecule with another system containing several layers of water, where the properties of bulk water are recovered. Our results so far show that upon applying the electric field the interfacial water seems to re-orient very weakly and may be dominated by the hydrogen bonding.

O 85: Poster Session - Supported Nanoclusters: Structure, Reactions, Catalysis

Time: Wednesday 18:15–20:00 Location: P2/EG

O 85.1 Wed 18:15 P2/EG

Bottom-up synthesis of free-standing nanocluster arrays supported by carbon — •Tobias Hartl[1], Moritz Will[1], Sophia Dellmann[1], Davor Čapeta[2], Virginia Boix de la Cruz[3], Rajendra Singh[4], Daniel Scheinecker[4], Paolo Lacovig[5], Silvano Lizzit[5], Jani Kotakoski[4], Jan Knudsen[3], Marko Kralj[2], Thomas Michely[1], and Pantelis Bampoulis[1] — [1]University of Cologne — [2]Institute of Physics, Zagreb — [3]MAX IV Laboratory, Lund — [4]University of Vienna — [5]Elettra Synchroton, Trieste

Cluster superlattices exhibit unique properties stemming from their small size and dimensionality. However, their use in applications is hampered by their low stability when exposed to application relevant conditions, e.g. ambient pressure, high temperature. We succeeded in synthesizing free-standing membranes hosting metal cluster superlattices which are stable at these conditions. We present, in detail, the fabrication process of such membranes. The cluster superlattices are grown on graphene on Ir(111), and subsequently embedded in a few nanometer thick carbon matrix. XPS and STM reveal that the carbon embedding is conformal to the clusters, anchors them to the graphene and greatly improves their thermal and mechanical stability. Removal of the membranes from the Ir(111) substrate by hydrogen bubbling is possible, when a substantial reduction of the graphene-Ir binding is accomplished by annealing at 850 K and intercalation of Eu. Post-removal TEM analysis of the cluster lattice membrane proves that the excellent order of the cluster lattice is maintained in the free-standing membrane.

O 85.2 Wed 18:15 P2/EG

Hydrogenation of small organic molecules with size-selected Pt_n clusters supported on thin-film SiO_2 and MgO — •Tobias Hinke, Marian Rötzer, Maximilian Krause, Andrew Crampton, and Ueli Heiz — Technische Universität München, Ernst-Otto-Fischer Straße 1, D-85748 Garching bei München

To gain fundamental understanding in heterogeneous catalysis processes, model systems and associated reactions, e.g. in UHV, are useful tools. Transition metal clusters on a single crystal and metal oxide support constitute highly tunable systems. The high degree of surface uniformity of metal single crystals governs an epitaxial growth of metal oxide thin-films, forming a suitable support, which are capable of modeling bulk oxide supports. Transition metal clusters with up to 50 atoms show significant, non-scalable size-effects. Additional properties of the support, like acidity, reducibility, film thickness and interfacial support interactions, in conjunction with the crystal (local) work function affect the cluster polarization. This induces a change in surface charge density, an important quantity for metal cluster reactivity. The activity and the change of the structural sensitivity of size-selected Pt_n-clusters (n=9, 10, 13) supported on SiO_2 and MgO thin-films are studied. Activity and structure sensitivity towards the hydrogenation of small organic molecules (ethylene and acetylene) as a model reaction are evaluated. Activity is monitored by pulsed molecular beam reactive scattering and temperature programmed desorption experiments. Characterization is performed through electronic (AES, MIES, UPS) and vibrational (IRRAS) spectroscopy.

O 85.3 Wed 18:15 P2/EG

Photocatalytic properties of graphene-supported titania clusters calculated from *first principles* — •Sabuhi Badalov[1], René Wilhelm[2], and Wolf Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn — [2]Institut für Organische Chemie, Technische Universität Clausthal, 38678 Clausthal-Zellerfeld

Among photocatalyst materials, titanium dioxide (TiO_2; titania) draws considerable interest because of its excellent photoactivity, high oxidation potential, nontoxicity, earth abundancy, and long-standing physical and chemical stability.[1,2,3] However, its application is hampered by the lack of response to visible light and the fast recombination rate of electron-hole pairs.

In the present study, we use density-functional theory in order to explore the potential of graphene and graphene nano-flakes for photosensitizing titania clusters. It is found that the size of the graphene nano-flakes has a significant effect on the bandgap of the composite material. Besides, spatial separation of photoexcited electrons and holes is observed, which indicates prolonged lifetimes of the photoexcitation. This finding can be expected to improve the photocatalytic activity.

References

(1) M. Fujihira et.al., Nature 293, 206-208 (1981).
(2) E. Wahlstrom et.al., Science 303, 511-513 (2004).
(3) J. Schneider et.al., Chem. Rev. 114, 9919-9986 (2014).

O 86: Poster Session - Organic Molecules on Inorganic Substrates: Electronic, Optical and other Properties II

Time: Wednesday 18:15–20:00 Location: P2/EG

O 86.1 Wed 18:15 P2/EG

STM and DFT study of BF4 anion migration on a triazatriangulenium SAM on Au(111) — •Sergii Snegir[1], Yannick Dappe[2], Dmitro Sysoiev[3], Olivier Pluchery[4], Thomas Huhn[1], and Elke Scheer[1] — [1]University of Konstanz, Konstanz, Germany — [2]SPEC, CEA, CNRS, University Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette Cedex, France — [3]Institute of Organic Chemistry and Biochemistry, Prague, Czech republic — [4]Institut des Nano-Sciences de Paris (INSP), Sorbonne Universités, CNRS, Paris, France

Chemical coupling of functional molecules with so-called platforms allows the formation of functional Self-Assembled Monolayer (SAM). An example is triazatriangulenium (TATA), with extended aromatic core, allowing the formation of good electronic contact with the metal surface. Here we present studies on SAMs of TATA-BF4 molecules on Au(111) by means of Scanning Tunneling Microscopy (STM) and Density Functional Theory (DFT). In solution, these molecules exist as ion pairs of TATA+ and BF4-. However, under electrochemical deposition on Au(111) [1], on the TATA+ cations formed SAMs the BF4- anions seemingly disappear. Our STM experiments reveal dissociation of the TATA-BF4 complex. The TATA+ remains stable within the SAM while the BF4- spontaneously migrates through the TATA SAM on the surface. DFT calculations show a reduction of the TATA-BF4 binding energy after deposition. [1]-S. Kuhn, U. Jung, S. Ulrich, R. Herges and O. Magnussen, Chemical Communications, 2011, 47, 8880-8882.

O 86.2 Wed 18:15 P2/EG

Pump-Probe Photoelectron Momentum Microscopy of Molecular Thin Films at a Free-Electron Laser — •Christian Metzger[1], Markus Scholz[2], Kiana Baumgärtner[1], Chul-Hee Min[1], Thiago R. F. Peixoto[1], Dmytro Kutnyakhov[3], Michael Heber[3], Federico Pressacco[4], Wilfried Wurth[3,4], Anders Madsen[2], and Friedrich Reinert[1] — [1]Experimentelle Physik 7, Universität Würzburg, Germany — [2]European XFEL, Germany — [3]DESY Hamburg, Germany — [4]Universität Hamburg, Germany

The analysis of the momentum distribution from static angle-resolved photoemission experiments has provided new insights into the electronic interaction at molecule-metal interfaces [1], electron-vibration coupling [2] as well as structural alignment [3] in the last decade [4]. Our pump-probe measurements focus on translating these previous achievements into the time-domain. To this end, we conducted dynamic experiments on pentacene bilayers on top of Ag(110) with a time-of-flight momentum microscope at a free-electron-laser facility [5]. Pentacene is an ideal archetype for this endeavor due to its broad applicability in electronic devices and its well characterized properties in static experiments [6]. Furthermore, it has the potential to showcase a variety of ultrafast photoinduced processes such as singlet fission.

[1] G. Zamborlini et al., Nat. Comm. 8, 335 (2017). [2] M. Graus et al., Phys. Rev. B 98, 195412 (2018). [3] B. Stadtmüller et al., EPL 100, 26008 (2012). [4] P. Puschnig et al., Science 326, 702 (2009). [5] M. Scholz et al., arXiv:1907.10434. [6] M. Grimm et al., Phys. Rev. B 98, 195412 (2018)

O 86.3 Wed 18:15 P2/EG

Application of periodic energy decomposition analysis to metallic systems — •Jan-Niclas Luy, Benedikt P. Klein, J. Michael Gottfried, and Ralf Tonner — Fachbereich Chemie, Philipps Universität Marburg, Germany

The Energy Decomposition Analysis (EDA) is a wavefunction based bonding analysis scheme that enjoys significant popularity in the molecular chemistry community [1]. Recently the method has been extended to surfaces and solids [2] and applied to organic surface chemistry [3]. It was shown that localized, covalent bonds in a periodic system can be interpreted in a similar fashion as their 0D molecular counterparts. Adsorption of organic molecules on transition metal surfaces, however, requires a more nuanced description [4]. In addition to covalent bonds, interactions are often characterized by large charge transfer, polarization and dispersion contributions. While for many alternant hydrocarbons (e.g. naphthalene) dispersion dominates on Cu(111), orbital interactions can be identified in non-alternant cases (azulene). With the more reactive Pt(111) surface, both naphthalene and azulene form strong chemisorptive bonds that show donor/acceptor and shared-e^- character.

[1] M. von Hopffgarten and G. Frenking, *WIREs Comput Mol Sci* **2012**, *2*, 43.
[2] M. Raupach, R. Tonner, *J. Chem. Phys.* **2015**, *142*, 194105.
[3] L. Pecher, S. Laref, M. Raupach and R. Tonner, *Angew. Chem. Int. Ed.* **2017**, *56*, 15150.
[4] B. P. Klein *et al.*, *Phys. Rev. X* **2019**, *9*, 011030.

O 86.4 Wed 18:15 P2/EG

Vibron-assisted spin excitation in a magnetically anisotropic molecule — •Garnier L.[1], Verlhac B.[1], Bachellier N.[1], Zaldívar J.[2], Rubio-Verdú C.[2], Abufager P.[3], Ormaza M.[1], Choi D.-J.[4,6], Bocquet M.-L.[5], Pascual J.I[2,6], Lorente N.[4], and Limot L.[1] — [1]Université de Strasbourg, CNRS, IPCMS, UMR 7504, F-67000 Strasbourg, France — [2]CIC nanoGUNE, 20018 Donostia-San Sebastián, Spain — [3]Instituto de Física de Rosario, CONICET and Universidad Nacional de Rosario, Av. Pellegrini 250 (2000) Rosario, Argentina — [4]Centro de Física de Materiales (CFM) & DIPC, 20018 Donostia-San San Sebastián, Spain — [5]PASTEUR, ENS, Sorbonne Universités, CNRS, 75005 Paris, France — [6]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

The electrical control and readout of molecular spin states is key for high-density storage. Expectations are that electrically-driven spin and vibrational excitations in a molecule should give rise to new conductance features in the presence of magnetic anisotropy, offering alternative routes to study and, ultimately, manipulate molecular magnetism. Here, we use inelastic electron tunneling spectroscopy to promote and detect the excited spin states of a prototypical molecule with magnetic anisotropy. We demonstrate the existence of a vibron-assisted spin excitation that can exceed in energy and in amplitude a simple excitation among spin states. The excitation, which can be quenched by chemical changes in the magnetic molecule, is explained using first-principles calculations and model calculations that include dynamical correlations.

O 86.5 Wed 18:15 P2/EG

Electronic properties of N-substituted pentacene derivatives on Au(111) — •Tanja Schmitt[1], Jakob Steidel[1], Marvin Hoffmann[2], Hilmar Reiss[3], Uwe Bunz[3], Andreas Dreuw[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg — [2]Interdisziplinäres Zentrum für Wissenschaftliches Rechnen, Universität Heidelberg — [3]Organisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg

N-heteropolycyclic aromatic compounds are promising candidates for n-channel semiconductors. The introduction of nitrogen into the π-electron-backbone of the polycyclic aromatic hydrocarbons stabilizes the frontier orbitals and increases the electron affinity, while the size of the HOMO-LUMO (optical) gap is nearly uneffected.

Thus, the electronic properties of N-functionalised pentacene derivatives were studied using two-photon photoemission (2PPE). With this powerful technique, the energetic positions of occupied, unoccupied and excitonic states were determined. In addition, the dynamics upon optical excitation can be investigated on a femtosecond time scale. Also, angle-resolved 2PPE can be performed in order to study the dispersion of present states.

Crucial properties such as optical and transport gap as well as binding energy was determined and compared to non-substituted pentacene using 2PPE. In addition, state-of-the-art quantum chemical theory was carried out.

O 86.6 Wed 18:15 P2/EG

Dehydrogenation Reactions of O-Heterocyclic LOHC Molecules — •Felix Hemauer, Philipp Bachmann, Fabian Düll, Johann Steinhauer, Hans-Peter Steinrück, and Christian Papp — Friedrich-Alexander-Universität, Erlangen, Germany

With the dwindling of fossil fuels and the alarming progression of global warming, the ecological and social demand for cleaner and more sustainable energy sources has never been as high. As renewable sources, such as wind and solar power, give no continuous and constant power output, hydrogen is a promising candidate for the chemical storage of energy. The concept of Liquid Organic Hydrogen Carriers (LOHCs) avoids unfavorable handling of elemental hydrogen.

Heterocyclic LOHC molecules display advantageous thermodynamic properties regarding their heat of dehydrogenation. Consequently, several N-heterocycles have been successfully investigated, e.g. the indole-based systems and their derivatives.

In order to investigate the feasibility of O-heterocyclic compounds as possible LOHCs, synchrotron radiation-based high resolution X-ray photoelectron spectroscopy and temperature-programmed desorption measurements of furan and benzofuran were performed on Pt(111) under UHV conditions. By applying heating ramps after the adsorption experiment, the respective dehydrogenation and decomposition reactions are monitored via evaluation of the characteristic spectra. This allows for fundamental insights into the reactivity and stability and helps assessing the viability of the compound class as LOHC.

O 86.7 Wed 18:15 P2/EG

How Metrology can improve Photoemission Tomography — •Hans Kirschner[1], Alexander Gottwald[1], Georg Koller[4], Peter Puschnig[4], Mike Ramsey[4], Mathias Richter[1], Serguei Soubtach[2,3], and Stefan Tautz[2,3] — [1]Physikalisch-Technische Bundesanstalt, 10587 Berlin, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]ülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, 52425 Jülich, Germany — [4]Institut für Physik, Karl-Franzens-Universität Graz, NAWI Graz, 8010 Graz, Austria

Photoemission tomography (PT) is a powerful tool to identify the electron orbital structure of mono-and bi-layers of molecules on surfaces. Using angle-resolved photoemission spectroscopy and assuming a basic plane wave as the final state of the photoelectrons, the molecular orbital can generally be represented by a Fourier Transformation of the resulting impulse map. Thus, detailed information on electronic and geometric structures, as well as orbital densities of molecular systems on different surfaces is extracted.

In order to receive accurate relative electron densities of the orbitals, it already has been shown that a normalization to the precise photon flux is essential. In this context, we seek to apply the PT method to experimental datasets for angle-resolved photoemission of atomic photoionization. The resulting impulse distributions will be compared to those, received from analytically calculated hydrogen-like atomic orbitals, in order to show and overcome differences in the electron densities of the orbitals due to the PT method.

O 86.8 Wed 18:15 P2/EG

The geometric and electronic properties of kekulene monolayers on Cu(111) and Cu(110) studied by density functional theory — •Alexander Reichmann[1], Anja Haags[2,3,4], Qitang Fan[6], Tim Naumann[6], Simon Werner[6], Jörg Sundermeyer[6], Xiaosheng Yang[2,3,4], Larissa Egger[1], Hans Kirschner[5], Francois C. Bocquet[2,3], Georg Koller[1], Alexander Gottwald[5], Mathias Richter[5], Michael G. Ramsey[1], J. Micheal Gottfried[6], Serguei Soubatch[2,3], F. Stefan Tautz[2,3,4], and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [3]Jülich Aachen Research Alliance (JARA), Germany — [4]Physics IV A, RWTH Aachen University, Germany — [5]Physikalisch-Technische Bundesanstalt (PTB), Germany — [6]Fachbereich Chemie, Philipps-Universität Marburg, Germany

Kekulene is a polycyclic aromatic hydrocarbon made of 12 fused benzene rings which has attracted renewed interest. For instance, its aromaticity is still debated and it may serve as a model for graphene pores. In this contribution, we use density functional theory to study kekulene adsorbed on the (111) and (110) surfaces of copper. We determine kekulene's adsorption height, site and its azimuthal alignment. Based on the relaxed adsorption geometry, we further analyze the electronic structure in detail by computing the molecular orbital projected density of states and by simulating angle-resolved photoemission (ARPES) band and momentum maps. Finally, we compare our results to experimental ARPES data.

O 86.9 Wed 18:15 P2/EG

Structure and Morphology of Tetracene Aggregates on HOPG — •Annika Bergmann, Christian Völkner, Kevin Oldenburg, Ingo Barke, and Sylvia Speller — University of Rostock, Institute of Physics, 18059 Rostock, Germany

Exciton formation in tetracene involves fascinating phenomena such as long-range triplet propagation and singlet fission, and fusion [1]. Our aim is to elucidate the spatially resolved population dynamics and energetics of these processes in tetracene nano- and microstructures at surfaces. Here we present scanning probe (AFM, LT-STM) and fluorescence microscopy data on tetracene aggregates on HOPG prepared by *ex-situ* deposition from a solution via drop-casting or immersion, as well as *in-situ* evaporation. For the latter polarization dependent fluorescence reveals highly ordered crystallites, while the structure of ex-situ prepared layers in the monolayer regime is more fragile. Since literature about tetracene on HOPG is scarce we compare the results to studies on pentacene on HOPG [2]. Formation of tetracene mono- and multilayers is discussed with regard to lying-down and standing-up molecular configurations, respectively.

[1] Akselrod et al., Nat. Commun. **5** (2014).
[2] Götzen et al., Phys. Rev. B **81** (2010).

O 87: Poster Session - Nanostructures at Surfaces: 1D and 2D Structures and Networks

Time: Wednesday 18:15–20:00 Location: P2/1OG

O 87.1 Wed 18:15 P2/1OG

Confinement and Tailoring of Surface 2DEGs in Temperature-driven Molecular Nano-porous Network — •Lu Lyu[1], Benito Arnoldi[1], Jin Xiao[2], Sina Mousavion[1], Johannes Stöckl[1], Maniraj Mahalingam[1], Benjamin Stadtmüller[1,3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern — [2]School of Science, Hunan University of Technology, Zhuzhou 412007, China — [3]Graduate School Materials Science in Mainz, Kaiserslautern

Controlling the quantum confinement of (spin-dependent) electronic states by design of two-dimensional (2D) organic nanoporous networks (NPNs) opens a unique avenue to accelerate the implementation of quantum technology in next-generation photonic and spintronic applications. In our previous study [1], a thermal-driven TPT NPN is found on Cu(111) surface. At low temperature, the formation of nanopores can confine the free 2D electron gas (2DEGs) of the surface into a regular array of quantum dots. Moreover, the electronic coupling between neighboring quantum dots induces a dispersive band structure in k-space near the Fermi level. Further, the confined 2DEGs can be modulated by the doped cobalt atoms. Combining the DFT and EBEM/EPWE (electron boundary elements and electron plane wave expansion methods), the details on spin-dependent electronic states are provided in Co-doped NPN. These findings pave the way to control 2DEGs in temperature-driven molecular networks.

[1] J. Phys. Chem. C 123, 26263 (2019)

O 87.2 Wed 18:15 P2/1OG

Modeling of molecular stripe formation on insulating surfaces — •Christoph Schiel[1], Maximilian Vogtland[2], Ralf Bechstein[2], Angelika Kühnle[2], and Philipp Maass[1] — [1]Fachbereich Physik, Universität Osnabrück, Germany — [2]Fakultät für Chemie, Universität Bielefeld, Germany

The interplay of intermolecular and molecule-surface interactions plays a decisive role for molecular structure formation. Insulating surfaces are interesting due to the weaker electronic coupling of the molecules to the substrate compared to metals. This allows for exploiting the rich variety of intermolecular interactions to a larger extent, in particular for pattern formation with specific applications in nanotechnology. Here we study theoretical approaches to model the stripe formation of 3-hydroxybenzoic acid (3-HBA) and 3-aminobenzoic acid (3-ABA) molecules on calcite (104). It is argued that adsorption-induced dipolar interactions cause an ordering towards a regular spacing between the molecular stripes [1]. We model the stripe formation by an anisotropic Ising model with dipole-dipole interactions. Stripe length and distance distributions are determined by Monte Carlo simulations and show good agreement with the experimental data. They allow us to give estimates for induced dipole moments and binding energies between molecules.

[1] J. L. Neff, H. Söngen, R. Bechstein, P. Maass, A. Kühnle, J. Phys. Chem. C **119**, 24927 (2015).

O 87.3 Wed 18:15 P2/1OG

Epitaxial growth of Bi on epitaxial graphene — •Chitran Ghosal[1], Johannes Aprojanz[1], and Christoph Tegenkamp[1,2] — [1]TU Chemnitz, Germany — [2]Leibniz Universität Hannover, Germany

The semimetal Bi still attracts a lot of interest because of its unique electronic properties such as a low carrier concentrations and large carrier mobilities. The mesocopic Fermi wavelength gives rise to pronounced quantum confinement effects, e.g the semimetal to semiconductor transition. The surface states on Bi(111) reveal strong spin polarization and ultrathin Bi films are topologically non-trivial. Therefore, proximity coupling of Bi nanostructures to graphene may be used to tune the transport properties of the 2D relativistic electron gas. In this work we studied the growth of the Bi on epitaxial graphene on SiC(0001) by means of LEED and STM. While for low coverages Bi(110) are formed, Bi(111) structures were found in the high coverage regime. This allotropic transition occurs around 14 bilayers (5.6 nm) and significantly larger than the transition reported on Si(111) [1]. Moreover, needle-like structures along three different directions were found. For various Bi coverages, the widths of these Bi-structures is around 12 nm, apparently, due to a lateral quantum confinement effect. Contrary, magic heights were now observed. In order to probe proximity effects, we will present also first magneto transport measurements. [1] T. Nagao, et al. Phys. Rev. Lett, 93, 105501 (2004).

O 87.4 Wed 18:15 P2/1OG

Coupling of Yu-Shiba-Rusinov states on 2*H*-NbSe$_2$ — •Eva Liebhaber[1], Lisa Rütten[1], Gaël Reecht[1], Kai Rossnagel[2,3], Felix von Oppen[1,4], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, Germany. — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany. — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany. — [4]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Germany.

A magnetic impurity adsorbed on a superconducting substrate leads to the formation of Yu-Shiba-Rusinov (YSR) states. These are low-energy bound states inside the superconducting energy gap. YSR wave functions of two adjacent magnetic adatoms can hybridize and form symmetric and antisymmetric linear combinations. Increasing the number of adatoms leads to the formation of Shiba bands. In adatom chains, the spin texture and hence, the underlying physics, is dictated by the inter-atomic distance as well as by the nature of the coupling [1].

We investigate magnetic atoms on the superconductor 2*H*-NbSe$_2$ which is a layered van der Waals material. Its strong 2D character leads to a large spatial extent of the YSR wave functions facilitating the coupling between them [2]. We assemble adatom chains with different interatomic spacings using a superconducting tip and track the evolution of the YSR states.

[1] F. Pientka *et al.*, *Phys. Rev. B* **89**, 180505 (2014).
[2] G.C. Ménard *et al.*, *Nature Phys.* **11**, 1013 (2015).

O 87.5 Wed 18:15 P2/1OG

Coadsorption of shape-persistent macrocycles and fullerene derivatives on graphite: Lithography with the STM tip — •Joshua Bahr, Annemarie Meyer, Tristan J. Keller, Sigurd Höger, and Stefan-Sven Jester — Kekulé-Institut für Organische Chemie und Biochemie, Bonn, Deutschland

Shape-persistent arylene-alkynylene macrocycles self-assemble into 2D crystalline nanopatterns at the solid/liquid interface of highly oriented pyrolytic graphite (HOPG) and 1-phenyloctane, and are imaged *in situ* by scanning tunneling microscopy (STM) with submolecular resolution. The physisorption and packing of such species is driven by long extraannular alkoxy substituents, which also guarantee sufficient compound solubility for processing. The ability of macrocycles to template the adsorption of fullerenes on HOPG has gained recent interest, as it does not require covalent bond formation.[1] Here, we report on patterns of macrocycles on HOPG, that are metastable upon addition of fullerene PC$_{61}$BM to the supernatant liquid phase. STM-tip induced local disturbance of such a system leads to desorption of the macrocycles and re-adsorption of cocrystals of both compounds. We discuss both potential and limits of STM-based supramolecular lithography at the solid/liquid interface. [1] G.-B. Pan, X.-H. Cheng, S. Höger, W. Freyland, *J. Am. Chem. Soc.* **2006**, *128*, 4218-4219.

O 87.6 Wed 18:15 P2/1OG

Isomorphic packing of carboxylic acid terminated arylene-alkynylenes and monodisperse oligomers on graphite — •David A. Hofmeister, Lucas Rothe, Tristan J. Keller, Sigurd Höger, and Stefan-S. Jester — Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany.

Arylene-alkynylenes form supramolecular nanopatterns at the solid/liquid interface of graphite (HOPG), that are imaged by scanning tunneling microscopy with submolecular resolution. The structure of the two-dimensional (2D) crystals depends on the exact geometry of the shape-persistent backbones, the substitution with functional groups that mediate the interaction of such species, and (intermolecularly interdigitating) alkoxy side chains. Here, we report on (i) arylene-alkynylenes that carry OC$_{16}$H$_{33}$ side chains and carboxylic end groups and are obtained in a stepwise synthesis, and (ii) monodisperse oligomers of alike systems obtained by oxidative Glaser coupling of acetylene-terminated precursors and subsequent separation by recycling gel permeation chromatography. Both species form isomorphous 2D packings, which is drawn back to alike spatial requirements of (i) carboxylic acid dimers that form after adsorption and (ii) butadiynylene units.

O 87.7 Wed 18:15 P2/1OG

Electronic and magnetic structure of oriented sandwich-molecular wires on graphene/Ir(110) — •Stefan Kraus[1], Alexander Herman[2], Felix Huttmann[1], Ken Bischof[1], Nico Rothenbach[2], Katharina Ollefs[2], Marco Bianchi[4], Raluca-Maria Stan[4], Ann Julie Holt[4], Jan Dreiser[5], Shigeru Tsukamoto[3], Nicolae Atodiresei[3], Philip Hofmann[4], Heiko Wende[2], and Thomas Michely[1] — [1]Universität zu Köln, Germany — [2]Universität Duisburg-Essen, Germany — [3]Forschungszentrum Jülich, Germany — [4]Aarhus university, Denmark — [5]Paul Scherrer Institut, Switzerland

Sandwich-molecular wires are one-dimensional arrangements of alternating metal atoms and cyclic molecules which, when synthesized on a surface, can interlock with each other and form islands. Here, we use europium as metal reactant and cyclooctatetraene as ligand. We choose the substrate Gr/Ir(110) which has a two-fold symmetric moiré, in order to achieve a global wire orientation. Excluding defects we observe wire formation only along the [001] direction, which allows for band structure investigations using ARPES. Although it is not possible to observe the π-derived bands, we find a flat band stemming from the 4f-states. The comparison with DFT calculations allows us to estimate the Hubbard U for the wires. While XMCD for these wires on Gr/Ir(111) shows a hyteresis at 5K, this hysteresis is suppressed in the oriented wires on Gr/Ir(110). We speculate that the more reactive binding of Gr/Ir(110) leads to this suppression, while the electronic configuration of Eu 4f^7 is left unchanged.

O 87.8 Wed 18:15 P2/1OG

Thermal- vs. Light-Induced on-Surface Polymerization — •Christophe Nacci and Leonhard Grill — Department of Physical Chemistry, University of Graz, 8010 Graz, Austria

The on-surface synthesis of covalently linked molecular precursors via Ullmann coupling reaction is an efficient approach to produce novel functional materials. The dissociation of specific bonds and the formation of new covalent ones can be induced by using different external stimuli. While many studies exist on the thermal control of the reaction, very few studies have reported a photochemical approach to form polymers at single-crystal surfaces. The purpose of this work is to get insight into the reaction pathways from individual molecular species to one-dimensional polymers by driving the reaction either by heat or by light illumination. The molecular precursors were deposited in ultrahigh vacuum onto a Au(111) surface where polymerization occurs. Two stimuli, thermal- and photo-induced polymerization by using UV light, were employed and systematically compared. The structural characterization of the product results by low-temperature scanning tunneling microscopy and the corresponding polymer length distributions will be shown.

O 88: Poster Session - Nanostructures at Surfaces: Other Aspects

Time: Wednesday 18:15–20:00 Location: P2/1OG

O 88.1 Wed 18:15 P2/1OG

Fabrication of metallic microstructures on optical fibers — •Alexander Fassbender and Stefan Linden — Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 12, D-53115 Bonn

We report on the fabrication of microstructured gold electrodes on the end facet of a single mode fiber. The basic idea is to use 3D direct laser writing based on multi-photon absorption to print microstructured sleeves, in which the cleaved optical fiber is inserted. Next, the optical fiber as well as the sleeve are metalized by thermal evaporation of gold or copper. The apertures in the sleeve define the electrodes during the evaporation process. In order to connect four electrodes on the end-facet with bond pads on the side of the fiber, we utilize two specially designed sleeve-structures and perform several evaporation runs from different directions. In- and outcoupling of light is not affected by the electrodes, since the core is protected by the sleeves. We envision that our microstructured fibers can be employed to realize compact ion traps.

O 89: Poster Session - Oxide and Insulator Surfaces: Structure, Epitaxy and Growth

Time: Wednesday 18:15–20:00 Location: P2/1OG

O 89.1 Wed 18:15 P2/1OG

High Pressure Oxidation of Copper - From Thin Films to Bulklike Materials — •Alexander Gloystein and Niklas Nilius — Institute of Physics, Carl von Ossietzky University Oldenburg, Germany

Copper oxidation at UHV-compatible O2 pressures only enables the formation of few-layer thick oxide films. In contrast, arbitrarily thick layers are produced by Cu deposition onto Au(111) followed by oxidation at 20-50 mbar O2. According to XPS, the Cu completely oxidizes to Cu2O in this case, while LEED reveals a highly uniform Cu2O(111) surface. The film morphology is governed by large hexagonal crystallites, being terminated by Cu-O six rings decorated with a sqrt3 shamrock structure known from bulk Cu2O(111). The latter indicates a high reducibility of the film, and even larger Cu aggregates emerge on the oxide surface upon vacuum annealing. The oxide reduction can also be followed in STM conductance spectra that evolve from a p-type behavior with a unique acceptor state above E(Fermi) to an almost stoichiometric conductance response. Further information on the Cu2O defect structure is obtained from temperature-controlled photoluminescence spectroscopy.

O 89.2 Wed 18:15 P2/1OG

Morphological study of vanadium dioxide (VO_2) thin films grown on the different substrates using STM — •Aman Baunthiyal, Simon Fischer, Jon-Olaf Krisponeit, and Jens Falta — Institute of Solid State Physics, University of Bremen, Germany

Vanadium dioxide (VO_2) is an interesting material for sensor and memory devices due to its metal-insulator transition (MIT) near room temperature (RT) that is accompanied by a structural change between a monoclinic insulator phase and a rutile metallic phase. This temperature can be varied by the choice of the substrate: TiO_2(110) and RuO_2(110) applies in-plane tensile strain to the rutile c-axis which leads to an increase of the transition temperature of VO_2, favoring the monoclinic phase.

RuO_2(110) islands were formed on the surface of a Ru crystal by oxidizing it while observing with in-situ LEEM and LEED. Then, VO_2 was deposited using molecular beam epitaxy (MBE). VO_2 growth on TiO_2(110) substrate was grown through the same process. To study the surface morphology of VO_2 grown on RuO_2(110) and TiO_2(110), we used STM (scanning tunneling microscope) at RT. In the case of VO_2/RuO_2, the surface of VO_2 was found flat with two rotational domains separated by 60 degrees. The thickness of VO_2 on RuO_2 was measured to be about 3 to 4 nm using XRR (X-ray Reflectometry). In the case of VO_2/TiO_2, the surface was also found to be flat but showing small grains of VO_2 on the TiO_2 surface. Next, we intend to study the effect of different substrates on the MIT transition of VO_2 by variable temperature STM (VT-STM) using single-point spectroscopy.

O 89.3 Wed 18:15 P2/1OG

Surface Charge patterning and mapping on SrTiO3 thin films — •Mirco Wendt[1], Eric Andersen[1], Regina Lange[1], Sven Kraft[1], Ronny Brandenburg[1,2], Ingo Barke[1], and Sylvia Speller[1] — [1]Institute of Physics, University of Rostock, 18059 Rostock, Germany — [2]Leibniz Institute for Plasma Science and Technology, 17489 Greifswald, Germany

Perovskites such as SrTiO3 are oxides with high permittivity which show ferroelectric behaviour under certain conditions [1]. We address the question whether surface charges can be stabilised by strong substrate polarisation which would be an interesting property for controlled adsorption, e.g. via command layers, and for biological applications. We use SrTiO3 thin films grown by pulsed laser deposition on SrTiO3(100) and expose them to electron beams through a mask at different kinetic energies in a scanning electron microscope (SEM). Detection is accomplished by force microscopy methods (AFM) with the aim to map the resulting charge distributions. Alternative techniques for charge deposition, detection and imaging are discussed.

[1] HW Jang, et al, Phys Rev Lett 104, 197601(2010)

O 89.4 Wed 18:15 P2/1OG

Muscovite Mica: Cleaved in UHV, Exposed to Water Vapour, Imaged with nc-AFM — •Sebastian Brandstetter, Michael Schmid, Markus Valtiner, Ulrike Diebold, and Martin Setvín — Institute for Applied Physics, TU Wien, Wiedner Hauptstraße 8-10, 1040, Vienna, Austria

The Muscovite Mica(001) surface is used as an atomically well defined model substrate in a variety of applications ranging from imaging DNA to high resolution studies of solid/liquid interface structures. To prepare a well defined substrate purified water is commonly used to rinse freshly cleaved muscovite to dissolve potassium cations. Little is known about the hydration and mobility of surface cations at the atomic scale. Here we present non-contact AFM measurements in ultrahigh vacuum (UHV) resolving single potassium atoms on the UHV-cleaved surface. We find evidence of hydrated potassium atoms after dosing sub-monolayer amounts of molecular H_2O to the cleaved sample below temperatures of 140 K. The as-cleaved surface presents domains of uncompensated charges while the adsorption of water molecules at the surface facilitates growth of ice-like structures at temperatures below 5 K.

O 89.5 Wed 18:15 P2/1OG

Epitaxial growth of RuO_2(110) thin films on TiO_2(110) substrates by pulsed-laser-deposition — •Philipp Kessler, Matthias Schmitt, Berengar Leikert, Philipp Schütz, Martin Kamp, Michael Sing, Ralph Claessen, and Simon Moser — Experimental Physics IV, Julius Maximilian University of Würzburg

Ruthenium dioxide (RuO_2) is a functional semimetal hosting a network of Dirac nodal lines in its bulk and a flat band state at its surface. For spectroscopic and transport measurements on this material, stoichiometric films of high crystalline quality and well-ordered surfaces are needed. Here we present a growth study of rutile RuO_2(110) thin films on TiO_2(110) substrates by pulsed-laser-deposition. In situ growth monitoring by RHEED in combination with ex situ characterization based on LEED, XPS, AFM and STEM reveal defect free epitaxial films up to 10 unit cells thickness, limited by formation of volatile species at the surface. Strategies to overcome this thickness limitation will be outlined.

O 90: Poster Session - Semiconductor Substrates: Metallic Nanowires, Overlayers, etc.

Time: Wednesday 18:15–20:00 Location: P2/1OG

O 90.1 Wed 18:15 P2/1OG

Dimerization, self-doping and step-step correlation of Au chains on Si(553) — Zamin Mamiyev, •Priyanka Yogi, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany

Adsorption of 0.48 of a monolayer of Au on the regularly stepped Si(553) surface leads to the formation of one double chain of Au per terrace by self-organization. They are considered as a prototype of a quasi one-dimensional system. However, since the interaction with the Si surface results in modifications of the Si surface states, this system turns out not to be purely 1D. In this study we explore the conditions of quasi-1D behavior in more detail by variation of the Au concentration, starting at the optimal concentration of 0.48 ML, as judged from maximum slope and intensity of plasmon dispersion. LEED shows an enhanced coupling between the Au wires at slightly smaller Au concentrations, while a Au surplus up to 0.03 ML adsorbed at RT, dopes the system, removes stacking faults from the wires and simultaneously enhances dimerization, but effectively decouples the wires. By annealing above 630° C the Au atoms are collected in $\sqrt{3}$-ordered clusters with a local concentration of 1ML. Concerning long range order of Au chains, the situation with 0.48 ML Au is restored. The same hold for the plasmon dispersion. Geometric models to explain these properties are discussed.

O 90.2 Wed 18:15 P2/1OG

DFT and ab-inito thermodynamics investigation of GdSi$_2$-nanowires on Si(001) — •Niklas Jöckel[1,2], Kris Holtgrewe[1,2], and Simone Sanna[1,2] — [1]Justus Liebig Universität, Giessen, Germany — [2]Center for Materials Research, Giessen, Germany

In a recent study, detailed STM images of GdSi$_2$-nanowires have been produced[1]. They show a structural connection between the quasi 1D wires and the two-dimensional silicide coverage. On this basis structural models were proposed which we further investigated by ab-initio calculations.

Employing density functional theory, we simulated STM images for different models of two-dimensional silicide layers and compared their stability by minimization of the Landau potential. The two most stable 2D structures that reproduced the experimental STM images were taken as the basis for quasi 1D nanowire models confined to 8 surface lattice constants.

A nanowire structure was found that accurately reproduces the experimental findings. The nanowire is found to be metastable since the system prefers a complete silicide coverage.

[1] Song et al, Sci. Rep. **9**, 1364 (2019)

O 91: Poster Session - Semiconductor Substrates: Structure, Epitaxy and Growth

Time: Wednesday 18:15–20:00 Location: P2/1OG

O 91.1 Wed 18:15 P2/1OG

A First-Principles Study of the Structure and Stability of Oxygen-Terminated Diamond(110) Surfaces — •Shayantan Chaudhuri[1,2] and Reinhard J. Maurer[2] — [1]EPSRC Centre for Doctoral Training in Diamond Science and Technology, University of Warwick, Coventry, CV4 7AL, United Kingdom — [2]Department of Chemistry, University of Warwick, Coventry, CV4 7AL, United Kingdom

Diamond is a material that possesses numerous properties and applications in a variety of fields, such as photonics and electrochemistry. Boron-doped diamond (BDD) is electrically-conducting and can be used as a working electrode for electrodeposition and electrochemical sensor applications. BDD crystals can be grown by chemical vapour deposition (CVD), which appears to favour the growth of the (110) facet amongst others. Under such reaction conditions, diamond surfaces will be partially oxidised and oxygen-terminated. Infrared (IR) and X-ray photoelectron spectroscopy (XPS) measurements in literature provide indications of the co-existence of different oxygen species. We have conducted density functional theory (DFT) calculations to understand the surface structure and chemical composition of the oxidised diamond(110) surface. By constructing a large set of possible terminations and coverages, we construct a phase diagram of surface terminations, which is dominated by an unexpectedly stable co-existence phase of keto and ether groups. By explicit simulation of IR and XPS signals, we establish the most likely dominant oxygenation state of the surface.

O 91.2 Wed 18:15 P2/1OG

Surface structure of MOVPE-prepared GaP(111)B — •Peter Kleinschmidt[1], Pingo Mutombo[2], Theresa Berthold[1,3], Agnieszka Paszuk[1], Matthias Steidl[1], Gernot Ecke[4], Andreas Nägelein[1], Christian Koppka[1,3], Oliver Supplie[1], Stefan Krischok[1,3], Oleksandr Romanyuk[2], Marcel Himmerlich[1,3,5], and Thomas Hannappel[1] — [1]Institut für Physik, Technische Universität Ilmenau PF 100565, 98684 Ilmenau — [2]Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10, 16200 Prague, Czech Republic — [3]Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, PF 100565, 98684 Ilmenau, Germany — [4]Institut für Mikro- und Nanoelektronik, Technische Universität Ilmenau, PF 100565, 98684 Ilmenau, Germany — [5]European Organization for Nuclear Research - CERN, 1211 Meyrin, Switzerland

The MOVPE-prepared GaP(111)B surface was studied by XPS, STM, LEED, AES and AFM as well as ab initio DFT. Deoxidation under TBP, followed by high-temperature annealing under pure hydrogen results in the formation of Ga-rich islands, whereas the regions in between are atomically flat. Atomically resolved STM of these regions shows a largely disordered surface, but small units of (2×2), $c(4 \times 2)$, and $(\sqrt{3} \times \sqrt{3})R30°$ordering can be identified. According to DFT calculations, these are the most favorable reconstructions under hydrogen-rich conditions. We conclude that STM images the dangling bonds of an otherwise hydrogen-terminated phosphorus face.

O 91.3 Wed 18:15 P2/1OG

Impact of Al on defect formation in GaP buffer layers grown on Si(100) substrates in CVD ambience — •Manali Nandy[1], Agnieszka Paszuk[1], Christian Koppka[1], Markus Feifel[2], Peter Kleinschmidt[1], Frank Dimroth[2], and Thomas Hannappel[1] — [1]Institute of Physics, TU Ilmenau, Ilmenau, Germany — [2]Fraunhofer Institute for Solar Energy Systems ISE, Freiburg, Germany

The performance of III-V-on-Si multi-junction solar cells is still limited by a high density of defects at the GaP/Si heterointerface and in the III-V buffer layer. Here, in order to improve the crystal quality of the GaP buffer layer grown on Si(100) substrates by MOCVD, we modify the GaP nucleation, which consists of 10 alternating pulses of TBP and TEGa, by substituting the first few selected TEGa pulses with TMAl. Crystal defects in the GaP(100) buffer layers are investigated by electron channeling contrast imaging. GaP buffer layers grown on the GaP nucleation exhibit short misfit dislocations (MDs), and therefore, a high density of threading dislocations (TDs), which are located at the ends of each MD. In contrast, in the GaP buffer layer grown on the AlGaP nucleation the MDs are significantly longer, which results in lower density of TDs. In addition, we find lower density of stacking faults and stacking fault pyramids compared to the GaP buffer layer grown on the GaP nucleation. We conclude that the Al induced in the GaP nucleation layer suppresses defect formation and improves crystal quality of the epilayer. Further studies of reciprocal space map by x-ray diffraction aim to investigate strain in both GaP buffer layers and its correlation to the defect density.

O 92: Poster Session - Ultrafast Electron Dynamics at Surface and Interfaces II

Time: Wednesday 18:15–20:00 Location: P2/1OG

O 92.1 Wed 18:15 P2/1OG

Electronic energy transfer during scattering of H$^+$/Al(111) studied with TDDFT-MD and adiabatic GGA — •Lukas Deuchler and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, CAU Kiel, 24098 Kiel, Germany

In order to quantify the electronic energy transfer that occurs during the scattering of hyperthermal H$^+$ ions incident on the on-top position of an Al(111) surface, Ehrenfest molecular dynamics simulations based on time-dependent density functional theory have been performed. The Al-surface is represented by a cluster geometry. We have used the Octopus code [1] by A. Rubio *et al.* Scattering and charge transfer of H$^+$ at Al surfaces has been studied experimentally and theoretically since long [2-4]. Here we extend our previous TDDFT-MD simulations of the charge transfer [4] and demonstrate how the electronic energy transfer (and thus the kinetic energy of the scattered hydrogen) is linked to the distance where the charge transfer occurs.

[1] X. Andrade *et al.*, Phys. Chem. Chem. Phys. **17**, 31371 (2015).
[2] H. Winter, J. Phys.: Condens Matter **8**, 10149 (1996).
[3] J. Merino *et al.*, Phys. Rev. B **54**, 10959 (1996).
[4] J. Merino *et al.*, Phys. Rev. B **57**, 1947 (1998).
[5] N. Schlünzen *et al.*, Contrib. Plasma Phys. e201800184 (2019).

O 92.2 Wed 18:15 P2/1OG

Describing the electronic nonequilibrium after ultrashort laser excitation — •Markus Uehlein, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

Laser-matter interaction is an important topic in fundamental research for industrial applications. The energy of ultrashort laser pulses in the visible range is only absorbed by the electrons of the solid and then transferred to the phonons. For this dynamics multiple descriptions exist, ranging from phenomenological models to kinetic simulations. Here, we want to compare an extension of the TTM [1] by a non-thermal electron distribution and its interactions [2], with a complete kinetic description applying complete Boltzmann Collision Integrals [3]. Both descriptions are applied for various metals. Results as well as the range of applicability of the models will be compared.

[1] S. I. Anisimov *et al.*, JETP **39**, 375 (1974)
[2] E. Carpene, PRB **74**, 024301 (2006)
[3] B. Y. Mueller and B. Rethfeld, PRB **87**, 035139 (2013)

O 92.3 Wed 18:15 P2/1OG

Dual-channel laser system with gap-less tuning from 250 - 1300 nm at megahertz repetition rates for time-resolved photoelectron-emission microscopy and spectroscopy — •Michael Schulz[1], Gregor Indorf[1], Ivanka Grguras[1], Jan-Heye Buss[1], Torsten Golz[1], Mark Prandolini[1,2], and Robert Riedel[1] — [1]Class 5 Photonics GmbH, Notkestrasse 85, 22607 Hamburg, Germany — [2]Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

A dual-channel, high-power laser system with gap-less tuning from 250 - 1300 nm at 30 - 50 femtoseconds pulse duration is presented as the ideal tool for time-resolved photo-emission microscopy and spectroscopy experiments in order to study ultrafast condensed phase and interface dynamics. The system integrates an industrial Yb-doped femtosecond laser, two independently tunable optical-parametric amplifiers, second-harmonic generation and third-harmonic generation, and features repetition rates from 0.1 - 4 MHz with maximum average power of 3 W per channel.

O 92.4 Wed 18:15 P2/1OG

Implementation of a bichromatic beamline for time-resolved two-photon momentum microscopy — •Martin Mitkov, Ralf Hemm, Florian Haag, Sebastian Emmerich, Sebastian Hedwig, Martin Aeschlimann, and Benjamin Stadtmüller — University of Kaiserslautern and Research Center OPTIMAS, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern

Mapping excited state dynamics in momentum space on a femtosecond time scale by time-resolved two-photon photoemission is an important prerequisite for understanding the optical and transport properties of new functional and materials. This is typically challenging for molecular materials due to their large ionization potential.

Here, we present a novel beamline for our momentum microscope [1] that is optimized for molecular spectroscopy with femtosecond time-resolution. It consists of a bichromatic UV beamline for 3 eV pump, 6 eV probe spectroscopy. The femtosecond time resolution will be demonstrated by cross-correlation measurements using a C$_{60}$ multilayer film evaporated on Cu(111) as model system. For comparison, we will show autocorrelation traces recorded for the 3 eV probe pulse on a clean Cu(111). Finally, the capability of our approach of time-resolved momentum microscopy for molecular materials will be discussed for the prototypical molecular system C$_{60}$ on Cu(111).

[1] F. Haag et al., Rev. Sci. Instr. 90, 103104 (2019)

O 92.5 Wed 18:15 P2/1OG

Energy and momentum streaking in subcycle THz-ARPES — •Jens Güdde[1], Johannes Reimann[1], Suguru Ito[1], Stefan Schlauderer[2], Christoph Schmid[2], Christoph Lange[2], Rupert Huber[2], and Ulrich Höfer[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, Germany — [2]Fakultät für Physik, Universität Regensburg, Germany

Recently, we have demonstrated a novel concept of subcycle THz-ARPES, which permits a direct access to carrier transport in non-trivial band structures with high time resolution [1]. This concept employs time- and Angle-Resolved Photoelectron Spectroscopy (ARPES) to observe how the carrier wave of a THz pulse accelerates Dirac fermions in the topological surface state of Bi$_2$Te$_3$.

Here, we will show that in addition to this acceleration within the sample, the THz electric field also leads to an energy and momentum streaking of the photoemitted electrons, the size of which depends on its polarization direction. For UV photoemission pulses that are much shorter than the period of the THz driving field, this streaking can be used for an in-situ sampling of the electric field at the sample surface, but also needs to be taken into account for a correct interpretation of the photoelectron spectra. We will discuss how the acceleration within the sample and the streaking in front of the surface both affect energy and momentum of the detected photoelectrons in a different manner, and how these contributions can be disentangled.

[1] J. Reimann *et al.* Nature **562**, 396 (2018).

O 92.6 Wed 18:15 P2/1OG

Localized linear photoemission from a cold field emitter — •Alexander Schröder, Jelto Jordan, Nora Bach, Christopher Rathje, and Sascha Schäfer — Institute of Physics, University of Oldenburg, Germany

Ultrafast transmission electron microscopy (UTEM) combines the femtosecond temporal resolution of a pump-probe approach with the nanometer spatial resolution of a TEM. Further improving the spatio-temporal resolution in UTEM requires the development of novel high-coherence photoelectron sources with stable laser-driven emission currents over long time periods.

Here, we report on the current status of our development of a laser-driven cold field emitter. Using a field ion microscope, we prepared atomically clean (311)-oriented sharp tungsten tips. Above a certain threshold potential localized photoemission from these tips is observed using a continuous-wave 355-nm laser beam focused onto the tip apex. Photocurrent characterization yields a stable, linear photoemission regime in the fA-range, ideally suited for application in UTEM.

O 92.7 Wed 18:15 P2/1OG

Momentum Microscope vs. Hemispherical analyzer - a quantitative comparison of electron analyzer performance for time-resolved ARPES experiments — Julian Maklar, Tommaso Pincelli, Samuel Beaulieu, Shuo Dong, Maciej Dendzik, Martin Wolf, Ralph Ernstorfer, and •Laurenz Rettig — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

For angle-resolved photoelectron spectroscopy (ARPES), an important element is the employed electron analyzer. While hemispherical analyzers with angle-dispersing electron lenses have been the working horse for decades, recently time-of-flight based momentum microscopes have shown a huge improvement in parallel detection efficiency, allowing for simultaneous detection of multiple Brillouin zones without the need to rearrange the sample geometry. However, one drawback of such instruments, in particular in time-resolved studies, arises from the large energy and momentum range covered simultaneously, which in combination with detection limitations of delay-line detectors can severely reduce the effective detection rate for selected energy-momentum regions compared to conventional hemispherical analyzers. Additionally, the high electron energies employed in the more complex electron lens system designs impose new constraints in terms of space charge. Using our XUV time-resolved ARPES system hosting both a hemispherical analyzer (SPECS Phoibos 150) and a momentum microscope (SPECS Metis 1000) in one experimental setup, we quantitatively compare the advantages and disadvantages of both types of analyzers for various kinds of trARPES experiments.

O 92.8 Wed 18:15 P2/1OG

Observation of electron excitation dynamics by time-resolved two-photon momentum microscopy based lifetime analysis — •Lars Pidde, Florian Haag, Tobias Eul, Eva Walther, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics and research center OPTIMAS, TU Kaiserslautern

The investigation of the dynamics of hot electrons are fundamental to understand many chemical and physical phenomena at surfaces, interfaces or in bulk materials. The evolution of such electrons on ultrafast timescales are dominated by inelastic and elastic scattering processes which simultaneously affect both the electron energy and their momentum. To capture these complex dynamics, we present a data analysis scheme based on time-resolved two-photon momentum microscopy [Rev. Sci: Instrum. 90, 103104 (2019)]. It incorporates the well established *tr-2PPE* experiments, momentum resolved *photoemission electron microscopy* and either *double hemispherical* or *time-of-flight* energy analyzers. To determine lifetimes of electrons in predefined energy and momentum regions we present a data analysis scheme to create so called lifetime maps at constant energies.

The capability of this approach is exemplary illustrated by the study of a metallic surface.

O 93: Surface Magnetism (joint session MA/O)

Time: Thursday 9:30–12:00 Location: HSZ 101

Invited Talk O 93.1 Thu 9:30 HSZ 101

Vacuum Resonance States as Atomic-Scale Probes of Noncollinear Surface Magnetism — •Anika Schlenhoff — Department of Physics, University of Hamburg (Germany)

Understanding the spin-dependent scattering of electrons at magnetic surfaces is highly relevant for the control of electron transport in future spintronic applications. However, its atomic-scale variations, e.g. on noncollinear magnetic surfaces, remained inaccessible, due to the laterally averaging nature of the established experimental approaches.

By means of spin-polarized scanning tunneling microscopy (SP-STM) and spectroscopy on unoccupied resonance states (RSs) located *in vacuo*, the reflection of electrons at noncollinear magnetic surfaces is investigated [1]. Even for energies up to 20 eV above the Fermi level, the RSs exhibit the same local spin quantization axis as the underlying spin texture. Mapping the spin-dependent electron phase shift upon reflection at the surface on the atomic scale demonstrates the relevance of all magnetic ground state interactions for the scattering of spin-polarized low-energy electrons. Moreover, while conventional SP-STM is restricted to probe at tip-sample distances of a few Å, tunneling into RSs allows for imaging atomic-scale spin textures at technically feasible distances in the nm regime [2]. Experimental results will be discussed in terms of the RS spin-splitting and the magnetic contrast as a function of bias and tip-sample distance, as well as in terms of the atomic-scale nature of the electron reflection at the surface.

[1] A. Schlenhoff, S. Kovaric, S. Krause, and R. Wiesendanger, Phys. Rev. Lett. **123**, 087202 (2019). [2] A. Schlenhoff *et al.*, in preparation.

O 93.2 Thu 10:00 HSZ 101

Dead magnetic layer at the interface - magnetic moment quenching in Mn on W(001) — •Sebastian Meyer[1], Martin Schmitt[2], Matthias Vogt[2], Matthias Bode[2], and Stefan Heinze[1] — [1]Institute for Theoretical Physics and Astrophysics, Christian-Albrechts University of Kiel, 24098 Kiel — [2]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, 97074 Würzburg

The magnetic moment of transition metals can vary strongly due to orbital bonding interactions with ligands, hybridization, or band structure changes induced by reduced coordination, often resulting in high spin–low spin transitions [1]. In contrast, the complete quenching of the magnetic moment, a so-called "dead magnetic layer", has not yet been observed [2]. Using density functional theory in combination with spin-polarized scanning tunneling microscopy, we show that the surface of a Mn double layer on W(001) exhibits a two-dimensional c(2×2) antiferromagnetic ground state. This result can only be confirmed by a complete moment quenching in the interfacial Mn layer caused by the combined action of hybridization and magnetic frustration.

[1] J. L. Fry, *et. al.*, Phys. Rev. B **36**, 868 (1987)

[2] C. A. F. Vaz, *et. al.*, Rep. Prog. Phys. **71**, 056501 (2008)

O 93.3 Thu 10:15 HSZ 101

Tunneling anisotropic magnetoresistance of Pb and Bi adatoms and dimers on Mn/W(110) — •Soumyajyoti Haldar, Mara Gutzeit, and Stefan Heinze — Institute of Theoretical Physics, University of Kiel, Leibnizstrasse 15, 24098 Kiel, Germany

Noncollinear magnetic structures at transition-metal interfaces are very promising candidates for spintronics applications [1]. A Mn monolayer on W(110) is a prominent example which exhibits a noncollinear cycloidal spin-spiral ground state with an angle of about 173° between neighboring spins. This allows to rotate the spin-quantization axis of an adatom or dimer quasicontinuously and is ideally suited to explore the angular dependence of the tunneling anisotropic magnetoresistance (TAMR) using scanning tunneling microscopy. Here [2], using density functional theory, we explored the TAMR effect of Pb and Bi adatoms and dimers adsorbed on this surface as these elements have a very strong spin-orbit coupling. Pb and Bi adatoms and dimers show a large TAMR up to 60% due to strong spin-orbit coupling (SOC) and the hybridization of 6*p* orbitals with 3*d* states of the magnetic layer. For dimers the TAMR also depends sensitively on the dimer orientation with respect to the crystallographic directions of the surface due to bonds formation with the surface and the symmetry of the SOC induced mixing.

[1] A. Fert et al. Nat. Nanotechnol. **8**, 152 (2013). [2] S. Haldar et al. Phys. Rev. B **100**, 094412 (2019)

O 93.4 Thu 10:30 HSZ 101

Dynamical spin-excitations of transition metal atoms deposited on superconducting surfaces — •Ana Montero, Filipe Souza Mendes Guimarães, Juba Bouaziz, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recently, the interest in superconductors has been renewed thanks to their application in topological quantum computing — for instance, in the context of qubits, such as Majorana zero modes, which are in-gap states that can arise in nanostructures deposited atop superconductors. Based on ab-initio simulations [1], we systematically scrutinize the electronic and magnetic properties of 3*d* adatoms deposited on various superconducting surfaces above their critical temperature, and investigate their dynamical spin-excitation as probed via inelastic tunneling spectroscopy (IETS). The excitation lifetime, damping and signature in the transport spectra will be presented with a focus on the potential generation of many-body states resulting from the interaction of electrons and spin-excitations.

This work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator Grant No. 681405-DYNASORE).

[1] B. Schweflinghaus et al. Phys. Rev. B **89**, 235439 (2014).

O 93.5 Thu 10:45 HSZ 101

Doping graphene with substitutional manganese atoms — •Renan Villarreal[1], Pin-Cheng Lin[1], Harsh Bana[1], Maya N. Nair[2], Ken Verguts[3,4], Steven Brems[4], Stefan De Gendt[3,4], Manuel Auge[5], Hans Hofsäss[5], Chris Van Haesendonck[1], and Lino M. C. Pereira[1] — [1]Quantum Solid-State Physics, KU Leuven, 3001 Leuven, Belgium — [2]CUNY Advanced Science Research Centre, 85 St. Nicholas Terrace, New York, N.Y. 10031, USA — [3]Departement Chemie, KU Leuven, 3001 Leuven, Belgium — [4]Interuniversitair Micro-electronica Centrum (imec), vzw, 3001 Leuven, Belgium — [5]II. Institute of Physics, University of Göttingen, Göttingen 37077, Germany

Several approaches have been explored for the functionalization of 2D materials: the use of different substrates, creation of intrinsic defects, adsorption and intercalation, substitutional doping, among others. For incorporation of substitutional dopants, a major challenge remains: the limited control over the concentration and form of incorporation. An alternative approach is to incorporate the foreign species by ultra-low energy (ULE) ion implantation, precisely tuning the number of implanted ions and their kinetic energy. Here, we demonstrate that it is possible to controllably incorporate manganese (Mn) in graphene as a substitutional dopant using ULE ion implantation. Our approach is based on a wide range of characterization techniques, including STM/STS, synchrotron-based XPS, ARPES, XMCD, transport measurements and Raman spectroscopy. These experimental studies are complemented by DFT and MD calculations.

15 min. break.

O 93.6 Thu 11:15 HSZ 101

Growth and Characterization of Thulium-Cyclooctatetraene-Compounds on Gr/Ir(111) with XANES and XMCD — •Lea Spieker[1], Alexander Herman[1], Benedikt Eggert[1], Tobias Lojewski[1], Nico Rothenbach[1], Stefan Kraus[2], Florin Radu[3], Chen Luo[3,4], Kai Chen[3], Fadi Choueikani[5], Thomas Michely[2], and Heiko Wende[1] — [1]University of Duisburg-Essen — [2]University of Cologne — [3]Helmholz Center Berlin for Materials and Energy — [4]TU Munich — [5]Synchrotron SOLEIL

The magnetic anisotropy and the magnetic coupling of localised 4f elements connected to an organic ligand in a molecular network are a notable point of interest in organic spintronics. We combine the lanthanide thulium (Tm) with the organic molecule cyclooctatetraene (Cot) for the growth of different phases on Gr/Ir(111). Using an undoped substrate Gr/Ir(111) leads the TmCot to self-assemble in a punctiform shape (Dot-phase). On the negatively doped substrate Gr/Eu/Ir(111) TmCot self-assembles in sandwich-molecular wires. As reference, these phases are compared to the metallic sample Tm/Ir(111) which is known to have an electronic configuration of 4f^{12}. The electronic and magnetic properties are analysed by X-ray Absorption Spectroscopy using the methods XANES and XMCD, at temperatures down to 1 K. Angular- and field-depended measurements at the thulium M$_{4,5}$-edge revealed magnetic anisotropies. By comparison to multiplet calculations the electronic configuration could be determined as 4f^{12} for the three phases. Financial support by DFG (WE 2623/17-1) is acknowledged.

O 93.7 Thu 11:30 HSZ 101

***Ab initio* simulations of hybrid magnetic 2D-materials** — •Nicolae Atodiresei, Vasile Caciuc, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich, Germany

We used density functional theory calculations to engineer the electronic and magnetic properties for two classes of two dimensional (2D) materials adsorbed onto Ir(111). In a 1st study, we investigated how to magnetically functionalize a nonmagnetic 2D system as MoS$_2$ by adsorbing a magnetic cluster made of three Fe atoms. In a 2nd study, we employed non-magnetic molecular systems characterized by different reactivity (e.g. electropositive BH$_3$ and electronegative NH$_3$ molecules) to chemically funtionalize a single layer of a magnetic 2D system such as CrI$_3$. Our *ab initio* simulations can be used as a guide on how the interaction between 2D, atomic clusters and molecules can be used to manipulate the (i) spin-polarization, (ii) magnetic exchange couplings, (iii) magnetic moments and (iv) their orientation of these hybrid 2D materials. This work has been supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project number 277146847 - CRC 1238 (C01). [1] V. Caciuc *et al.*, Phys. Rev. Mat. **2**, 084001 (2018). [2] V. Caciuc *et al.*, Phys. Rev. Mat. **3**, 094002 (2019).

O 93.8 Thu 11:45 HSZ 101

Emerging 2D-ferromagnetism and strong spin-orbit coupling at the surface of valence-fluctuating EuIr$_2$Si$_2$ — •Susanne Schulz[1], Ilya A. Nechaev[2], Monika Güttler[1], Georg Poelchen[1], Steffen Danzenbächer[1], Silvia Seiro[3], Kristin Kliemt[4], Evgueni V. Chulkov[5], Clemens Laubschat[1], Eugene E. Krasovskii[5], Christoph Geibel[6], Cornelius Krellner[4], Kurt Kummer[7], and Denis V. Vyalikh[5] — [1]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [2]Centro de Física de Materiales CFM-MPC and Centro Mixto CSIC-UPV/EHU, Donostia/San Sebastián, Spain — [3]IFW Dresden, Germany — [4]Kristall- und Materiallabor, Goethe-Universität Frankfurt, Germany — [5]Donostia International Physics Center, Donostia/San Sebastián, Spain — [6]MPI für Chemische Physik fester Stoffe, Dresden, Germany — [7]European Synchrotron Radiation Facility, Grenoble, France

Here, we present the valence-fluctuating material EuIr$_2$Si$_2$, where in contrast to its non-magnetic bulk, the Si-terminated surface reveals controllable 2D ferromagnetism. Close to the surface the Eu ions prefer a magnetic divalent configuration and their large $4f$ moments order below 48 K. The emerging exchange interaction modifies the spin polarization of the 2D surface electrons originally induced by the strong Rashba effect. The temperature-dependent intermediate valence of the bulk allows to tune the energy and momentum size of the projected band gaps to which the 2D electrons are confined. This gives an additional degree of freedom to handle spin-polarized electrons at the surface.

O 94: 2D Materials and their Heterostructures II (joint session DS/O/HL)

Time: Thursday 9:30–10:45 Location: CHE 89

O 94.1 Thu 9:30 CHE 89

Longitudinal Nonlinear Spin Sensitive Response in two-dimensional Materials — •Dominik Kreil, Mario Graml, and Helga M. Böhm — Institute of Theoretical Physics, Johannes Kepler University Linz, Altenbergerstr. 69, A-4040 Linz, Austria

Future spin- and valleytronic devices will demand a deeper understanding of electronic systems. [1] With increasing intenstitys of state of the art terahertz lasers linear approximations become more imprecise. Nonlinear plasmonic effects arising from coherent oscillations of free charge carriers in metals or highly doped semiconductors serve to enhance optical processes. The underlying dynamics of electrons (or holes) was successfully treated semi-classically [2] in three-dimensional (3D) nanostructures; quantum expressions for up to the third order of the longitudinal nonlinear polarizabilities of the 3D, 2D and 1D homogeneous electron gases as well as graphene are also known. We here present a general discussion of higher order response functions resulting from time-dependent perturbation theory. Using the random phase approximation as in Ref. [3] we also derive a closed formula for longitudinal nonlinear spin sensitive response functions in arbitrary order. It holds for all the above listed systems and for imbalanced spin- or valley-polarizations. An application to the 2D spin-polarized electron gas with parabolic dispersion and in graphene [4,5] is presented.

References: [1] Vitale et al., Small 14, 1801483 (2018). [2] Krasavinet al., Laser & Photonics Reviews 12, 1700082 (2018). [3] Mikhailov, Phys. Rev. B. 93, 085403 (2016). [4] D. Kreil et al., Phys. Rev. B. 92, 085403 (2015). [5] D. Kreil et al., Lithuanian J. Phys. 59, 35 (2019).

O 94.2 Thu 9:45 CHE 89

Predicting Exfoliability of MAX Phases into MXenes Using Ab-initio Thermodynamics — •Ali Muhammad Malik, Delwin Perera, Jochen Rohrer, and Karsten Albe — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

In recent years, research on 2D MAX-derived MXenes has expanded significantly due to their potential application in energy storage systems, electromagnetic interface shielding, electrocatalysis and gas detection. Almost 40 MAX phases have been predicted to be exfoliable based on force constant calculations and exfoliation energies. However, in experiment only 21 have so far been chemically exfoliated. In this work, we present a descriptor that combines calculated reaction energies and surface stabilities under experimentally relevant conditions.

In agreement with experiments, we show that this descriptor is indeed capable of predicting the exfoliability of MXenes from Ti-based MAX phases in HF, whereas Cr-based MAX phases are predicted to decompose into Cr_3C_2 (carbide). We suggest that this descriptor is capable to guide experimental synthesis efforts in particular with respect to the choice of etchant and concentration.

O 94.3 Thu 10:00 CHE 89

Characterization and Stability of Janus TiXY (X/Y= S, Se, and Te) Monolayers — Aybey Mogulkoc[1], Yesim Mogulkoc[1], Seymur Jahangirov[2], and •Engin Durgun[2] — [1]Department of Physics, Ankara University, 06100, Ankara, Turkey — [2]UNAM and Institute of Materials Science and Nanotechnology, Bilkent University, 06800, Ankara, Turkey

The addition of third element to binary 2D structures can lead to superior properties, hence extensive analyses on the characterization of such systems are required to reveal their full potential. In this study, we examine the structural, mechanical, electronic, thermal, and optical properties of TiXY (X/Y= S, Se, and Te) monolayers by using first-principles techniques. The stability of 1T and 2H-phases are revealed by phonon spectrum analysis and molecular dynamics simulations. Following the investigation of the mechanical response, electronic structures are examined together with partial density of states analysis. While monolayers of 1T-TiXY are found to be semimetals, monolayers of 2H-TiXY are semiconductors with indirect band gap. The optical spectrum is obtained by calculating the imaginary dielectric function and is correlated with the electronic structure. The variation of heat capacity with temperature is investigated and low/high temperature response is shown. Finally, possible structural distortions are also taken into account and charge density wave transition in 1T-TiSeS due to Peierls instability is demonstrated. Our results not only reveal the stable Janus monolayers of TiXY but they also point out these systems as promising candidates for nanoscale applications.

O 94.4 Thu 10:15 CHE 89

Semiconducting defect-free polymorph of borophene: Peierls distortion in two dimensions — Semran Ipek[2], Aybey Mogulkoc[1], •Seymur Cahangirov[2], and Engin Durgun[2] — [1]Department of Physics, Ankara University, 06100, Ankara, Turkey — [2]UNAM and Institute of Materials Science and Nanotechnology, Bilkent University, 06800, Ankara, Turkey

In contrast to the well-defined lattices of various two-dimensional (2D) systems, the atomic structure of borophene is sensitive to growth conditions and type of the substrate which results in rich polymorphism. By employing ab initio methods, we reveal a thermodynamically stable borophene polymorph without vacancies which is a semiconductor unlike the other known boron sheets, in the form of an asymmetric centered-washboard structure. Our results indicate that asymmetric distortion is induced due to Peierls instability which transforms a symmetric metallic system into a semiconductor. We also show that applying uniaxial or biaxial strain gradually lowers the obtained band gap and the symmetric configuration is restored following the closure of the band gap. Furthermore, while the Poisson's ratio is calculated to be high and positive in the semiconducting regime, it switches to negative once the metallicity is retrieved. The realization of semiconducting borophene polymorphs without defects and tunability of its electronic and mechanical response can extend the usage of boron sheets in a variety of nanoelectronic applications

O 94.5 Thu 10:30 CHE 89

First-principles study of hydrogenation on bilayer GaN — •Anh Khoa Augustin Lu[1], Tetsuya Morishita[1,2], Tomoe Yayama[3], and Takeshi Nakanishi[1,2] — [1]MathAM-OIL, AIST, Sendai, Japan — [2]CD-FMat, AIST, Tsukuba, Japan — [3]Department of Applied Physics, Kogakuin University, Tokyo, Japan

In the last decade, a large number of two-dimensional materials has been discovered. In recent years, two-dimensional III-V materials have arisen with the experimental demonstration of two-dimensional GaN. Here, we focus on the case of bilayer GaN. While the atomic structure of pristine bilayer GaN is relatively well understood, the impact that hydrogenation remains unclear since unlike transition metal dichalcogenides, pristine GaN has dangling bonds. In that respect, the present work focuses on the atomic structure, stability and electronic properties of bilayer GaN passivated by hydrogen atoms, with a large range of hydrogen coverage. First-principles calculations based on the density functional theory were performed to identify the structures with the lowest energy. While previous studies have focused on structures oriented along the c-plane, our results reveal that depending on the hydrogen concentration, the plane orientation of the most stable structure (c-, m-, or a-plane) is different. In particular, at high hydrogen concentration, structures oriented along the m- and a-planes have the lowest energy. Their stability is confirmed by first-principles molecular dynamics simulations performed at finite (room) temperature. By modulating the hydrogen concentration, one can therefore tailor the atomic structure and properties of bilayer GaN.

O 95: Thin Oxides and Oxide Layers I (joint session DS/HL/O)

Time: Thursday 9:30–10:45 Location: CHE 91

O 95.1 Thu 9:30 CHE 91

Atomically sharp epitaxial interface between Ba_2SiO_4 and Si(001) — •Julian Koch and Herbert Pfnür — Leibniz Universität Hannover, Institut für Festkörperphysik

Epitaxial growth of Ba_2SiO_4 on Si(001) is a challenge, since neither crystal symmetry nor lattice constants match in a simple manner, but as we show, it has the potential to become the first high quality crystalline high-k gate dielectric. We combined X-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED) and aberration-corrected scanning transmission electron microscopy (STEM) in order to optimize the epitaxial growth by molecular beam epitaxy. The films were grown by a co-deposition method that requires no diffusion of Si from the substrate. While 400 °C turned out to be sufficient to form chemically homogeneous films, crystalline films required an annealing step to $670-690\,^{\circ}C$ with the break-up of interfacial Si-O bonds as crucial step. STEM confirms that the interface is atomically sharp and that a single layer of the silicate is changed to a (2×3) structure at the interface from the (2×1.5) bulk structure. Electrical measurements on MOS-diodes with this material show small hysteresis in CV-curves, low interface trap densities ($< 6\times10^{10}$ cm^2eV^{-1}) and low leakage currents.

O 95.2 Thu 9:45 CHE 91

Nano-scale spectroscopic analysis of $LaAlO_3/SrTiO_3$ interfaces using scattering-type Scanning Near-field Optical Microscopy — •Yigong Luan[1], Julian Barnett[1], Marc Rose[2], Felix Gunkel[2], Martin Lewin[1], and Thomas Taubner[1] — [1]Institute of Physics (IA) RWTH Aachen — [2]PGI-3, Forschungszentrum Jülich

In the group of functional oxide materials, the interface of bulk insulators $LaAlO_3$ and $SrTiO_3$ (LAO/STO) attracts attention due to its highly confined and conductive two-dimensional electron gas (2DEGs), which could be interesting for high-electron-mobility transistors. 2DEGs at oxide interfaces result from electronic reconstruction, which is highly dependent on the local structure [1]. The extraction of their electronic properties is difficult for far-field spectroscopy and conventional nano-resolved microscopy (e.g. STM), as the conducting layer is highly confined and buried below an insulating layer (LAO). We overcome these limitations by using scattering-type Scanning Near-field Optical Microscopy for a quantitative extraction of electron properties from "phonon-enhanced spectroscopy", as the presence of free charge carriers leads to significant changes to the phonon resonance due to plasmon-phonon coupling [2]. We use an improved model (Finite Dipole Model) combining with Transfer Matrix Method to interpret the experimental results, investigating the influence of both LAO layer and 2DEGs on the STO phonon near-field resonance in detail, which allows us to extract the local electronic properties.

[1] A. Ohtomo et al., Nature 427, 423 (2004)
[2] M. Lewin et al., Adv. Funct. Mater, 28. 1802834 (2018)

O 95.3 Thu 10:00 CHE 91

Optoelectrical properties of VO_2 ultra-thin films — •Maximilian Obst[1], Laura Rodríguez[2], Gustau Catalan[2,3], Susanne C. Kehr[1], and Lukas M. Eng[1,4] — [1]Institute of Applied Physics, Technische Universität Dresden, Germany — [2]Institut

Catalá de Nanociéncia i Nanotecnologia and The Barcelona Institute of Nanoscience and Technology, Campus UAB, Barcelona, Catalonia — [3]ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Catalonia — [4]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, Technische Universität Dresden, Germany

Vanadium dioxide (VO_2) is a material that is in the central research focus due to its metal-to-insulator phase transition (MIT) at room temperature. Experimentally, this temperature-regime is easily accessible, and hence allows profound MIT-studies while dreaming of interesting applications, such as phase-change memories. Although thicker VO_2 films are intensively investigated, the properties and physical behavior of ultrathin VO_2 layers are far from being understood.

In this work, an epitaxial VO_2-film of 10 nm grown on a rutile(001) single-crystal is explored, applying a broad set of electrical and optical methods. While Raman-spectroscopy revealed no structural phase transition of the film, electrical transport measurements as well as spectrally-resolved (UV to mid-IR) reflectivity measurements clearly show the MIT at ~300 K. In conclusion, the structural and electrical phase transition seems to be completely disentangled in these ultrathin films. However, thin VO_2-films might easily oxidize to V_2O_5, as was indicated by measuring the vanadium $2p_{3/2}$-peak using XPS.

O 95.4 Thu 10:15 CHE 91

Towards quasi two-dimensional β-Ga2O3 — •Constance Schmidt, Mahfujur Rahaman, and Dietrich R. T. Zahn — Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

β-Ga2O3 is a transparent oxide semiconductor with outstanding properties due to its wide bandgap (Eg = 4.9 eV). It is already intensively studied in its bulk and thin film form. Studies on ultrathin films or even quasi-2D films are less common. Nevertheless, for nano electronics quasi-2D β-Ga2O3 can be beneficial as semiconductor or insulator, depending on layer thickness and doping [1]. β-Ga2O3 is not a van-der-Waals material, which makes conventional exfoliation challenging. Attempts show that layer thicknesses below 60 nm are not yet possible by exfoliating β-Ga2O3 [2]. To overcome this difficulty, we use a van-der-Waals material (GaSe), exfoliate thin flakes on Si with 300 nm SiO2, HOPG and Mica substrates, and oxidize these flakes by thermal annealing ((600 - 1000)°C, 30 min, in air) to obtain quasi 2D β-Ga2O3. In this work, we show the preparation of Se free quasi-2D β-Ga2O3 by annealing using temperatures higher than 700°C. The thin flakes obtained have thicknesses in the range of (0.5 - 50) nm as measured with atomic force microscopy. Energy dispersive X-ray spectra reveal the chemical composition of the 2D flakes and most importantly the absence of Se. Raman spectroscopy (excitation: 325 nm) verifies the β-Ga2O3 phase.

[1] J. Su, et al., J. Phys. Chem. C 122 43 24592-24599 (2018) [2] Y. Kwon, et al., APPLIED PHYSICS LETTERS 110 131901 (2017)

O 95.5 Thu 10:30 CHE 91

Thermal phase transformations through iron oxides/ oxide substrates interfaces — •Mai Hussein Hamed[1,2], David N. Mueller[1], Tomáš Duchoň[1], Ronja Hinz[1], Claus M. Schneider[1,3], and Martina Müller[1,4] — [1]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich GmbH, Germany — [2]Faculty of Science, Helwan University, Cairo, Egypt — [3]Fakultät für Physik, Duisburg-Essen Universität , Germany — [4]Experimentelle Physik I, Technische Universität Dortmund, Germany

Oxide heterostructures possess a wide range of electrical and magnetic properties arising, in particular, vie interactions across their interfaces. Therefore, our primary goal is understanding, controlling and tuning the interface properties. In this study, using hard X-ray photoelectron spectroscopy (HAXPES), we demonstrate phase transformations from Fe_3O_4 to either γ-Fe_2O_3 or FeO through active redox reactions across three relevant interfaces, i.e. (1) the outside atmosphere/Fe_xO_y film interface, (2) the interface between phase-transformed Fe_xO_y/Fe_xO_y intralayers and (3) the Fe_xO_y/oxide substrate interface. We find that the "active" oxide substrates ($SrTiO_3$ or YSZ) play an important role as an additional oxygen supplier or scavenger. This leads to a clear alteration of the standard temperature-pressure phase diagram of iron oxides. Accordingly, we calculate the effective oxygen pressure through the interfaces and adjust the phase diagram. Our findings allow us not only to control the interfaces but more importantly, to tune their physical functionalities by a controlled thermal phase design, giving access to far from equilibrium phases.

O 96: Overview Talk: Charlie Sykes

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

Topical Talk O 96.1 Thu 9:30 TRE Phy

Single-Atom Alloy Catalysts: Born in a Vacuum, Tested in Reactors, and Understood In Silico — •Charles Sykes — Tufts University, Medford, MA, USA

In this talk I will discuss a new class of metallic alloy catalysts called Single Atom Alloys in which precious, reactive metals are utilized at the ultimate limit of efficiency. These catalysts were discovered by combining atomic-scale scanning probes with more traditional approaches to study surface-catalyzed chemical reactions. This research provided links between the atomic scale surface structure and reactivity which are key to understanding and ultimately controlling important catalytic processes. Over the last five years the concepts derived from our surface science and theoretical calculations have been used to design Single Atom Alloy nanoparticle catalysts that can perform industrially relevant reactions at realistic reaction conditions. For example, alloying elements like platinum and palladium with cheaper, less reactive host metals like copper enables 1) dramatic cost savings in catalyst manufacture, 2) more selective chemical reactions, 3) reduced susceptibility to CO poisoning, and 4) higher resistance to deactivation by coking. I go on to describe very recent theory work predicts reactivity trends of 16 different Single Atom Alloy combinations for important reaction steps like activation of H-H, C-H, N-H, O-H and C=O bonds. This project illustrates that the field of surface science is now at the point where it plays a critical role in the design of new heterogeneous catalysts.

O 97: Wetting and Liquids at Interfaces and Surfaces I (joint session CPP/O/DY)

Time: Thursday 9:30–13:00 Location: ZEU 255

O 97.1 Thu 9:30 ZEU 255

Designing Pickering Emulsions for Catalysis: Influence of Nanoscale Particle Properties on Microscale Droplets — •Sebastian Stock[1], Annika Schlander[1], Kai Spanheimer[1], Maresa Kempin[2], Dmitrij Stehl[1], Anja Drews[2], Markus Gallei[3], and Regine von Klitzing[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]HTW Berlin, Berlin, Germany — [3]Universität des Saarlandes, Saarbrücken, Germany

Pickering Emulsions (PEs) describe emulsions stabilized by surface-active particles. The aim of the present work is to design PEs as a reaction environment for catalytic reactions. As a model reaction the hydroformylation of 1-dodecene is investigated. Due to the PEs high stability separation methods with outstanding energy efficiency are applicable e. g. the separation of the oil phase by nanofiltration. Many microscopic and macroscopic PE properties are dominated by the nanoscale properties of the particles. In order to distinguish the impact of particle surface charge both positively and negatively charged silica spheres were prepared. This was achieved by adequate surface modification. The resulting nanoscale particle properties concerning size, shape, charge, and hydrophobicity were investigated via Transmission Electron Microscopy (TEM), ζ-potential and sessile drop measurements, the effect on the microscopic emulsion properties were studied with microscopy and the PEs reaction behavior including yield and stability was evaluated.

O 97.2 Thu 9:45 ZEU 255

A Thermodynamic Consistent, Instantaneous Dividing Surface to Study Wetting Phenomena — •Amal Kanta Giri and Marcello Sega — Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Fürther Straße 248, 90429 Nürnberg, Germany

A detailed knowledge of the microscopic structure and dynamics in the interfacial region of soft materials is a necessary step on the way to develop novel materials and is also key to a deeper understanding of the statistical mechanics of fluid interfaces out of equilibrium. The presence of thermal capillary waves, however, hinders efforts to investigate the local structure of interfaces by smearing out observable quantities computed in the global reference frame. To recover a detailed picture of the interface neighborhood, one needs to compute observables in the local, instantaneous reference frame located at the interface, although the determination of this frame is, in general, not unique.

Here, we report on the possibility of using computational geometry approaches to determine the set of instantaneous surface atoms in a way which is thermodynamically consistent with the Gibbs (equimolar) dividing surface. We apply these methods to the determination of the instantaneous, fluctuating contact line of droplets on solid substrates, with an outlook on the problem of dynamic wetting of soft, deformable substrates.

O 97.3 Thu 10:00 ZEU 255

Concentration measurements in binary liquids via Raman spectroscopy — •Alena K. Bell and Robert W. Stark — Physics of Surfaces, Materialwissenschaften, TU Darmstadt, Alarich-Weiss-Str. 16, 64287 Darmstadt, Deutschland

The optical measurement of concentration gradients in liquid mixtures plays a crucial role in understanding transport processes in various technical applications such as printing or medical technology. In particular Raman spectroscopy offers a direct approach to identify the substances and to quantify the concentration of the components in a binary liquid. In order to quantify concentration gradients confocal Raman spectroscopy can provide the necessary spatial and temporal resolution that is needed to monitor transport processes as they occur during the evaporation of binary droplets or during mixing processes in microchannels. To this end, chemically similar substances such as alcohols of different molecular weight need to be differentiated either through the analysis of the fingerprint region or through chemical labelling. However, using the weak Raman signals in fingerprint region reduces the temporal resolution drastically which makes chemical labelling much more convenient. We discuss the advantages and disadvantages of chemical labelling in order to discriminate spectroscopically between the components of a binary liquid. By using this approach concentration gradients can be calculated by comparing relative peak intensities and correlating these results with calibration curves. Thus, the temporal and spatial evolution of concentration gradients in binary mixtures of chemically similar fluids can be analysed.

O 97.4 Thu 10:15 ZEU 255

Hard sphere electrolyte solutions at heterogeneously charged substrates — •Maximilian Mussotter[1], Markus Bier[2], and S. Dietrich[1] — [1]Max-Planck Institut für Intelligente Systeme und Universität Stuttgart, 70569 Stuttgart, Germany — [2]University of Applied Sciences Würzburg-Schweinfurt, 97421 Schweinfurt, Germany

The structure of a dilute electrolyte solution close to a surface carrying a non-homogeneous surface charge distribution is investigated by means of classical density functional theory (DFT) within the approach of fundamental measure theory (FMT). In the case of electrolyte solutions, the effects of these inhomogeneities are particularly severe due to the corresponding length scale being the Debye length, which is large compared to molecular sizes. A fully three-dimensional investigation is performed, which accounts explicitly for the sol- vent particles, and thus provides insight in effects of ion-solvent coupling. The present work introduces a powerful framework to study a broad range of possible surface charge heterogeneities even beyond the linear response regime, showing a sensitive dependence of the density profiles of the fluid components and of the electrostatic potential on the magnitude of the charge as well as on the short ranged details of the surface charge pattern.

O 97.5 Thu 10:30 ZEU 255

Core-shell latex colloids as interfaces for tailoring wetting properties — Calvin J. Brett[1,2,3], Joakim Engström[3,4], Volker Körstgens[5], Peter Müller-Buschbaum[5,6], Eva Malmström[4], and •Stephan V. Roth[1,4] — [1]DESY, 22603 Hamburg, Germany — [2]KTH, Dept. Mechanics, SE-10044 Stockholm, Sweden — [3]WWSC, SE-10044 Stockholm, Sweden — [4]KTH, Dept. Fibre and Polymer Technology, SE-10044 Stockholm, Sweden — [5]TUM, Physik Department, 85748 Garching, Germany — [6]MLZ, TUM, 85748 Garching, Germany

Facile surface functionalisation of latex colloids makes them most promising materials for broad thin film applications. However, the effect of these colloids on chemical film and wetting properties is not easily evaluated. Core-shell particles can deform and coalesce on the nanoscale during thermal annealing yielding tailored physical properties. We investigated two different core-shell systems (soft and rigid) with identical shell but with chemically different core polymer and core size. These core-shell colloids are probed during thermal annealing on surfaces in order to investigate their behavior as a function of nanostructure size and rigidity. X-ray scattering allows us to follow the re-arrangement of the colloids and the structural evolution in situ during annealing. Evaluation by real-space imaging techniques reveals a disappearance of the structural integrity and a loss of colloids' boundaries. We present the possibility to tailor and fine-tune the wettability by tuning the core-shell colloid morphology in thin films, thus providing a facile template methodology for repellent surfaces.

O 97.6 Thu 10:45 ZEU 255

Depleting Hydrogels with Oil Flows — •Philipp Baumli[1], Emanuela Lorusso[2], Lukas Hauer[1], Azadeh Sharifi-Aghili[1], Katharina Hegner[1], Maria D'Acunzi[1], Burkhard Duenweg[1], Jochen Gutmann[2], Hans-Jürgen Butt[1], and Doris Vollmer[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Deutsches Textilforschungszentrum Nord-West ÖP GmbH, Adlerstraße 1, 47798 Krefeld, Germany.

Hydrogels are ubiquitous in our daily lives. Applications range from jelly pudding and diapers to scaffolds in tissue engineering. A hydrogel-coating is covalently attached to a micropillar array. Swelling the hydrogel-coating with water establishes a liquid-infused surface (LIS). On LIS, liquid-depletion is synonymous with loss of functionality.

We demonstrate that the hydrogel-based LIS can be kept lubricated upon a shear-flow of oil for a wide variety of flow conditions independent of the exact nature of the hydrogel-coating. Dehydration of the hydrogel-coating is followed by confocal laser scanning microscopy and progresses linearly independent of flow conditions and hydrogel. The mechanism is explained with the help of an extended diffusion model.

O 97.7 Thu 11:00 ZEU 255

Tracking nematic flows at microscales using small angle X-ray scattering — •Paul Steffen[1], Eric Stellamanns[2], Michael Sprung[2], Fabian Westermeier[2], and Anupam Sengupta[3] — [1]Göttingen — [2]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [3]Physics of Living Matter, Dept. of Physics and Materials Science, University of Luxembourg, Luxembourg

Liquid crystal microflows play a fundamental role in materials, modern display technologies, and biological systems. However, a quantitative, dynamic and spatially resolved measurement of the director field and surface anchoring remain a significant challenge. Here we present small angle X-ray measurements on stationary flows of 4-Cyano-4-pentylbiphenyl (5CB) in circular Kapton capillaries (under homeotropic and random planar anchoring) at temperatures between 280 and 310 K, and Ericksen numbers ranging from 0 to 200, with a spatial resolution of 1/1000 of the capillary dimension. The angular dependence of the scattering peaks from both periodic length scales was approximated by a double Gaussian fit with four parameters: amplitude, angle, width and background amplitude. The peak angles were found to be in good agreement with the director fields calculated using the Leslie-Ericksen theory. The width and the amplitude of the scattering patterns obtained from the larger length scale are less affected by the temperature than those from the smaller length scale.

15 min. break

O 97.8 Thu 11:30 ZEU 255

Macroscopic Capillary Number for Characterization of Two-phase Flow in Porous Media — •Hu Guo and Rudolf Hilfer — Institute for Computational Physics, Universität Stuttgart, Stuttgart, Germany

The Capillary number (Ca) defined as the ratio of viscous force to capillary force is widely used to qualitatively characterize multiphase flow in porous media as in carbon dioxide geologic sequestration and chemical enhanced oil recovery (EOR). The main difficulty is to characterize forces porperly. There exists 22 definitions for Ca (Guo et al, IOR 2020). The most concise definition is $Ca = \frac{v\mu}{\sigma}$ with velocity v, viscosity μ and interfacial tension σ (Saffman and Taylor, 1958). It is supported by core flooding tests and most widely used. However, this definition is less sound than the one that involves the wettability parameter (Moore and Slobod, 1955). Meanwhile, the values of these Ca are regarded as too small to reflect the actual force balance (Dullien, 1979). It was shown theoretically, that this Ca is microscopic in nature and incorrectly used (Hilfer and Øren, 1996, Trans. Porous Media).

We study the new macroscopic capillary number $Ca = \frac{\mu\phi v L}{K P_b}$ with viscosity μ, porosity ϕ, velocity v, permeability K, length L and capillary breakthrough pressure P_b (Hilfer et al, 2015, Physical Review E). The new Ca explains some of the latest observations (Doorwar and Mohanty, 2017, SPE J; Qi et al, 2017, SPE J; Rabbani et al, 2018, PNAS; Zhao et al, 2019, PNAS) that contradict predictions obtained from the microscopic Ca. EOR field practice also verified that the macroscopic Ca is more profound.

O 97.9 Thu 11:45 ZEU 255

Drop Impact on Hot Plates: Contact, Lift-Off and the Formation of Holes — •Kirsten Harth[1,2], Sang.Hyeon Lee[3], Maaike Rump[2], Minwoo Kim[3], Detlef Lohse[2], Kamel Fezzaa[4], and Jung Ho Je[3] — [1]Institute of Physics, Otto von Guericke University Magdeburg — [2]Physics of Fluid and Max Planck Center, University of Twente, The Netherlands — [3]X-Ray Imaging Center, Pohang University of Science and Technology, Korea — [4]X-Ray Science Division, Argonne Ntnl. Laboratory, USA

Everyone who poured water into a hot pan has experienced the manifold boiling behaviours of drops impacting on a hot plate, a problem which is of high relevance in many technical applications. When the drop is gently deposited, and the surface temperature is sufficiently high, it hovers on a vapour layer (Leidenfrost effect). For impacting drops, this critical temperature for a contact-less rebound is substantially increased, and much harder to determine. In fact, determining contact times between drops and smooth substrates from side view imaging is impossible for most temperatures above the boiling point.

We combine High-Speed Total Internal Reflection and synchrotron X-Ray measurements to reliably determine contact times and the Leidenfrost temperature for drops impacting on smooth hot surfaces. Furthermore, we study the lift-off characteristics. A local minimum in lift-off times correlates with spontaneous lamella rupture and the morphology of the contact.

O 97.10 Thu 12:00 ZEU 255

Lucas-Washburn equation applies for four phase contact point — •Peyman Rostami[1,2] and Günter Auernhammer[1,2] — [1]Max Planck Institute for Polymer Research, 55128, Mainz, Germany — [2]Leibniz Institute of Polymer Research, 01069, Dresden, Germany

A four-phase contact point, e.g., in merging of immiscible drops, is the point where the liquid-liquid interface advances along the contact line of one drop. The dynamics of drop merging involve various driving and dissipating forces in the dynamics of the four-phase contact point. The viscous friction, i.e. the flow field, within liquids is influenced by the different boundary conditions on the different interfaces (liquid-gas, liquid-liquid, liquid-solid). Additionally, Marangoni stresses between the two liquids and the spreading coefficients along the contact lines play a role. Effectively, these effects lead to a capillary force acting on the four-phase contact point. In total, the situation resembles the capillary flow in open V-shaped groove. The important difference is that, in the classical problem, the grooves are made out of two solid walls, but in the present case one of the *walls* is liquid, i.e., flowable and deformable. We investigate a range of liquids with different combination of physical properties (viscosity ratio, surface and interfacial tensions). The results show a good qualitative agreement for different liquids of the experimental results with the classical Washburn equation (h~square root of time), where h is the filled length of the *groove*.

O 97.11 Thu 12:15 ZEU 255

Simulations of Thermal Fluctuations with a Thin Film Lattice Boltzmann Model — •Stefan Zitz[1], Jens Harting[1,2], and Andrea Scagliarini[3] — [1]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Nuremberg, Germany — [2]Eindhoven University of Technology, Eindhoven, The Netherlands — [3]Consiglio Nazionale delle Ricerche, Rome, Italy

The effect of thermal fluctuations on thin film flows is an interesting yet challenging phenomenon. Although in experiments their presence is undeniable thermal fluctuations are often neglected in the analysis of the results. Also in simulations their inclusion is far from being trivial due to the stochastic nature of the fluctuations.

Here we present a numerical approach to include the influence of thermal fluctuations. Based on our newly developed lattice Boltzmann method we show how to effectively match the thin film regime and further how to include thermal fluctuations in a self consistent matter [1].

One problem of deterministic thin film simulations is the discrepancy between experimental and simulated rupture times in dewetting experiments. It has been shown that the experimental rupture times are shorter than the ones predicted by deterministic simulations. We will show that adding fluctuations does reduce the rupture time to better match the experimental results. To this end we will also address the importance of the fluid substrate interaction, e.g. the equilibrium contact angle θ_{eq}.

S. Zitz, J. Harting et al., Phys. Rev. E 100:3, 033313, 2019

O 97.12 Thu 12:30 ZEU 255

Impact of submillimetre-sized droplets on freely suspended liquid membranes — •Florian von Rüling, Alexey Eremin, and Ralf Stannarius — Otto von Guericke University Magdeburg, Germany

Droplet impact and splashing phenomena at solid and fluid interfaces remain an exciting research topic with vast application possibilities [1]. Impact scenarios are primarily governed by capillary forces, inertia, oscillation dynamics of the droplets, and the dynamics of the thin air cushion entrapped between droplet and surface during impact [2,3]. We experimentally investigated the impact of large submillimetre- to millimetre-sized droplets on freely suspended smectic films. We were able to vary the droplet diameter from several hundred microns to one millimetre. Droplets can either be trapped or reflected by the film or tunnel through it, depending on geometrical and dynamical parameters. The film remains intact in all these scenarios. In addition to the drop size and impact velocity, material properties and the film thickness can affect the behaviour of both droplet and film.

[1] A. M. Worthington, The Splash of a Drop; Romance of Science. Society for the Promotion of Christian Knowledge, London, 1895.

[2] C. Antonini, A. Amirfazli, M. Marengo, Drop impact and wettability: From hydrophilic to superhydrophobic surfaces, Phys. Fluids 24 102104 (2012).

[3] S. Dölle, R. Stannarius, Microdroplets impinging on freely suspended smectic films: three impact regimes, Langmuir 31 6479 (2015).

O 97.13 Thu 12:45 ZEU 255

Imbibition-Induced Deformation Dynamics in Nanoporous Media — •Juan Sanchz[1], Zhuoqing Li[2], Michael Froeba[3], and Patrick Huber[4] — [1]Institute of Materials Physics, Hamburg University of Technology — [2]Institute of Materials Physics, Hamburg University of Technology — [3]Institute of Anorganic and Applied Chemistry, Hamburg University — [4]Institute of Materials Physics, Hamburg University of Technology

We present time-dependent macroscopic dilatometry experiments on the deformation of nanoporous monoliths (carbon and silica) upon spontaneous, capillarity-driven invasion of water. We find two distinct dynamical regimes. One of them can be quantitatively traced to deformations originating in changes in the surface stress at the inner pore walls (dynamic Bangham's regime) upon water invasion, whereas the second one results from Laplace pressure effects. Our study demonstrates that it is possible to dynamically monitor imbibition dynamics by simple dilatometry measurements.

O 98: Graphene I: Growth, Structure and Substrate Interaction (joint session O/TT)

Time: Thursday 10:30–12:00 Location: GER 37

O 98.1 Thu 10:30 GER 37

Design principles for doping graphene for electrochemical CO2 reduction: Insights from Theory — •Sudarshan Vijay[1], Joseph Gauthier[2], Hendrik Heenen[1], Vanessa Bukas[1], Henrik Kristoffersen[1], and Karen Chan[1] — [1]CatTheory, Department of Physics, Technical University of Denmark — [2]SUNCAT Center for Interface Science and Catalysis, Department of Chemical Engineering

Graphene based 2D catalysts hold great promise for CO2 reduction to CO and CH4. Recent experimental investigations [1,2] show metal doped Iron-Nitrogen-Carbon (Fe-N-C) catalysts are able to reduce CO2 to CO at low overpotentials and with high selectivity. However, modelling these materials in an electrochemical environment poses several open challenges. In this work, we present a theoretical investigation on Fe-N-C catalysts which includes the effect of potential, interfacial pH, change in local spin states to properly elucidate the mechanism for CO2 reduction. We find that the electronic structure of Fe-N-C resembles graphene more than it does a metal, with significantly fewer states at the fermi level. Charge dependence of binding energies of key intermediates depend on the position of the highest energy d-orbital with respect to the fermi level. Using computed reaction energetics coupled with mean-field kinetic models, we are able to ascertain the mechanism for CO2 reduction and compare our results with experimental findings. We extend this analysis to other 2D material systems and propose rational design principles.

[1] Science 14 Jun 2019: Vol. 364, Issue 6445, pp. 1091-1094 [2] ACS Energy Lett. 2018, 3, 4, 812-817

O 98.2 Thu 10:45 GER 37

Graphene/S/Ru(0001): a model system for studying intercalation — •Lars Buss[1,2], Jens Falta[2,3], Moritz Ewert[1], Polina Sheverdyaeva[4], Paolo Moras[4], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Institute for Solid State Physics, University of Bremen, Bremen, Germany — [3]MAPEX Center for Materials and Processes, University of Bremen, Bremen, Germany — [4]Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Trieste, Italy

The epitaxial growth of single-layer graphene on transition-metal substrates enables the growth of micrometer-sized islands with excellent crystalline quality, but the possibly strong binding to the substrate has proven detrimental to its materials properties. However, intercalation of foreign atoms lifts the interlayer coupling, restoring its unique electronic structure. We have investigated the intercalation of sulfur underneath graphene on Ru(0001) with low-energy electron microscopy (LEEM) and micro-diffraction (μLEED). We find that sulfur deposited from a molecular precursor at elevated temperatures intercalates through the edge of the island, eventually leading to wrinkles in the graphene. Intriguingly, the overlaying graphene limits the number of possible S/Ru(0001) reconstructions below, preventing the formation of less dense reconstructions like the p(2×2)-S and $(\sqrt{3}\times\sqrt{3})$-S surface phases. Intensity-voltage LEEM and angle-resolved photoemission (ARPES) prove the free-standing character of the sulfur intercalated graphene, which is found to be p-doped by 380 meV.

O 98.3 Thu 11:00 GER 37

Au intercalation under epitaxial graphene on Ru(0001): the role of graphene edges — •Sebastian Günther[1], Tevfik Onur Mentes[2], Robert Reichelt[1], Elisa Minussi[2], Benito Santos[2], Alessandro Baraldi[2], and Andrea Locatelli[2] — [1]TUM, Dept. Chemie, Lichtenbergstr.4, D-85748 Garching — [2]Sincrotrone Trieste, AREA Science Park I-34149 Trieste

Au intercalation at the graphene-Ru(0001) interface is investigated at elevated temperature by using low energy electron - and x-ray photoelectron emission microscopy (LEEM/XPEEM). Graphene (g) growth by ethylene decomposition at 1030 K on a Au pre-covered Ru surface pushes the Au adatoms towards the g-free surface area. When instead, evaporating Au on a partly g-covered surface, a modified Stranski-Krastanov growth on Ru with two atomic wetting layers followed by 3D islands is observed. At 970 K the growth follows a precise order: 1)The first wetting Au layer is grown exclusively on the g-free area of the Ru surface. 2)After completion of the Au/Ru layer, Au intercalation below g-flakes sets in. 3)Having completed the g/Au/Ru layer, second wetting Au layer growth ouside the g-covered area takes place. 4)After completion of the Au/Au/Ru layer, intercalation of the second Au layer underneath g sets in. At 970 K, Au is shown not to stick to g-covered surface regions. This crucial finding singles out the g-edges as the only intercalation channel. Chemical maps at different stages during Au growth point to a pronounced kinetic barrier at the g-edges preventing intercalation before the Au monolayer is completed outside the g-covered regions.

O 98.4 Thu 11:15 GER 37

Covalent functionalization of epitaxial graphene on cubic-SiC(001) — •Dmitrii Potorochin[1,2,3], Olga Molodtsova[1,2], Victor Aristov[1,4], Alexander Chaika[4], Maxim Rabchinskii[5], Marina Baidakova[2,5], Nikolai Ulin[5], Pavel Brunkov[2,5], Dmitry Marchenko[6], and Serguei Molodtsov[2,3,7] — [1]DESY, Hamburg, Germany — [2]ITMO University, Saint Petersburg, Russian Federation — [3]TU Bergakademie Freiberg, Freiberg, Germany — [4]ISSP RAS, Chernogolovka, Russian Federation — [5]Ioffe Institute RAS, Saint Petersburg, Russian Federation — [6]Helmholtz-Zentrum Berlin, Berlin,Germany — [7]European XFEL, Schenefeld, Germany

Some properties of graphene, although being unique, can serve as a deterrent factor to its use in some fields of technology. For instance, the bandgap absence complicates the fabrication of graphene-based logic elements of electronics. Furthermore, the transparency in the visible spectral region imposes a restriction on the use of graphene as an active material for elements of photonics (photodetectors, photovoltaics, etc.). Covalent functionalization of graphene is a promising approach to overcome such limitations. In the current report, we present an investigation of the electronic structure and morphology of epitaxial graphene on cubic-SiC(001) covalently modified by organic dyes. Results of high-resolution X-ray photoelectron spectroscopy (HR-XPS), photoemission electron microscopy (PEEM), and scanning tunneling microscopy (STM) studies are given. This work was supported by RAS, RFBR (Grant Nos. 17-02-01139, 17-02-01291), and Minobrnauki of Russia (Project 3.3161.2017/4.6).

O 98.5 Thu 11:30 GER 37

Controlled formation of nanobubbles in graphene — •Pin-Cheng Lin[1], Renan Villarreal[1], Harsh Bana[1], Ken Verguts[2,3], Steven Brems[3], Stephen de Gendt[2,3], Manuel Auge[4], Felix Junge[4], Hans Hofsäss[4], Hossein Ghorbanfekr[5], M Fallh[5], François Peeters[5], Mehdi Neek-Amal[5], Chris Van Haesendonck[1], and Lino da Costa Pereira[1] — [1]Quantum Solid State Physics, KU Leuven, 3001 Leuven, Belgium — [2]Departement Chemie, KU Leuven, 3001 Leuven, Belgium — [3]imec, 3001 Leuven, Belgium — [4]II. Institute of Physics, University of Göttingen, Göttingen 37077, Germany — [5]Department of Physics, University of Antwerp, 2020 Antwerp, Belgium

Strained nanobubbles have been used to engineer the electronic structure of graphene through the creation of pseudomagnetic fields (e.g. via strain imposed by a selected substrate or mechanical actuators), however, they provide limited controllability. Here we report on the controlled formation of noble gas (He, Ne, Ar) nanobubbles in graphene (on various substrates) using ultra-low energy (ULE) ion implantation. ULE ion implantation allows us to precisely tune the number of implanted ions and their kinetic energy, which in turn controls the bubble formation efficiency and bubble density. Our experimental approach is based on scanning tunneling microscopy/spectroscopy (STM/STS), synchrotron X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, among others, complemented by density functional theory (DFT) and molecular dynamics calculations (MD), which give insight into the bubble formation and stability mechanisms.

O 98.6 Thu 11:45 GER 37

Simulating the scattering of a hydrogen atom from graphene using a high-dimensional neural network potential. — •Sebastian Wille[1,2], Marvin Kammler[2], Martín L. Paleico[3], Jörg Behler[3], Alec M. Wodtke[1,2], and Alexander Kandratsenka[2] — [1]Institute for Physical Chemistry, Georg-August University Göttingen, Germany — [2]Department of Dynamics at Surfaces, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany — [3]Theoretical Chemistry, Georg-August University Göttingen, Germany

Understanding the formation of covalent bonds due to atomic-scale motions and energy dissipation pathways involved is an ongoing challenge in the field of chemistry. Recent measurements of the translational energy loss distribution of hydrogen atoms scattered from graphene showed a bimodal pattern. The second generation reactive empirical bond order potential was fitted to ab initio electronic structure data obtained from embedded mean-field theory to generate a potential energy surface (PES). First-principles dynamics simulations using the provided PES were able to reproduce the bimodal feature of the energy loss spectrum and were in qualitative agreement with experimental results. But these investigations could not fully provide a detailed description of the scattering and sticking mechanisms. Therefore, we developed a full-dimensional neural network PES by fitting to the density functional theory data in order to further reduce the remaining errors by the fitting procedure of the PES underlying molecular dynamics simulations performed.

O 99: Organic Molecules on Inorganic Substrates VI: Adsorption, Growth and Networks

Time: Thursday 10:30–13:30 Location: GER 38

O 99.1 Thu 10:30 GER 38

Electric Field/ Light-Induced Switching of Spiropyran Derivative on Graphite — •HIMANI MALIK[1], THOMAS HALBRITTER[2], ALEXANDER HECKEL[2], and THIRUVANCHERIL G. GOPAKUMAR[1] — [1]Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur-208016, India — [2]Institute for organic chemistry and chemical biology, Goethe-University Frankfurt, Germany

Spiropyran (SP) and its derivatives are known for their switching ability by UV light. SP (closed form), shows reversible ring openings by cleavage of C-O bond and converted into merocyanine (MC, open form). The open form is planar, conjugated and possesses a large dipole moment due to the stabilization of a zwitterion form [1]. The closed and the open forms are distinguished on Au(111) surface as reported before [2]. In the current work, we discuss the self-assembly of SP derivative with a carboxylic group attached to the indoline ring. The carboxylic group offers strong hydrogen bonding interaction, which facilitates the formation of ordered patterns. We show the electrical field and light-induced switching of an adlayer of SP derivative. The SP films are prepared from the solution phase on highly oriented pyrolytic graphite. The microscopic structure and electronic properties are measured using scanning tunnelling microscopy and atomic force microscopy.

1.G. Cottone, et al., Chem. Phys. Lett 2004, 388, 218-222 2.C. Bronner, et al., J. Phys.: Conden. Matter 2011, 23, 484005-12

O 99.2 Thu 10:45 GER 38

Electron transmission through alpha-helical polyalanine investigated by STM and STS — •Nguyen Thi Ngoc Ha[1], Diana Slawig[2], Yossi Paltie[3], and Christoph Tegenkamp[1,2] — [1]TU Chemnitz, Germany — [2]Leibniz University, Hannover, Germany — [3]Department of Applied Physics, Hebrew University of Jerusalem, Israel

Alpha-helical molecules recently have attracted much attention in view of electron propagation along the helical backbone structure which comes along with an efficient spin polarization [1]. In this study, we investigated the growth and electronic levels of molecular monolayer structures of helical polyalanine-based peptides (PA) on Au(111) and HOPG surfaces by scanning tunneling microscopy (STM), spectroscopy (STS) under ambient conditions. The self-assembled monolayer (SAM) films revealed a high degree of lateral and rotational order [2]. Due to formation of Au-S bonds on Au(111), resulting from the termination of the helix by cysteine, the PA molecules are oriented and their intrinsic dipole moment is tilted with respect to the surface normal, contrary to HOPG. This charge ordering within the SAM facilitates internal electric fields, which obviously renormalize the molecular orbital energies along the helix, thus enabling a high conductance through these peptides. [1] K. Kitagawa et al., Journal of Polymer Science Part A: Polymer Chemistry 41, 3493, (2003). [2] Nguyen T.N.Ha et al. The Journal of Physical Chemistry C 123, 612, (2019).

Invited Talk O 99.3 Thu 11:00 GER 38

Exploration of complex interfacial networks and 2D tesselations — •Johannes V Barth — Physics Department E20, TU Munich - www.e20.ph.tum.de

A major objective in modern surface and nanoscale science relates to complex interfaces and the development of protocols for their control, both in the static and dynamic regime. Interfacial molecular engineering employing optimized assembly procedures and carefully selected molecular tectons represents a powerful tool for constructing a variety of intriguing materials. Herein we report advances towards surface-confined complex networks using different fabricaton schemes. Specifically, we realized networks and tesselations via (i) supramolecular organization of organic tectons, (ii) metal-directed assembly, notably exploiting rare-earth centers, (iii) flexible molecular units, and (iv) multi-step convergent synthesis where sequential chemical conversions of a simple organic species mediate the expression of a semiregular archimedean tiling. Our approach illustrates novel avenues to construct complex materials via specific interactions and interfacial adaptation or transformations of adsorbed molecular species. Moreover, the findings and employed methodology contributes to the general understanding of the emergence of complexity and hierarchic systems in chemistry and biology.

O 99.4 Thu 11:30 GER 38

Explaining Misleading Surface Diffraction Patterns with DFT and Machine Learning — •Andreas Jeindl[1], Jari Domke[2], Malte Schulte[3], Falko Sojka[2], and Oliver T. Hofmann[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany — [3]Experimental Physics 1, TU Dortmund, Germany

The determination of the structure of organic thin films and monolayers on inorganic substrates commonly relies on surface diffraction methods, such as LEED. Although the spectra obtained by these methods contain all the necessary information (except the phase) required to directly reconstruct the atomistic structure, in practice the interpretation is far from straightforward. In cases when multiple different models satisfactorily explain the experiment, good scientific practice suggests applying occam's razor and selecting the simplest structure possible.

Here, we highlight several instances where diffraction pattern misleadingly suggest too simple structures due to the presence of orientational domains, disorder, or small structure factors. Using caffeine on Au(111) and acenequinones on Ag(111) as examples, we perform a comprehensive first-principles structure search to independently determine the correct geometry, which is often complex. We discuss the difficulties and interpretation possibilities when trying to compare LEED-data of organic monolayers with theoretically predicted structures for different organic/inorganic interfaces.

O 99.5 Thu 11:45 GER 38

On-surface synthesis of triazine-based porous nanoribbons — •Mirunalini Devarajulu, Martin Haller, Min-Ken Li, Shadi Sorayya, and Sabine Maier — Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Covalent triazine frameworks are 2D materials that provide a high chemical stability and plenty of nitrogen sites, which are important for host-guest chemistry and applications as membranes and energy storage materials. Here, we present a low-temperature scanning tunneling microscopy study on the on-surface synthesis of triazine-based porous carbon nanoribbons on Ag(111) using 1,3,5-tris(3-bromophenyl)triazine as a precursor. We followed a thermally induced sequential synthesis based on an Ullmann-type reaction to covalently couple the molecules and a preprogrammed isomerization combined with a dehydrogenation reaction to fabricate the ribbons, as previously reported for all-carbon porous nanoribbons.[1,2] Despite the structural similarity of the precursors, the triazine-based molecules lacked a strong conformational selectivity in the first reaction step, which prevented the ribbon formation. We demonstrate that this can be successfully resolved by following either a bimolecular or a kinetically controlled synthesis, respectively. Finally, we will show that the triazine-based porous nanoribbons are suitable for host-guest experiments using single metal atoms.

[1] M. Ammon, T. Sander, S. Maier, JACS, 2017, 139 (37), 12976.

[2] M. Ammon, et al., ChemPhysChem 2019, 20, 2333.

O 99.6 Thu 12:00 GER 38

Controlling molecular cluster formation by molecule-surface interaction — •Ole Bunjes[1], Lucas A. Paul[2], Tobias Claus[1], Emmanouil Stavroulakis[1], Inke Siewert[2], and Martin Wenderoth[1] — [1]IV. Physical Institute, University of Göttingen, Germany — [2]Institute of Inorganic Chemistry, University of Göttingen, Germany

Deposition of self-assembling molecules on a surface is a promising approach to control the growth of large scale structures with nanometer precision, as it is necessary in the context of molecular electronics. We use scanning tunneling microscopy (STM) to study the self-assembly of molecular clusters. Sub-monolayer films of the thermally stable complex *fac*-Re(bpy)CO_3Cl (bpy = 2,2′-bipyridine) were deposited on a clean Ag(100) surface at 300 K, and investigated by STM at low temperatures. The initial steps of cluster formation are found to strongly depend on the presence of step edges with a specific geometric orientation. Attached molecules affect Ag atom diffusion so that the neighboring step segments preferentially align along the same direction, thereby increasing the probability for further molecules to attach to the clusters. This molecule-surface interaction is found to play a major role for the growth of *fac*-Re(bpy)CO_3Cl-structures of different dimensions, e.g., for chain and monolayer growth. We acknowledge the financial support by the DFG via the SFB 1073 (projects C4 and C1).

O 99.7 Thu 12:15 GER 38

Electrospray Controlled Ion Beam Deposition as a powerful tool to deposit biomolecules on a solid support under UHV with subsequent STM imaging — •Karolina Stoiber, Andreas Walz, Peter Knecht, Anthoula Papageorgiou, Joachim Reichert, Annette Huettig, Hartmut Schlichting, and Johannes V. Barth — Physics E20, Technical University of Munich, Germany

Biomolecules gain interest in surface science and nanotechnology as potential building blocks in nano-sized structures or new materials. Their thermal fragility and lack of sublimation capacity make them ineligible for classical deposition technologies such as OMBE. Our new preparative approach based on electrospray ionization with controlled ion beam deposition (ES-CIBD) unlocks this potential. Data obtained with plasmid DNA, insulin and spermine are presented, representing three chemical classes (nucleic acids, proteins, polyamines) and molecular masses from 200 Da to 2 MDa. We applied negative and positive spray modes and tested different conformations introduced by variation of pH, ionic strength or by enzymatic manipulation. The ionization principle described by the charge residue model and chain ejection model is primarily determined by the outer shape of the molecule: here we experimentally compare globular and elongated forms. Parameters to evaluate the preparation process and quality of deposition are mass spectra to assess selectivity, ion currents for efficiency and imaging the deponents on Ag(111) and Cu(111) by UHV-STM for integrity. In conclusion, ES-CIBD is a versatile tool to selectively and efficiently deposit biomolecules on solid supports while the structure is preserved.

O 99.8 Thu 12:30 GER 38

Molecule-Surface Collision Explores the Chemical and Conformation Space of a Molecule — •Kelvin Anggara — Max Planck Institute for Solid State Research, Stuttgart

Molecule-surface collision is fundamental in wide array of contemporary topics, ranging from material science to structural biology. From scattering experiments at gas-surface interface, much of the collision dynamics is known for diatomic molecules colliding with a surface - but not for polyatomics. Here, we study the dynamics of polyatomic-surface collision in vacuo by combining electrospray ionization and single-molecule microscopy. Using the electrospray ion-beam deposition (ES-IBD) technique, a beam of polyatomic ions was aimed normal to a metal surface with a known translational energy. The resulting collision outcome was imaged using Scanning Tunnelling Microscopy (STM) to allow inference of the collision dynamics. The key finding here is that, upon collision, the molecular translation is converted to low-frequency molecular vibrations, which consequently trigger: (i) a chemical reaction at 5 - 50 eV collision energy; or (ii) a conformation change at 0.5 - 5 eV. The former is exemplified by a Reichardt Dye colliding with a Cu(100) surface that gave a bond-selective reaction via mechanical compression of the whole molecule; While, the latter is exemplified by a Cellohexaose colliding with Cu(100) that resulted in an exploration of the conformation space, i.e. folding motifs, of the oligosaccharide. The general approach described here thus allows the use of molecule-surface collision as a means to explore different regions of potential energy surface for any molecule that can be electrosprayed.

O 99.9 Thu 12:45 GER 38

Global approach to prediction and modeling of biomolecules on surfaces — •Johann Christian Schön[1], Juan Cortes[2], Nathalie Tarrat[3], Bohdan Andriyevsky[4], Sabine Abb[1], Stephan Rauschenbach[5], and Klaus Kern[1,6] — [1]MPI FKF, Stuttgart, Germany — [2]LAAS-CNRS, Toulouse, France — [3]CEMES-CNRS, Toulouse, France — [4]TU Koszalin, Koszalin, Poland — [5]Dept. Chemistry, University Oxford, Oxford, UK — [6]EPFL, Lausanne, Switzerland

Biomolecules on surfaces exhibit a large variety of individual conformations and self-assembly patterns, whose prediction is a great challenge. We have developed a systematic global energy landscape based approach to generate models for individual molecules and their assemblies[1]. Individual molecules are globally optimized in the gas phase, and the optimal configurations are placed on the substrate for a second global search using a rapidly-growing random-tree based algorithm, followed by an ab initio relaxation and energy ranking. Finally, the best conformations are used as building blocks for models of the assembly and / or as input conformations for global optimizations of multi-molecule patterns; the resulting multi-molecule assemblies can then be compared with experimental data. We demonstrate this approach at the example of two disaccharides, trehalose[2] and sucrose[3], that had been deposited on a Cu-100 surface and imaged via STM.

[1] J. C. Schön et al., Z. Naturf. B, 2016, 71:351-374 [2] S. Abb et al., RSC Advances, 2019, 9:35813-35819 [3] S. Abb er al., Angew. Chemie, 2019, 131:8424-8428

O 99.10 Thu 13:00 GER 38

Growth of N-heterocyclic carbenes on a deactivated semiconductor surface — •Martin Franz[1], Sandhya Chandola[2], Maximilian Koy[3], Robert Zielinski[2], Matthias Freitag[3], Conor Hogan[4], Frank Glorius[3], Norbert Esser[2], and Mario Dähne[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., 12489 Berlin, Germany — [3]Organisch-Chemisches Institut, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany — [4]Istituto di Struttura della Materia-CNR (ISM-CNR), 00133 Rome, Italy

Self-assembled monolayers based on N-heterocyclic carbenes (NHCs) are promising for surface functionalization as ultra-stable alternatives to thiol based systems. Here, we report on the ordered growth of NHCs on silicon, demonstrating the versatility of NHCs as anchors for surface functionalization. In a detailed scanning tunneling microscopy and first principles calculations study, we investigate the adsorption of the prototypical NHC 1,3-bis(dimethyl)imidazolium (IMe) on the deactivated Si(111)$\sqrt{3}\times\sqrt{3}$R30°-B surface. We find a vertical adsorption geometry of the molecules above the Si adatoms of the substrate. At low IMe coverage, a rotation of the molecules leads to a round appearance in the STM images, while at high NHC coverages an ordering of the molecules into a $2\sqrt{3}\times\sqrt{3}$R30° superstructure is observed.

O 99.11 Thu 13:15 GER 38

Gas adsorption on hydrophobic surfaces near the critical point — •Mike Moron, Göran Surmeier, Marc Moron, Jennifer Bolle, Julia Nase, Michael Paulus, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44227 Dortmund, Germany

Hydrophobic surfaces and their interaction with their environment are of great importance in current research. One important example is the interaction between the so-called surfactants in the alveoli of the lung and the surrounding gas. The surfactants form monolayers inside the alveoli, that are orientated with their hydrophobic hydrocarbon chains towards the gas space. Together with various proteins, the surfactants are involved in the gas exchange and the stabilization of the alveoli. Since the surfactant monolayers are in direct contact with the inhaled air, including argon and CO_2, it is essential to investigate the interaction in order to understand the processes involved. Another important example is the adsorption of CO_2. The usage of metal-organic frameworks (MOFs) appear to be a promising method for storaging CO_2. A self-assembled octadecyltrichlorsilane (OTS) monolayer on a silicon wafer, served as hydrophobic surface. The gases under investigation were CO_2 and Ar at different gas pressures. Besides, we used hexafluorethane (C_2F_6) to study the effect of different gases on the adsorption behavior. We performed an X-ray-reflectivity experiment with a beam energy of 27 keV at the beamline BL9 at DELTA, allowing to resolve the formed structures and gas adsorption layers.

O 100: Electronic Structure of Surfaces II

Time: Thursday 10:30–13:00 Location: REC C 213

O 100.1 Thu 10:30 REC C 213

Scanning tunneling spectroscopy on Be(0001) — •Hermann Osterhage, Roland Wiesendanger, and Stefan Krause — Department of Physics, University of Hamburg, Germany

Beryllium is an alkaline earth metal with peculiar electronic properties. The bulk material behaves similar to a semiconductor with a partial bandgap around the Fermi energy. In contrast, on the Be(0001) surface there is a delocalized electron system contributing substantially to the electronic density of states (DOS) at the Fermi energy.[1] Large amplitudes of Friedel oscillations seen in STM near the Fermi level disagree with a nearly free electron model.[2] A charge density wave and electron-phonon coupling were proposed as possible explanations for this deviation. More recently, the presence of Dirac node lines of surface bands in alkaline earth metals was identified as another possible cause for the unusually large amplitude observed in STM.[3]

While the surface bands of Be(0001) have been studied in angle resolved photoemission spectroscopy,[4] investigations using scanning tunneling spectroscopy have been lacking so far. We recorded tunneling spectra on a clean Be(0001) surface and mapped the charge oscillations at cryogenic temperatures. The energy dependence of the charge oscillations' wave vector will be compared to the surface state dispersion derived from previous photoemission studies.
[1] P. J. Feibelmann *et al.*, Phys. Rev. B **50**, 17480 (1994).
[2] P. T. Sprunger *et al.*, Science **275**, 1764 (1997).
[3] R. Li *et al.*, Phys. Rev. Lett. **117**, 096401 (2016).
[4] K. B. Ray *et al.*, Surf. Sci. **285**, 66 (1993).

O 100.2 Thu 10:45 REC C 213

Measuring the scattering phase shifts of single non-magnetic impurity atoms buried in Cu by STM — •Thomas Kotzott[1], Mohammed Bouhassoune[2], Henning Prüser[1], Samir Lounis[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Germany

Scattering in a solid due to impurity atoms and other crystal imperfections has been subject of research for decades because of its fundamental significance for our understanding of matter and its application in technology. Various experimental approaches have been used to access bulk scattering properties, especially the phase shift, which can be determined by transport properties or the de Haas-van Alphen effect. Here, we use a UHV-low temperature scanning tunneling microscope (STM) to measure the effective scattering phase shift of a single, non-magnetic impurity buried below a Cu(100) surface. We compare silver and germanium atoms by their LDOS surface signature which is created by standing electron waves in the crystal due to electron focusing. We reproduce the experimental topographies accurately with a simple tight-binding model that we use to determine the phase shift. The experimental values match for both species with calculations based on density functional theory. Furthermore, in energy-dependent data we find that the simple model of a Lorentzian scatterer has to be extended to characterize a non-magnetic atom on the local scale. This work was supported by DFG projects LO 1659/5-1 and WE 1889/8-1.

O 100.3 Thu 11:00 REC C 213

Observation of anisotropic vortices on clean superconducting Nb(110) — •Felix Friedrich, Artem B. Odobesko, Robin Boshuis, Stefan Wilfert, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The quest for Majorana zero modes in solid state systems requires the possibility to distinguish between true zero energy modes and the variety of other, trivial, modes that can occur inside the superconducting gap. Large values of the gap facilitate the analysis of these in-gap states. We suggest the clean Nb(110) surface that we obtain by electron beam heating [1] as a suitable platform for future investigations of possible topological states due to its large superconducting gap $\Delta_{\mathrm{Nb}} \approx 1.53\,\mathrm{meV}$. We use low-temperature STM/STS to examine the response of the Nb(110) surface to an external magnetic field. As a type-II superconductor, Nb(110) develops an Abrikosov lattice of vortices. Spectroscopy measurements at the vortex core reveal conductance peaks around zero bias, which we attribute to Caroli-de Gennes-Matricon states. Intriguingly, $\mathrm{d}I/\mathrm{d}U$ maps recorded at bias voltages corresponding to energies inside the superconducting gap uncover an anisotropic shape of the vortices. We explain this observation with the pronounced nesting of the Fermi surface of Nb(110).
[1] A. B. Odobesko *et al.*, Phys. Rev. B **99**, 115437 (2019).

O 100.4 Thu 11:15 REC C 213

Scanning Tunneling Microscopy of Sub-Surface Atomic Structure of the Phase Change Material $\mathrm{GeSb_2Te4}$ **Enabled via Surface Antiresonances** — •Philipp Küppers[1], Peter Schmitz[2], Marcus Liebmann[1], Albert Ratajczak[3], Hilde Hardtdegen[4], Detlev Grützmacher[3], Riccardo Mazzarello[2], and Markus Morgenstern[1] — [1]II. Inst. Phys. B and JARA-FIT, RWTH Aachen University — [2]Institut für Theoretische Festkörperphysik, RWTH Aachen University — [3]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI 9) — [4]Forschungszentrum Jülich GmbH, Ernst Ruska Centre for Microscopy and Spectroscopy with Electrons (ERC-2)

The detailed atomic structure of phase change materials including its disorder is crucial for the understanding of many of its key features. A detailed mapping of the atomic disorder is challenging by standard approaches such as transmission electron microscopy, atom probe tomography or scanning tunneling microscopy. The latter suffers from the fact that the surface is covered by the well ordered Te layer. Here, we show by comparison of scanning tunneling spectroscopy and density functional theory data that details of the subsurface layer consisting of Ge, Sb and vacancies can be mapped by exploiting states that are suppressed towards the surface, so-called surface antiresonances. Probing such states becomes apparent as a honeycomb structure consisting of the Te layer and a significant contribution from the subsurface arrangement.

O 100.5 Thu 11:30 REC C 213

Layer thickness dependence of the electronic correlation in the surface alloy CeAg_x **on Ag(111)** — •Katharina Kissner, Hendrik Bostelmann-Arp, and Friedrich T. Reinert — Experimentelle Phyik VII, Universität Würzburg

Ce-based compounds present a role model for the investigation of electronic correlation. At low temperatures the local interaction of conduction band electrons with the single *4f*-electron provided by Ce leads to distinct features in the electronic structure in CeAg_x on Ag(111). These features appear in the valence band electronic structure in terms of the Kondo resonance, its spin orbit partner and the *4f*-ionization peak, as well as in the Ce *3d*-core levels. The appearance of Kondo physics strongly depends on the local environment of the Ce ion in the lattice and can therefore be modified by varying the alloy film thickness or by doping with different adatoms [1, 2].
In this study we investigate the electronic structure and stoichiometry of different surface alloy film thicknesses of CeAg_x on Ag(111) by means of Angle Resolved and X-Ray Photoelectron Spectroscopy (ARPES and XPS). Furthermore we study the surface lattice structure by Low Energy Electron Diffraction and Scanning Tunneling Microscopy (LEED and STM). This provides us with the opportunity to tune the strength of the electronic correlation in CeAg_x on Ag(111).
[1] H. Schwab, Phys. Rev. B, 85, 2012; [2] C. Praetorius et al., Phys. Rev. B 92, 045116, (2015)

O 100.6 Thu 11:45 REC C 213

Multiple scattering x-ray photoelectron diffraction study on the Ni-doped SrTiO3 (100) films — •Fatima Alarab[1,2], Sylvain Tricot[3], Berengar Leikert[4], Matthias Muntwiler[5], Karol Hricovini[2], Didier Sébilleau[3], and Ján Minár[1] — [1]NTC, University of West Bohemia, Pilsen, Czech Republic — [2]LPMS, Université de

Paris Seine, Neuville sur-Oise, France — [3]IPR, Université de Rennes, Rennes, France — [4]RCCM, Universität Würzburg, Würzburg, Germany — [5]PSI, Villigen, Switzerland

The atomic surface structure of Ni-doped SrTiO3(100) films grown by pulsed laser deposition (PLD) method with (Ni=6 at% and 12 at%) was investigated by x-ray photoelectron diffraction (XPD) at the PEARL beamline of the Swiss-Light-Source. The main goal is to define Ni impurity locations (Substitutional and/or interstitial positions) in the hosting lattice. The results have been compared to similar XPD measurements on pure SrTiO3(100) films. Ekin of all recorded spectra was chosen to be in the range of 190-198 eV. In this interval of energy, the photoelectron diffraction peaks are assigned by considering not only the forward scattering of photoelectrons by the atomic potential near the emitter atom, but also the backward scattering effects. This makes XPD more sensitive on an atomic scale and useful for local atomic structure analysis down to the monolayer and surface relaxation. With the large number of elastic scattering events, it was necessary to use the multiple scattering package for spectroscopies (MsSpec) in which same experimental conditions used for the XPD data acquisition were applied for the multiple scattering calculations.

O 100.7 Thu 12:00 REC C 213

In operando angle-resolved photoemission on a graphene device — •Davide Curcio[1], Alfred Jones[1], Jyoti Katoch[2], Klara Volckaert[1], Deepnarayan Biswas[1], Ryan Muzzio[2], Charlotte E. Sanders[3], Pavel Dudin[4], Cephise Cacho[4], Jill A. Miwa[1], Søren Ulstrup[1], and Philip Hofmann[1] — [1]Aarhus University, Denmark — [2]Carnegie Mellon University, USA — [3]Central Laser Facility, STFC Rutherford Appleton Laboratory, UK — [4]Diamond Light Source, UK

The electronic structure and properties of two-dimensional (2D) materials are widely tuneable via the choice of substrate, vertical electric fields or subtle structural features, and surprising new properties such as gate-switchable superconductivity have been observed in transport experiments. The directly accessible surface of 2D materials permits, at least in principle, a simultaneous study of transport properties and electronic structure using in-operando angle-resolved photoemission spectroscopy (ARPES). So far, this has been achieved for applied gating voltages but not in presence of a steady state current through the device, mainly because a large voltage drop within the area of the UV light spot proves detrimental to the energy resolution of the experiment. Here, using a graphene device as a model system, we show that this restriction can be overcome with a nano-scale light spot. We demonstrate non-invasive nanoARPES spectroscopy of the spectral function in a graphene device for current densities of up to 10^7Acm^{-2}, mapping properties such as the local doping, many-body effects, conductivity, and carrier mobility.

O 100.8 Thu 12:15 REC C 213

Spectroscopic evidence for a charge-density wave in monoclinic TaTe2 — •Sanjoy K Mahatha[1], Florian Diekmann[2], Sebastian Rohlf[2], Matthias Kalläne[2,3], and Kai Rossnagel[1,2,3] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [3]Ruprecht-Haensel-Labor, Christian-Albrechts-Universität zu Kiel und Deutsches Elektronen-Synchrotron DESY, 24098 Kiel und 22607 Hamburg, Germany

Layered transition-metal dichalcogenides have been a subject of intense research for the last 40 years or so as they are characterized by a plethora of interesting physical phenomena including the formation of charge-density waves (CDWs). Recently, considerable interest in the electronic properties of transition-metal ditellurides has been sparked by the discoveries of Weyl fermions and extremely large magnetoresistance in WTe2 [1]. Within the ditelluride family, however, one compound, TaTe2, has received very little attention until now. Monoclinic TaTe2 undergoes a first-order structural transition around 170 K [2] that has been suggested to originate from a CDW instability. Yet, spectroscopic signatures of the interplay between the complex lattice distortion and charge-density modulation are still missing. Here, we will give a detailed account of the experimental geometric and electronic structure of this "neglected" material.

[1] M. N. Ali, et al., Nature 514, 205 (2014). [2] J. J. Gao, et al., Phys. Rev. B 98, 224104 (2018).

O 100.9 Thu 12:30 REC C 213

Investigation of strong correlation and topological phase in Thulium monochalcogenides TmSe$_{1-x}$Te$_x$ — •Simon Müller[1], Chul-Hee Min[2], Celso Fornari[1], Chang-Jong Kang[3], Byung Il Min[4], Yong Seung Kwon[5], and Friedrich Reinert[1] — [1]Institut für Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany. — [2]IEAP, Christian-Albrechts-Universität zu Kiel, Germany. — [3]Departement of Physics and Astronomy, Rutgers University, New Jersey, USA. — [4]PCTP, Pohang University of Science and Technology, Republic of Korea. — [5]Department of Emerging Materials Science, DGIST, Daegu, Republic of Korea.

To understand the possible interplay between strong correlation and topology it is necessary to find a compound possessing these properties. Surface states with strongly localized 4f character is a good starting point, but the Dirac point has not been clearly identifying by experiments, yet. Our investigation of TmSe$_{1-x}$Te$_x$, which belongs to a mixed valence [1] and is predicted to show a band inversion in our DFT studies, has two main focuses. On the one hand, we try to continuously tune the lattice parameter of the system to a region, which for single crystalline samples was not reachable in ambient pressure, and on the other hand, we want to investigate other facets that are not possible to achieve by cleaving single crystals. In this talk, we will present experimental results of the single crystals but also first results of the grown film. [1] H. Launois, et al., PRL 44, 1271 (1980)

O 100.10 Thu 12:45 REC C 213

Understanding chemical constrast in field ion microscopy — •Christoph Freysoldt, Shyam Katnagallu, Baptiste Gault, Michael Ashton, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40273 Düsseldorf

Field ion microscopy (FIM) was the first technique to image surfaces with atomic resolution. In FIM, rare gas atoms are ionized near the surface of a nano-sharp tip subject to a very high voltage. FIM has recently seen renewed interest as a 3D imaging technique for crystallographic features: by applying additional voltage pulses, the surface atoms can be slowly evaporated, revealing the atomic structure of the tip layer by layer. Today's machinery of automated image processing allows then for a reconstruction of the tip's atomic structure.

While the FIM imaging contrast (which strongly depends on field strength, geometrical, and electronic structure) is generally not well understood, recent combined FIM and atom-probe tomography experiments demonstrated and proved a high chemical contrast in a Ni-based model superalloy, where Re atoms are imaged much brighter than the Ni matrix. To explain this effect from a density-functional theory perspective, we exploit a hitherto unknown formal equivalence in the theory of electron tunneling between FIM and scanning tunneling microcopy (STM). The calculations show not only a significant enhancement of the local density of states above Re atoms in a Ni matrix, but also show that adsorbed rare gas atoms may act as 'tunneling lenses' that generally improve lateral contrast.

O 101: Ertl Young Investigator Award Competition

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

O 101.1 Thu 10:30 TRE Ma

Magnetic resonance imaging of single atoms on a surface — •Philip Willke[1,2,3], Aparajita Singha[1,2], Xue Zhang[1,2], Kai Yang[3], Yujeong Bae[1,2,3], Taner Esat[1,2], Christopher Lutz[3], Andreas Heinrich[1,2], and Taeyoung Choi[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Ewha Womans University, Seoul 03760, Republic of Korea — [3]IBM Almaden Research Center, San Jose, USA

Combining electron spin resonance (ESR) with scanning tunneling microscopy (STM) allowed for spin resonance experiments on individual atoms on surfaces[1], for remote sensing of atomic spins[2] and for accessing the nuclear spin of single atoms in an STM[3]. In this talk, we focus on the interaction of the atomic spin system on the surface with the magnetic STM tip. We show that the tip field allows to tune the spin system into resonance similar to the external magnetic field, and that it can even fully replace the latter[4]. By utilizing this tip magnetic field, we establish magnetic resonance imaging of single atoms[5], exceeding the spatial resolution of other scanning field-gradient techniques by one to two orders of magnitude. We find that MRI scans of different atomic species and with different probe tips lead to unique resonance images revealing the magnetic interaction between tip and atom. [1] Baumann et al., Science, 350, 417-420 (2015). [1] Choi et al., Nat. Nano 12, 420-424(2017). [3] Willke et al., Science 362, 336-339 (2018) [4] Willke, Singha, Zhang et al., Nano Lett. 19, 8201-8206 (2019) [5] Willke et al. Nat. Phys. 15, 1005-1010 (2019).

O 101.2 Thu 11:00 TRE Ma

Probing surface electronic structure and reaction intermediates in situ — •Kelsey Stoerzinger — Oregon State University, Corvallis, Oregon USA — Pacific Northwest National Laboratory, Richland, Washington USA

Catalysts are important constituents in numerous energy conversion and storage processes. Rational design of catalysts with greater activity for higher efficiency devices requires an understanding of the material surface's electronic structure in situ, as well as the reaction intermediates involved.

Many surface science techniques, such as X-ray photoelectron spectroscopy (XPS), collect information from inherently surface-sensitive low-energy processes, requiring operation in ultrahigh vacuum. This constraint is lifted for ambient pressure XPS, which can probe the surface in equilibrium with the gas phase at pressures up to ~a few Torr, or with thin liquid layers using a higher incident photon energy. I will discuss the insights obtained with this technique regarding the electronic structure of well-defined epitaxial oxides in equilibrium with a gaseous atmosphere of small molecules (e.g. O2, H2O, CO2, CH3OH, NO), the adsorption of such species, and their subsequent transformation upon driving a desired reaction by heat, voltage, or additional reactant. Adsorption and reactivity can be manipulated by the oxide composition and electronic structure, crystallographic orientation, strain, and local environment in amorphous materials. This molecular-level understanding of interfacial interactions can guide the rational design of high-surface-area oxide catalysts for technical applications.

O 101.3 Thu 11:30 TRE Ma

Control of molecular spins on surfaces — •Manuel Gruber — IEAP, Christian-Albrechts-Universität zu Kiel, Germany

Controlling the spin of individual molecules is attractive for molecular spintronics, quantum computing, and may turn useful to study many-body physics in yet unexplored regimes. I will report on three approaches pursued in our group. (i) A direct approach is to employ spin-crossover (SCO) complexes, which exhibit an intrinsic spin bistability. Having first demonstrated SCO of Fe^{2+} compounds, we recently extended controlled and reversible switching to single Fe^{3+} complexes on a Cu_2N surface. (ii) We integrated a spin switching functionality into robust complexes. It relies on the mechanical movement of an axial ligand strapped to a porphyrin ring. Thus spin and coordination are interlocked and we demonstrate reversible electron-induced switching in this new class of compounds on Ag(111). (iii) Spin is induced in molecules and to some extent controlled through supramolecular manipulation. Spin detection is based on the Yu-Shiba-Rusinov resonances that result from the interaction of the induced spin with Cooper pairs of a superconducting substrate. The induced magnetic moment is fine tuned through the control of the electrostatic potential engendered by neighboring molecules. These experiments notably allow to probe the Yu-Shiba-Rusinov physics caused by fractional charges.

This work has been done in collaboration with the groups of Profs. Berndt, Herges, Rossnagel and Tuczek. Support via SFB 677 and the European Union's Horizon 2020 research and innovation programme (766726) is acknowledged.

O 101.4 Thu 12:00 TRE Ma

Determination and control of charge states of individual molecules — •Shadi Fatayer, Florian Albrecht, Nikolaj Moll, and Leo Gross — IBM Research - Zurich

The physicochemical properties of molecules adsorbed on surfaces are charge-state dependent. Insulating films serve as an ideal platform to study the physics and chemistry of charged molecules, because these films avoid charge leakage. However, investigating individual charged molecules on insulators is experimentally challenging. The atomic force microscope (AFM), operable on insulating substrates and capable of single-electron sensitivity and atomic resolution, is suitable to be used with insulators. Using the AFM, I will first show how the charge state of molecules can be controlled. Then, I will present how different aspects of charged molecules can be accessed with the AFM: (i) How using the AFM as a single-electron current meter allows for tunneling spectroscopy to be performed on insulators and electron-transfer properties probed, (ii) how reversible chemical reactions can be performed via charging molecules and (iii) the insights gained via resolving the atomic structure of individual molecules in different charge states.

O 101.5 Thu 12:30 TRE Ma

Discovery of chiral topological semimetals with multifold fermions and maximal Chern numbers — •Niels Schröter — Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland

Chiral topological semimetals (which possess neither mirror nor inversion symmetries) are expected host numerous novel phenomena, such as multifold fermions with large topological charge, long Fermi-arc surface states, unusual magnetotransport and lattice dynamics, and a quantized response to circularly polarized light - the first quantized response in metals. Until recently, all experimentally confirmed topological semimetals crystallized in space groups that contain mirror operations, which means that the aforementioned phenomena cannot appear.

Here I will present the first experimental evidence that AlPt and PdGa are chiral topological semimetals. Using angle-resolved photoelectron spectroscopy and ab-initio calculations, we show that these compounds host multifold fermions that carry the maximal Chern number that can be realized for linear band crossings in any material, which imposes an upper limit to the magnitude of many topological phenomena. Furthermore, by comparing two enantiomers (crystals with mirrored structure that do not coincide), we observe a reversal of their Fermi-arc velocities, which demonstrates that the handedness of chiral crystals can be used as a tuning parameter to manipulate the sign of their Chern numbers. I will furthermore demonstrate how time-reversal symmetry breaking can create novel topological multifold fermions that are elusive in non-magnetic compounds.

O 102: Heterogeneous Catalysis on Metals

Time: Thursday 10:30–13:30 Location: TRE Phy

Invited Talk O 102.1 Thu 10:30 TRE Phy

Video STM of particle diffusion on crowded surfaces — •Joost Wintterlin — Dept. of Chemistry, University of Munich, Germany

Fast surface diffusion of adsorbed particles is important for catalytic reactions as it randomizes the adsorption layer and determines transport to active sites. However, under reaction conditions a catalyst can be highly covered by particles. One expects that surface diffusion is then no longer a simple hopping of separate particles but that interactions and correlations in the "crowded layer" play a role. Such effects have been investigated by means of variable-temperature high-speed STM. Movies consisting of several 1000 frames were recorded over extended temperature ranges, providing the amount of data necessary for a statistical analysis. The experiments were performed with coadsorbed oxygen atoms and CO molecules on a Ru(0001) surface, which can be seen as a catalytic model system. Individual O atoms surprisingly moved through an ordered layer of CO molecules almost as fast as on the bare surface. It was shown that this high mobility can be understood by a new surface diffusion mechanism in which fast density fluctuations in the CO layer drive the diffusion of the oxygen atoms. Because combinations of similar types of adsorbates are present in many catalytic reactions the mechanism may play a general role.

O 102.2 Thu 11:00 TRE Phy

Diffusion of oxygen atoms on a highly CO-covered Ru(0001) surface — •Hannah Illner, Ann-Kathrin Henss, and Joost

Wintterlin — Chemie Department, Ludwig-Maximilians-Universität München, Deutschland

It was recently shown that oxygen atoms on a Ru(0001) surface covered with 0.33 monolayers (ML) of coadsorbed CO could travel through the CO layer by means of a new diffusion mechanism (Henß et al., Science 2019). The term "door-opening mechanism" indicated that the diffusion of the O atoms was facilitated by fluctuations in the CO layer that frequently opened low-energy paths for the oxygen. Here we report about investigations at higher CO coverages (0.50 ML). The experiments were performed between 239 and 280 K by means of a variable-temperature, high-speed STM that achieves imaging rates of up to 60 frames per second. In the investigated temperature range an ordered $(2\sqrt{3}$ x $2\sqrt{3})$R30° CO structure, which was observed at 70 K, had undergone on order-disorder transition. The trajectories of the O atoms through the disordered CO layer were analyzed, and hopping frequencies and an activation energy were extracted. It turned out that the surface diffusion of the O atoms was even faster than at the lower CO coverage and also faster than on the bare surface. We explain this finding by the weakened binding strength of the O atoms to the surface caused by CO.

O 102.3 Thu 11:15 TRE Phy

Active site representation in first-principles microkinetic models: Data-enhanced computational screening for improved methanation catalysts — •Martin Deimel, Mie Andersen, and Karsten Reuter — Chair for Theoretical Chemistry and Catalysis Research Center, Technical University of Munich, Germany

Reductionist first-principles microkinetic models have largely contributed to our trend understanding and computational screening of transition metal (TM) and TM alloy catalysts. As a key enabling step, these models draw much of their computational efficiency from scaling relations that reduce the required first-principles input to only a few adsorption energies of key reaction intermediates. Not withstanding, as these relations need to be established separately for every surface site considered, the predictive power of existing such models might be jeopardized by an overly simplistic representation of the active catalyst surface. Here we employ a recently established compressed-sensing approach [1] that (once trained) provides the required adsorption energies of ALL involved reaction intermediates at ALL high-symmetry sites from a single density-functional theory calculation of the clean TM or binary TM alloy surface. This enables refined microkinetic models considering multiple active sites. We revisit existing work investigating methanation catalysts on the basis of a less detailed microkinetic model [2] and show that the explicit consideration of hitherto neglected step and terrace sites indeed yields new mechanistic insights and highly active materials. [1] M. Andersen *et al.*, ACS Catal. **9**, 2752 (2019); [2] A. C. Lausche *et al.*, J. Catal. **307**, 275 (2013).

O 102.4 Thu 11:30 TRE Phy

Fluctuating nature of adsorbate layers on metal surfaces — •Sung Sakong and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

The dynamics of adlayers on surfaces is a fundamental feature influencing heterogeneous catalysis and electrocatalysis, because they determine whether adsorbed reaction partners can meet on a catalyst surface. Recently, video scanning tunneling microscopy (V-STM) experiments have addressed the O adatom dynamics in CO adlayers on a Ru(0001) surface [1] and of CO molecules on a Pt(111) electrode [2]. In spite of advances in the scan rate, the experiments are not capable of imaging all microscopic details of the adlayer dynamics due to the limited time resolution. Here, quantum chemistry can play a decisive role in elucidating the adlayer dynamics on the atomic level. We will discuss the fluctuating nature of CO adlayers on Ru(0001) and Pt(111) based on first-principles calculations and kinetic Monte Carlo simulations and demonstrate how fluctuations through a so-called door-opening mechanism can facilitate adatom diffusion on a crowded surface.

[1] A.-K. Henß, S. Sakong, P. K. Messer, J. Wiechers, R. Schuster, D. C. Lamb, A. Groß, and J. Wintterlin, Science **363**, 715-718 (2019).

[2] J. Wei, R. Amirbeigiarab, Y.-X. Chen, S. Sakong, A. Groß, and O. Magnussen, submitted.

O 102.5 Thu 11:45 TRE Phy

Chemical bond formation showing a transition from physisorption to chemisorption — Ferdinand Huber[1], •Julian Berwanger[1], Svitlana Polesya[2], Sergiy Mankovsky[2], Hubert Ebert[2], and Franz J. Giessibl[1] — [1]University of Regensburg, 93040 Regensburg, Germany — [2]LMU Munich, 81377 Munich, Germany

Surface molecules can transition from physisorption through weak van der Waals forces to a strongly bound chemisorption state by overcoming an energy barrier [1,2]. We show that a carbon monoxide (CO) molecule adsorbed to the tip of an atomic force microscope (AFM) [3] enables a controlled observation of bond formation, including its potential transition from physisorption to chemisorption. During imaging of copper (Cu) and iron (Fe) adatoms on a Cu(111) surface, the CO was not chemically inert but transited through a physisorbed local energy minimum into a chemisorbed global minimum, and an energy barrier was seen for the Fe adatom. Density functional theory reveals that the transition occurs through a hybridization of the electronic states of the CO molecule mainly with s-, p_z-, and d_z^2-type states of the Fe and Cu adatoms, leading to chemical bonding. The absence of hybridization 200 pm off-center the individual Fe and Cu adatoms results in the appearance as repulsive tori [4] in the AFM's image [5].

[1] A. Zangwill, Physics at Surfaces, Cambridge Univ. Press (1988)
[2] H. Ibach, Physics at Surfaces and Interfaces, Springer (2006)
[3] L. Gross et al. Science **325**, 1110 (2009)
[4] M. Emmrich et al. Science **348**, 6232 (2015)
[5] F. Huber et al. Science **366**, 235 (2019)

O 102.6 Thu 12:00 TRE Phy

Combining Planar Laser-Induced Fluorescence with Stagnation Point Flows for Small Single-Crystal Model Catalysts: CO Oxidation on a Pd(100) — Jianfeng Zhou[1], •Sebastian Matera[2], Sebastian Pfaff[1], Sara Blomberg[1,3], Edvin Lundgren[1], and Johan Zetterberg[1] — [1]Lund University, SE-22100 Lund, Sweden — [2]Freie Universität Berlin, D-14195 Berlin, Germany — [3]Lawrence Berkeley National Laboratory, Berkeley, CA 94720-8229, USA

Mass transfer limitations can have a tremendous impact on catalysts characterization and must be accounted for by an appropriate modelling and, if possible, reactor design. We present a stagnation flow reactor for reaction product imaging by planar laser-induced fluorescence (PLIF), which amenable to efficient low order modelling. Using CO oxidation over a Pd(100) single crystal as a showcase, we discuss the peculiarities for the case of small single-crystal model catalysts. While the ideal stagnation flow equations are not valid in this limit, a slightly modified theory can be derived, which exploits the information encoded in the PLIF signal. This combination of PLIF and half-theory/half-data driven modelling allows to efficiently analyse the experimental and to estimate the turnover frequency and the CO_2, CO and O_2 concentrations at the surface from solely the CO_2 profile at some distance of the surface.

O 102.7 Thu 12:15 TRE Phy

Ligand-Induced Heterogeneous Catalysis: Selective Hydrogenation of Acrolein on Ligand-Modified Pd(111) — •Carsten Schröder, Marvin C. Schmidt, and Swetlana Schauermann — Physikalische Chemie, CAU Kiel, Max-Eyth-Str. 2, 24118 Kiel

A major challenge in heterogeneous catalysis is obtaining control over selectivity in multi-pathway transformations of hydrocarbons. Recently, a new approach was introduced, which is based on employing catalytic surfaces functionalized with organic ligands. The intermolecular interactions between the reactants and the co-adsorbed ligand species were shown to be capable of promoting the desired reaction pathway. In our recent studies, on acrolein hydrogenation over Pd, almost 100% selectivity in the formation of the target product unsaturated alcohol propenol was detected, which arises from the presence of the oxopropyl-ligand species formed at the initial stages of reaction. In this contribution, we present a mechanistic study on hydrogenation of acrolein over ligand-modified Pd(111) surface. We employ a combination of infrared reflection adsorption spectroscopy and scanning tunneling microscopy along with the molecular beam techniques to obtain detailed information on the mechanisms and kinetics of acrolein partial hydrogenation to propenol. First experiments show, that the induction period of the formation of propenol, which is typically observed for acrolein hydrogenation, can be significantly reduced by precovering the surface with 2-methyl-2-pentenal as a ligand. Spectroscopic observations suggest fast formation of the desired reaction intermediate - propenoxy-species - on the ligand-modified surface.

O 102.8 Thu 12:30 TRE Phy

Exploring electrochemical CO_2 reduction towards C_2+-

products beyond copper — •Georg Kastlunger, Hendrik H. Heenen, and Karen Chan — Department of Physics, Technical University of Denmark

Electrochemical reduction of CO_2 and CO into high value chemical fuels would represent an ideal candidate for sustainable energy storage and conversion. Its application is, however, limited by the availability of efficient and selective catalysts for the production of longer chain hydrocarbons. To this day, no viable catalyst other than copper based materials lead to reasonable faradaic efficiencies.

In this contribution we present a density functional theory based study which focusses on understanding the general requirements for a catalyst to be viable for the electrochemical production of C_{2+} products. A larger scale theoretical study of this reaction cascade has historically been limited by the correct description of the crucial C-C coupling step and its potential dependence. Explicitly taking into account this key ingredient, we conducted a volcano type analysis exploring which interplay of the potential dependent binding energy of relevant intermediates opens up the path towards the desired products. Based on the discovered design principles, an alloy screening study going beyond copper will be presented, extending the palette of potential materials for the conversion of CO_2 into higher value hydrocarbons.

O 102.9 Thu 12:45 TRE Phy

Atomistic simulation of the surface reactions: O2, H2O and CO adsorption and dissociation on Zr- and B-terminated ZrB2(0001) surfaces — •Yanhui Zhang and Stefano Sanvito — CRANN, Trinity College Dublin, Dublin, Ireland

ZrB2 as a prototypical ultra-high temperature ceramic (UHTC) in combustion environment of aerospace applications are exposed to chemically aggressive gases like O, CO and H2O etc.. A detailed picture of the different channels of surface reactions involved are important for the development of ablation-resistant hot sections of the next generation aircraft. In this work, we have systematically studied the adsorption and dissociation of O2, CO and H2O on multiple active sites of ZrB2 (0001) surfaces by atomistic simulations based on density functional theory. The adsorption strength of O2 is the highest, followed by CO, and lastly H2O. Meanwhile, the hollow and bridge sites are largely preferred. The dissociative adsorption of O2 without activation barriers prevail in case of lateral approaching. Interestingly, the surface reconstruction of B-terminated (0001) surface is also observed to mediate surface reaction processes. Additionally, the surface reaction phase diagrams have been built up by searching the reaction barriers by climbing-image NEB method. Our results indicate the activation energy barriers of CO are the highest, while those of O2 are the lowest. This work provides insights into the initial processes of surface reactions at atomistic scale, and highlights the importance of surface treatment to the final performance of UHTC materials.

O 102.10 Thu 13:00 TRE Phy

Characterisation of Disordered Porous Solids: Perspectives from the Serially Connected Pore Model — •Henry R. N. B. Enninful[1], Richard Kohns[1,2], Dirk Enke[1], and Rustem Valiullin[1] — [1]Universität Leipzig, Leipzig, Germany — [2]Philipps Universität Marburg, Marburg, Germany

Elaborate determination of the pore structure of mesoporous solids offers important guidance towards optimal design of various applications such as catalysis, molecular separations and adsorption, among others. Routinely used characterisation tools, such as gas sorption, typically utilise the general adsorption isotherm (GAI) equation derived for ordered pore systems. The complex morphology of disordered porous solids, with its resulting cooperativity effects in thermodynamic phase transitions, renders characterisation more complex than what the GAI provides.

In this talk, we present a recently developed serially connected pore model (SCPM), which extends the GAI by incorporating cooperativity effects in phase transitions arising from pore complexity. Modelled as statistically disordered linear chain of pores, the SCPM will be validated with data from phase transitions in a synthesized porous silica material of similar pore construct, MCM-41. As an analogue to gas sorption (adsorption/desorption) studies, solid-liquid phase transitions (freezing/melting) of water in porous materials will be employed to correlate with the theoretical model.

References [1] Scientific Reports, 7, 7216, 2017. [2] Journal of Physical Chemistry C, 123, 16239, 2019.

O 102.11 Thu 13:15 TRE Phy

Adsorption Geometry of 2-Iodotriphenylene on Ag(111) and Cu(111) — •Alexander Ihle[1], Sebastian Ahles[2], Tobias Schlöder[3], Doreen Mollenhauer[3], Hermann A. Wegner[2], Andre Schirmeisen[1], and Daniel Ebeling[1] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Germany — [2]Institute of Organic Chemistry, Justus Liebig University Giessen, Germany — [3]Institute of Physical Chemistry, Justus Liebig University Giessen, Germany

On-surface chemistry is a powerful tool for building covalent molecular structures. In particular, the catalytic properties of the metal substrate as well as the 2D confinement facilitate the synthesis of new structures that are not accessible via solution chemistry. In order to control the bottom up formation process precise knowledge about the adsorption geometry of the molecular precursors is needed since this will help to understand the reaction mechanisms in detail. Here we studied the adsorption geometry of 2-iodotriphenylene on Ag(111) and Cu(111). By using low temperature atomic force microscopy with CO-functionalized tips we are able to identify the precise adsorption position of the molecules and their orientation with respect to the substrate lattice. On both substrates we find one preferred and one less preferred adsorption configuration, which are directed by metal atoms in the surface and the sub-surface layer. Due to different molecule-substrate interactions these adsorption configurations differ significantly from each other for the two substrate materials. Hence, the adsorption position can be actively controlled by the choice of substrate material.

O 103: Topology and Symmetry Protected Materials I

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

O 103.1 Thu 10:30 WIL A317

Zero Energy Bound States in the Proximity Induced Topological Superconductor System Bi2Te3 on Nb(110) — •Felix Kuester[1], Yunyi Zhang[1], Matthew Gilbert[2], Paolo Sessi[1], and Stuart Parkin[1] — [1]Max-Planck-Institute for Microstructure Physics, Halle (Saale), Germany — [2]University of Illinois, Urbana-Champaign, USA

Majorana bound states can be hosted by states on the surface of a strong topological insulator coupled to an ordinary s-wave superconductor and localized inside Abrikosov vortices (Fu and Kane 2008). This prediction provided the ingredients needed to find topologically protected, robust quantum states suited to form Qbits and motivated experimental research to investigate such structures thoroughly. We observed, by measuring differential conductance spectra and maps, zero-energy bound states inside vortices on 5 QL Bi2Te3 grown by MBE on Nb(110) to create a proximity induced topological superconductor system. Bi2Te3 is a strong topological insulator with a single Dirac cone at the gamma point which was confirmed by ARPES data on our sample. A comparison shows that neither the bare Nb(110) nor a proximity induced Pt film on the Nb(110) substrate exhibit a zero-energy peak in the vortex core or other anomalous features observed on the Bi2Te3 film. Therefore we suggest that the observed phenomena of unconventional superconductivity originate from the topological character of the Bi2Te3 surface.

O 103.2 Thu 10:45 WIL A317

Electronic and magnetic structure of the intrinsic magnetic topological insulator system $(\mathbf{Bi_2Te_3})_n(\mathbf{MnBi_2Te_4})$ ($n = 0, 1$) — •Thiago R. F. Peixoto[1,5], Raphael C. Vidal[1,5], Alexander Zeugner[2,5], Simon Moser[3,5], Michael Ruck[2,5], Bernd Büchner[4,5], Anna Isaeva[4,5], Hendrik Bentmann[1,5], and Friedrich Reinert[1,5] — [1]Exp. Phys. VII, Universität Würzburg — [2]Faculty of Chemistry and Food Chemistry, TU Dresden — [3]Exp. Phys. IV, Universität Würzburg — [4]Leibniz IFW Dresden and Faculty of Physics, TU Dresden — [5]Würzburg-Dresden Cluster of Excellence *ct.qmat*

Recently, $MnBi_2Te_4$ has been established as the first antiferromagnetic

(AFM) topological insulator [1,2], and represents the $n = 0$ member of the layered series $(Bi_2Te_3)_n(MnBi_2Te_4)$. For $n = 1$, we confirm a non-stoichiometric composition proximate to $MnBi_4Te_7$, and featuring an AFM state below 13 K, followed by a state with net out-of-plane magnetization below 5 K [3]. Here we present the spectroscopic signatures of these magnetic topological phases by means of angle-resolved photoemission (ARPES) and X-ray magnetic linear and circular dichroism (XMLD/XMCD) experiments on $MnBi_2Te_4$ and $MnBi_4Te_7$ single crystals. Both compounds reveal topologically non-trivial Dirac surface states on the (0001) surface, providing a versatile platform for the realization of magnetic topological states of matter.

[1] M. M. Otrokov *et al.*, ArXiv:1809.07389 (2019).
[2] R. C. Vidal *et al.*, Phys. Rev. B **100**, 121104(R) (2019).
[3] R. C. Vidal *et al.*, ArXiv:1906.08394 (2019).

O 103.3 Thu 11:00 WIL A317

Room temperature in-situ measurement of the spin voltage of a $BiSbTe_3$ thin film — •Arthur Leis[1,2,3], Michael Schleenvoigt[2,4], Abdur Rehman Jalil[2,4], Vasily Cherepanov[1,2], Gregor Mussler[2,4], Detlev Grützmacher[2,4], F. Stefan Tautz[1,2,3], and Bert Voigtländer[1,2,3] — [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]Experimentalphysik IV A, RWTH Aachen University, 52074 Aachen, Germany — [4]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

One of the hallmarks of topological insulators (TIs), the intrinsic spin polarisation in the topologically protected surface states, is investigated at room temperature in-situ by means of four-probe scanning tunnelling microscopy (STM) for a $BiSbTe_3$ thin film. To achieve the required precision of tip positions for measuring a spin signal, a precise positioning method employing STM scans of the local topography with each individual tip is demonstrated. From the transport measurements, the spin polarisation in the topological surface states (TSS) is estimated as p $\sim$ 0.3 - 0.6, which is close to the theoretical limit.

O 103.4 Thu 11:15 WIL A317

Mid-infrared-pump terahertz-probe spectroscopy on the topological insulator $(Bi_{1-x}Sb_x)_2Te_3$ — •Chris Reinhoffer[1], Andrea Bliesener[1], Gertjan Lippertz[1], Semyon Germanskiy[1], Yu Mukai[1,2], Yoichi Ando[1], Zhe Wang[1], and Paul H.M. van Loosdrecht[1] — [1]Institute of Physics II, University of Cologne, Cologne, Germany — [2]Department of Electronic Science and Engineering, Kyoto University, Kyoto, Japan

$(Bi_{1-x}Sb_x)_2Te_3$ is a series of topological insulators with the electronic properties tunable by varying the ratio between Bi and Sb. To get a better understanding of the inter-band scattering processes we performed mid-infrared-pump terahertz-probe spectroscopic measurements on three different $(Bi_{1-x}Sb_x)_2Te_3$ compounds, in which the Fermi energy was chemically tuned by varying x to be in the conduction-, valence-band, and bulk bandgap, respectively. The non-equilibrium response was studied systematically for pump energies above and below the bandgap of 200 meV and as a function of temperature down to 5 K. Our measurements show evident differences in the pump-probe response in the different compounds, which are compared with different theoretical scenarios.

O 103.5 Thu 11:30 WIL A317

Photoelectron spectroscopy on the transition metal doped topological insulator V:$(Bi,Sb)_2Te_3$. — •Philipp Kagerer[1], Thiago R. F. Peixoto[1], Raphael Crespo Vidal[1], Sonja Schatz[1], Martin Winnerlein[2], Steffen Schreyeck[2], Celso I. Fornari[1], Katharina Kissner[1], Charles Gould[2], Karl Brunner[2], Laurens W. Molenkamp[2], Hendrik Bentmann[1], and Friedrich Reinert[1] — [1]Experimental Physics VII, University of Würzburg — [2]Experimental Physics III, University of Würzburg

On the path towards combining topological surface states with ferromagnetism, transition-metal doped topological insulators have shown to be promising material systems. Here, we focus on V-doped $(Bi,Sb)_2Te_3$ thin films, which exhibit the quantum anomalous Hall effect (QAHE) at low temperatures and a ferromagnetic ground state with a comparably high T_c. Nevertheless, the electronic structure is still not comprehensively understood. We present a detailed study of the electronic structure of V:$(Bi,Sb)_2Te_3$ films based on angle-resolved photoemission spectroscopy (ARPES) in laboratory- and synchrotron-based experiments. Using systematic photon-energy dependent measurements, including resonant photoemission at the V L-edge, we study the electronic states close to the Fermi energy. Our results show that the topological surface state overlaps energetically with a dispersionless V impurity band. In our studies we will investigate the interplay between those states and search for possibilities of material engineering by tuning the position of the Fermi energy.

O 103.6 Thu 11:45 WIL A317

Core level and valence band dynamics of Bi_2Se_3 — •Michael Heber[1], Kevin Kühlmann[2], Dmytro Kutnyakhov[1], Federico Pressacco[3], Nils Wind[3], Davide Curcio[4], Klara Volckaert[4], Yves Acremann[2], Philip Hofmann[4], Kai Rossnagel[1,5], and Wilfried Wurth[1,3] — [1]DESY Photon Science, Hamburg, Germany — [2]Department of Physics, ETH Zürich, Switzerland — [3]Physics Department, University of Hamburg, Germany — [4]Aarhus University, Denmark — [5]IEAP, CAU Kiel, Germany

Bi_2Se_3 is one of the text book examples of a topological insulator. We investigated the ultrafast dynamics in the electronic structure of Bi_2Se_3 with time- and angle-resolved photoelectron spectroscopy. A time-of-flight-based momentum microscope in a pump-probe setup allows simultaneous detection of the three-dimensional band structure, with both parallel momentum components and binding energy, as well as the delay time in a single scan. Using the monochromatized XUV radiation delivered by the XUV beamline PG2 of FLASH provides the possibility to study the temporal response of the valence band simultaneous with the Se 3*d* and Bi 5*d* core levels. The relaxation dynamics of the core levels and the valence band will be presented with a focus on the excited electrons in the surface state above E_F.

O 103.7 Thu 12:00 WIL A317

Electronic structure of antimonene layers on Bi2Se3: insight from ab-initio calculations — •Kris Holtgrewe[1,2], Conor Hogan[3], and Simone Sanna[1,2] — [1]Justus Liebig University, Giessen, Germany — [2]Center for Materials Research, Giessen, Germany — [3]CNR-ISM, Rome, Italy

Topological insulators exhibit unconventional physical effects that have attracted the interest of the scientific community, especially when coupled to trivial insulators. A topologically insulating Bi_2Se_3 substrate covered by the trivial insulator antimonene is an ideal testbed to study the interfacial phenomena [1], and is furthermore interesting for applications such as topological pn-junctions [2].

Much research effort has been dedicated to the preparation of antimony layers on Bi_2Se_3 surfaces [3] and recently, the phase transition between two phases of the system has successfully been explained by *ab-initio* thermodynamics [4]. However, the Sb-coverage dependent spin texture is still not fully understood. Our work concentrates on the theoretical investigation of the relationships between structural motifs, band structures and STM patterns. Thereby, we show how an approach beyond local density functional theory, including both spin-orbit coupling and dispersion, is crucial for the correct modelling of the system.

[1] Jin et al, Phys Rev B **93**, 075308 (2016)
[2] Kim et al, ACS Nano **11**, 9671 (2017)
[3] Flammini et al, Nanotechnology **29**, 065704 (2018)
[4] Hogan et al, ACS Nano **13**, 10481 (2019)

O 103.8 Thu 12:15 WIL A317

Surface and bulk electronic structure of the 3D topological insulator HgTe(001) — •Raphael Crespo Vidal[1], Julia Issing[1], Lukas Lunczer[2], Giovanni Marini[3], Lena Fürst[2], Simon Moser[4], Giorgio Sangiovanni[5], Domenico Di Sante[5], Hartmut Buhmann[2], Gianni Profeta[3], Laurens W. Molenkamp[2], Hendrik Bentmann[1], and Friedrich Reinert[1] — [1]Experimental Physics VII, University of Würzburg, Germany — [2]Experimental Physics III, University of Würzburg, Germany — [3]Department of Physical and Chemical Sciences & SPIN-CNR, University of L'Aquila, Italy — [4]Experimental Physics IV, University of Würzburg, Germany — [5]Theoretical Physics I, University of Würzburg, Germany

Since the discovery of topological insulators HgTe proved itself to be a versatile material system, exhibiting a variety of topologically non-trivial states depending on adjustable structural parameters. Despite its persistent relevance in the field of topological materials a comprehensive understanding of its electronic band structure is still lacking. Here we will present an extensive angle-resolved photoemission (ARPES) study of epitaxially grown HgTe on CdTe(001). The lattice mismatch induces a strain of 0.3% which drives the system in its 3D

TI phase. The surface preparation for ARPES was done by cleavage of a Te capping layer as well as *in situ* transfer. Structural and chemical characterisation by LEED and core-level spectroscopy ensure a pristine surface quality. We find good agreement of our ARPES data with *ab initio* DFT calculations regarding band positions and dispersions as well as the orbital symmetry of the bands.

O 103.9 Thu 12:30 WIL A317

Unveiling the complex band structure of the potential non-symmorphic topological insulator TaNiTe$_2$ — •Tim Figgemeier[1], Jennifer Neu[2], Simon Moser[3], Johannes Hessdörfer[1], David J. Singh[4], Theo M. Siegrist[2,5], Hendrik Bentmann[1], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universität Würzburg — [2]National High Magnetic Field Laboratory, Tallahassee, Florida — [3]Experimentelle Physik IV, Universität Würzburg — [4]University of Missouri, Columbia, Missouri — [5]College of Engineering, FAMU-FSU, Tallahassee, Florida

NbNiTe$_2$ and TaNiTe$_2$ are layered van-der-Waals systems. While NbNiTe$_2$ was discussed as a Weyl-semimetal candidate lately [1,2], TaNiTe$_2$ (space group #53, *Pmna*) is predicted to be a topological insulator with non-symmorphic crystal structure, characterized by a topological inavriant of $Z_4 = 1$, that have rarely been studied experimentally up to now [3]. In this study we investigated the electronic structure of TaNiTe$_2$ by means of angle-resolved photoemission (ARPES) experiments and first-principle calculations. Systematic photon-energy- and polarization-dependent measurements allow us to disentangle the highly complex band structure. More than that, we discuss indications for the presence of a topological surface state.

[1] Wang et al., PRB 95, 165114 (2017)
[2] Neu et al., PRB 100, 144102 (2019)
[3] Vergniory et al, Nature 544, 480-450 (2019)

O 103.10 Thu 12:45 WIL A317

Drumhead surface state in ZrSiTe probed by scanning tunneling microscopy — •Brandon Stuart[1], Seokhwan Choi[1], Jisun Kim[1], Mohamed Oudah[1], Raquel Queiroz[2], Lukas Muechler[3], Leslie Schoop[4], Douglas Bonn[1], and Sarah Burke[1] — [1]Stewart Blusson Quantum Matter Institute, University of British Columbia,Vancouver, British Columbia, Canada V6T 1Z4 — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel — [3]Center for Computational Quantum Physics, The Flatiron Institute, New York, New York, 10010, USA — [4]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA

The family of materials ZrSiX (X = S, Se, Te) are topological nodal-line semimetals characterized by linear band crossings in 1-dimensional lines or loops in momentum space, rather than discrete points as in Dirac or Weyl semimetals. ZrSiTe is host to four nodal lines, two of which form loops in the BZ, one encircling the gamma point and the other encircling the Z point, and the other two forming lines that extend through the BZ. It was theoretically predicted that in the surface projection of ZrSiTe, the area between the nodal loops would contain a drumhead state, a topologically protected 2-dimensional surface state that links the nodal loops together [1]. Here, we show the first observed signature of electronic scattering within the drumhead state using low-temperature STM and QPI measurements.

[1] Muechler et al., arXiv:1909.02154

O 103.11 Thu 13:00 WIL A317

Fully radial spin texture in the chiral crystal of Te — Gianmarco Gatti[1], Daniel Gosálbez-Martinez[1], Michele Puppin[1], Serhii Polishchuk[1], Philippe Bugnon[1], Ivana Vobornik[2], Oleg Yazyev[1], Marco Grioni[1], and •Alberto Crepaldi[1] — [1]École polytechnique fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — [2]C.N.R. - I.O.M., Strada Statale 14, km 163.5, Trieste 34149, Italy

Chiral crystals are the new frontier in the field of topological materials. The absence of mirror-symmetry protects special fermions that have no counterparts in high-energy Physics [1], such as the Kramers-Weyl fermions [2]. These special nodes manifest unique magneto-electrical and optical properties, as consequence of their unique fully radial spin texture.

Trigonal tellurium (Te) is among the simplest realization of a gyrotropic chiral crystal, and our high-resolution ARPES data, supported by ab initio calculations, reveal the existence of multiple Kramers-Weyl points [3]. By using spin-resolved ARPES, we have resolved the monopole-like spin texture of the Fermi surface, whose experimental determination represent a fundamental piece to clarify the complex puzzle of the magneto-transport properties of Te [4]. Our results indicate that this material might constitute a major breakthrough in the field of topological materials.

References: [1] B. Bradlyn et al., Science 353, aaf5037 (2016). [2] G. Chang et al., Nat. Materials 17, 978 (2018). [3] G. Gatti in preparation. [4] S. S. Tsirkin et al., Phys. Rev. B 97, 035158 (2018).

O 104: Ultrafast Electron Dynamics III (joint session O/MA)

Time: Thursday 10:30–12:45 Location: WIL B321

O 104.1 Thu 10:30 WIL B321

THz-induced oscillations of the band structures in the topological insulator Bi$_2$Te$_3$ — •Suguru Ito[1], Johannes Reimann[1], Stefan Schlauderer[2], Christoph Schmid[2], Fabian Langer[2], Sebastian Baierl[2], Josef Freudenstein[2], Manuel Meierhofer[2], Konstantin Kokh[3], Oleg Tereshchenko[3], Akio Kimura[4], Christoph Lange[2], Jens Güdde[1], Rupert Huber[2], and Ulrich Höfer[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, Germany — [2]Fakultät für Physik, Universität Regensburg, Germany — [3]Novosibirsk State University, Russia — [4]Graduate School of Science, Hiroshima University, Japan

Time- and angle-resolved photoemission spectroscopy (time-resolved ARPES) is a powerful tool to map ultrafast dynamics occurring in electronic band structures. New opportunities arise in combination with THz excitation. As demonstrated recently for the topological surface bands of Bi$_2$Te$_3$, THz-ARPES is capable of mapping the dynamics of electrical currents in k-space with sub-cycle time resolution [1]. Here, we show that the THz light field also induces oscillations of the electronic bands on a time scale longer than the duration of the field transient. Frequency analysis implies the origin in atomic displacements but reveals the existence of oscillation modes that cannot be attributed to phonons in bulk Bi$_2$Te$_3$. Our results suggest another perspective of THz-ARPES, the capability to track band-structure engineering by light. We will discuss the experiment and compare with electronic structure calculations.

[1] J. Reimann *et al.* Nature **562**, 396 (2018).

O 104.2 Thu 10:45 WIL B321

Spin-, time- and angle-resolved photoemission spectroscopy on WTe2 — •Mauro Fanciulli[1,2], Jakub Schusser[1,3], Christine Richter[1,2], Cephise Cacho[4], David Bresteau[2], Thierry Ruchon[2], Jan Minár[3], and Karol Hricovini[1,2] — [1]LPMS, CY Cergy Paris Université, Cergy, FR — [2]LIDYL, CEA Saclay, Gif-sur-Yvette, FR — [3]NTC, University of West Bohemia, Pilsen, CZ — [4]Diamond Light Source, Didcot, UK

We combined a spin-resolved photoemission spectrometer with a high-harmonic generation (HHG) laser source in order to perform spin-, time- and angle-resolved photoemission spectroscopy (STARPES) experiments on the transition metal dichalcogenide bulk WTe2, a possible Weyl type-II semimetal. Measurements at different femtosecond pump-probe delays and comparison with spin-resolved one-step photoemission calculations provide insight into the spin polarization of electrons above the Fermi level in the region where Weyl points of WTe2 are expected. We observe a spin accumulation above the Weyl points region, that is consistent with a spin-selective bottleneck effect due to the presence of spin polarized cone-like electronic structure. Our results support the feasibility of STARPES with HHG, which despite being experimentally challenging provides a unique way to study spin dynamics in photoemission.

O 104.3 Thu 11:00 WIL B321

Mode-resolved reciprocal space mapping of electron-phonon interaction in the Weyl semimetal candidate *Td*-WTe$_2$ — •Petra Hein[1], Stephan Jauernik[1], Hermann Erk[1], Lexian

Yang[2], Yanpeng Qi[3], Yan Sun[4], Claudia Felser[4], and Michael Bauer[1] — [1]Institute of Experimental and Applied Physics, CAU Kiel, Germany — [2]State Key Laboratory of Low Dimensional Quantum Physics, Tsinghua University, China — [3]School of Physical Science and Technology, ShanghaiTech University, China — [4]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The selective excitation of coherent phonons provides unique capabilities to control fundamental properties of quantum materials on ultrafast time scales. For instance, in the presence of strong electron-phonon coupling, the electronic band structure can become substantially modulated. Recently, it was predicted that by this means even topologically protected states of matter can be manipulated: Pairs of Weyl points in Td-WTe$_2$ are expected to annihilate as an interlayer shear mode drives the material towards a centrosymmetric phase [1].

Here, time- and angle-resolved photoelectron spectroscopy is used to monitor the changes in the electronic structure of Td-WTe$_2$ upon absorption of 1.5 eV femtosecond laser pulses. We provide direct experimental evidence that the coherent excitation of the shear mode acts on the electronic states near the Weyl points. By comparison with higher-frequency coherent phonon modes, we finally prove the shear mode-selectivity of the observed changes in the electronic structure.

[1] E. J. Sie *et al.*, Nature **565**, 61-66 (2019).

O 104.4 Thu 11:15 WIL B321

Ultrafast Light-Induced Lifshitz Transition — •Samuel Beaulieu[1], Shuo Dong[1], Nicolas Tancogne-Dejean[2], Maciej Dendzik[1], Julian Maklar[1], Tomasso Pincelli[1], R. Patrick Xian[1], Martin Wolf[1], Angel Rubio[2,3], Michael A. Sentef[2], Laurenz Rettig[1], and Ralph Ernstorfer[1] — [1]Fritz-Haber- Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Max Planck Institute for the Structure and Dynamics, of Matter and Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010

Fermi surface is at the heart of our understanding of the properties of metals and strongly correlated many-body systems. An abrupt change in the Fermi surface topology, also called Lifshitz transition, can lead to the emergence of fascinating phenomena like colossal magnetoresistance and superconductivity. While Lifshitz transitions have been demonstrated for a broad range of materials and using different types of static external perturbations like strain, doping, pressure and temperature, a nonequilibrium route toward ultrafast and transient switching of the Fermi surface topology has not been demonstrated yet. Using time-resolved multidimensional photoemission spectroscopy combined with TDDFT+U simulations, we demonstrate a scheme based on ultrafast laser-driven band renormalization that drives a Lifshitz transition in the topological type-II Weyl semimetal $\mathrm{T_d-MoTe_2}$, due to transient modification of effective electron-electron interactions.

O 104.5 Thu 11:30 WIL B321

Time-resolved Momentum Microscopy of an Ultrafast Charge-Density-Wave-to-Metal Transition — •Julian Maklar[1], Shuo Dong[1], Samuel Beaulieu[1], Tommaso Pincelli[1], Maciej Dendzik[1], Philip Walmsley[2], Ian Fisher[2], Ralph Ernstorfer[1], Martin Wolf[1], and Laurenz Rettig[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland — [2]GLAM, Department of Applied Physics, Stanford, California, USA

Complex solids exhibit a multitude of competing and intertwined orders. A promising approach to disentangle relevant interactions and energy scales is by perturbation via ultrafast photoexcitation. However, this requires tracking of the electronic structure upon photoexcitation across a large energy and momentum range with femtosecond (fs) time-resolution in order to capture all relevant electronic processes.

Here, we investigate the evolution of the electronic band structure of the prototypical 2D charge-density-wave (CDW) compound TbTe$_3$ after photo-excitation. We utilize a new method, i.e. XUV time-resolved momentum microscopy, to simultaneously map a large energy- and momentum region with 40 fs temporal resolution. This allows us to identify collective excitations of the CDW as well as a strong coupling to a distinct phonon mode across multiple Brillouin zones.

O 104.6 Thu 11:45 WIL B321

Heavy fermion dynamics in semimetallic and insulating phases — •chul-hee min[1], michael heber[2], simon müller[3], lukas wenthaus[2], steffen palutke[2], dmytro kutnyakhov[2], federico pressacco[4], lenart dudy[5], mathieu silly[5], celso fornari[3], kiana baumgärtner[3], hendrik bentmann[3], woojae choi[6], yong seung kwon[6], markus scholz[7], friedrich reinert[3], wilfried wurth[2,4], and kai rossnagel[1,2] — [1]IEAP, CAU Kiel, Germany — [2]DESY, Hamburg, Germany — [3]EP7 and ct.qmat, University of Würzburg, Germany — [4]Department of Physics, University of Hamburg, Germany — [5]Synchrotron-SOLEIL, Saint-Aubin, France — [6]Department of Emerging Materials Science, DGIST, Republic of Korea — [7]European XFEL GmbH, Schenefeld, Germany

Due to time–energy correlation, heavy fermion systems with hard-to-detect meV energy scales are expected to show relatively slow dynamics on ps time scales, which are relatively easy to measure. Using the free-electron laser FLASH, we have performed time-resolved pump-probe photoemission spectroscopy of mixed valent TmSe$_{1-x}$Te$_x$. The system is composed of two magnetic $4f^{12}$ and $4f^{13}$ configurations in the ground state and can be tuned from semimetallic to insulating behavior via the Te concentration x without destroying the periodicity of the Tm ions. Here, we present and discuss the transient dynamics of the $4f$ states near E_F showing a remarkably strong dependence on x.

O 104.7 Thu 12:00 WIL B321

Polarisation effects in real space and real time in Xe-Cs solvatomers on Cu(111) — John Thomas[1], •Cord Bertram[1,2], Ping Zhou[1], Manuel Ligges[1], Karina Morgenstern[2], and Uwe Bovensiepen[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44780 Bochum, Germany

For understanding solvation under spatial constraints, morphology and ultrafast electron dynamics of solvent-solute complexes on surfaces are essential. In this contribution, we present the influence of the rare-gas, non-polar solvent xenon on the electronic structure of Cs/Cu(111) investigated by Scanning Tunneling Microscopy (STM) and Two-Photon-Photoelectron Spectroscopy (2PPE). After adsorption of xenon onto Cs precovered Cu(111), Cs agglomerates in xenon islands to a distance within the islands that is limited by Coulomb repulsion. The cesium antibonding resonance attributed to the Cs 6s orbital shifts up in energy with increasing Xe coverage and the lifetime of the antibonding resonance is increased from 15 fs to 81 fs. We interpret these results as an enhanced localization of the antibonding resonance and a decoupling of Cs from Cu(111), mediated by the polarization response of Xe in the close vicinity of Cs. Such effects will be discussed in the context of solvation and de-solvation of Cs-Xe complexes on Cu(111). We acknowledge that this contribution is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy - EXC 2033 - Projektnummer 390677874.

O 104.8 Thu 12:15 WIL B321

Investigation of coherent phonons at the interface of GaP/Si(001) heterostructures — •Steven Youngkin[1], Gerson Mette[1], Kunie Ishioka[2], Wolfgang Stolz[1], and Ulrich Höfer[1] — [1]Fachbereich Physik, Philipps Universität Marburg, Germany — [2]National Institute for Material Science, Tsukuba, Japan

Breaking of the bulk lattice atomic ordering by a surface leads to a plethora of novel and interesting physical phenomena such as new vibronic states, commonly known as surface phonon modes. However, very little is known about the vibronic states that arise at an interface of two solids.

Here, we use coherent phonon spectroscopy to study the interface vibronic system of GaP/Si(001) heterostructures, which represent a structurally well characterized model system of a polar/non-polar inorganic semiconductor interface. By measuring the transient reflectivity change of the probe beam at various pump photon energies, we can monitor the energy dependence of the coherent excitation of phonon modes with a resolution limited by the ultrashort laser pulses. Our studies reveal the existence of a low-frequency phonon mode with a frequency of 2 THz. This vibrational mode is absent in both bulk systems and is therefore assigned to originate from the buried interface between GaP and Si.

O 104.9 Thu 12:30 WIL B321

Three time-resolved photoelectron spectroscopies in one setup - time-of-flight momentum microscope at free electron laser. — •D. Kutnyakhov[1], R.P. Xian[2], M. Dendzik[2], M. Heber[1], F. Pressacco[3], S.Y. Agustsson[4], L. Wenthaus[1], H. Meyer[3], S. Gieschen[3], K. Bühlman[5], S. Däster[5], R. Gort[5], D. Curcio[6], K. Volckaert[6], M. Bianchi[6], Ch. Sanders[6], J.A. Miwa[6], S. Ulstrup[6], A. Oelsner[7], C. Tusche[8,9], Y.-

J. Chen[8,9], D. Vasilyev[4], K. Medjanik[4], G. Brenner[1], S. Dziarzhytski[1], S. Dong[2], J. Hauer[2], L. Rettig[2], J. Demsar[4], K. Rossnagel[1,10], H.-J. Elmers[4], Ph. Hofmann[6], R. Ernstorfer[2], G. Schönhense[4], Y. Acremann[5], and W. Wurth[1,3] — [1]DESY, Hamburg — [2]FHI Berlin — [3]CFEL, Univ. Hamburg — [4]Univ. Mainz — [5]ETH Zürich — [6]Univ. Aarhus — [7]Surface Concept GmbH, Mainz — [8]FZ Jülich GmbH — [9]Univ. Duisburg-Essen — [10]IEAP, CAU Kiel

Time-resolved photoemission with ultrafast pump and probe pulses is an emerging technique with wide application potential. Combining valence-band and core-level spectroscopy with photoelectron diffraction in a single efficient photoelectron-detection setup for electronic, chemical and structural analysis requires soft X-ray pulses (width few 10 fs) with some 10 meV spectral resolution. This is feasible at high repetition rate free-electron lasers using parallel imaging with segmented single-shot detectors with increased multi-hit capabilities. We have constructed and optimized a versatile setup commissioned at FLASH/PG2 that combines free-electron-laser capabilities with a multidimensional recording scheme for photoemission studies.

O 105: Scanning Probe Techniques II: Method Development (joint session O/CPP)

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

O 105.1 Thu 10:30 WIL C107

Identifying the atomic configuration of the tip apex using STM and FM-AFM with CO on Pt(111) — •Oliver Gretz, Alfred J. Weymouth, and Franz. J. Giessibl — Institute of Experimental and Applied Physics, Department of Physics, University of Regensburg, 93053 Regensburg

We investigated individual CO molecules adsorbed on Pt(111) with a metal tip using scanning tunneling microscopy (STM) and frequency-modulation atomic force microscopy (FM-AFM). When tips terminate in multiple atoms, the individual atoms are visible not only in the FM-AFM image but also in the raw STM image. This is in contrast to CO on Cu(111), where individual atoms cannot be identified in the raw STM image [J. Welker and F. J. Giessibl, Science 336, 444 (2012)]. We consider the mechanisms behind the higher spatial resolution on Pt, and rule out the increase stiffness of the adsorbed CO, concluding that CO bending does not strongly affect the STM image on either Cu or Pt.

O 105.2 Thu 10:45 WIL C107

Atomic Force Microscopy study of the complex surface unit cell of CaF_2(111) with a CO-terminated tip — •Alexander Liebig[1], Prokop Hapala[2], Alfred J. Weymouth[1], and Franz J. Giessibl[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Universitätsstraße 31, D-93053 Regensburg, Germany — [2]Department of Applied Physics, Aalto University, 00076 Aalto, Espoo, Finland

A chemically inert tip apex of an atomic force microscope (AFM), such as a carbon-monoxide (CO) molecule, allows to enter the repulsive interaction regime without destroying tip or sample. Imaging in a gentle repulsive regime has led to unprecedented spatial resolution of organic molecules [1] and opened the way for numerous results on different sample systems [2,3]. Here, we probe the ionic CaF_2 (111) surface with a CO-terminated tip over a range of distances, starting from a regime, where short-range electrostatics dominate the AFM contrast, down to distances, where Pauli repulsion and CO bending lead to a complete reversal of the atomic-scale contrast. By comparing the data to simulations, we demonstrate that a mechanical model using the overlap of electron densities [4] as well as the Lennard-Jones potential [5] is reproducing experimental AFM images even at tip-sample distances, where strong lateral forces cause strong lateral deflection of the CO molecule at the tip apex. [1] L. Gross et al., Science 325, 1110 (2009). [2] P. Jelínek, J. Phys.: Condens. Matter 29, 343002 (2017). [3] F. Huber et al., Science 366, 235 (2019). [4] M. Ellner et al., ACS Nano 13, 786 (2019). [5] P. Hapala et al., PRB 90, 085421 (2014).

O 105.3 Thu 11:00 WIL C107

Tip induced configuration change of a CO molecule on a copper surface — •Norio Okabayashi[1], Thomas Frederiksen[2,3], and Franz J. Giessibl[4] — [1]Kanazawa University — [2]Donostia International Physics Center — [3]Basque Foundation for Science — [4]University of Regensburg

Live coverage of a reaction process between the two atomic scale objects is one of the central goals in nanoscience. This can be achieved by combining atomic force microscopy to measure the potential energy between the tip apex and a molecule on a surface and inelastic electron tunneling spectroscopy (IETS) to measure the vibrational state of the molecule in the force field [1,2]. Here we demonstrate that the configuration change of a CO molecule in the force field produced by the tip can be traced with unprecedented quality by combining these two techniques and density functional theory (DFT). We found that when the tip is located laterally just above the CO molecule with upright configuration on a copper surface and approaches to the molecule, the CO molecule keeps the upright configuration from the attractive force regime to the beginning of the repulsive force regime; with further approaching the tip, the CO molecule suddenly changes its configuration from upright to tilted with the angle of 20 degree from the surface normal. This scenario is confirmed by IETS with adopting isotope 13C16O and 12C18O molecules. [1] N. Okabayashi, A. Peronio, M. Paulsson, T. Arai, and F. J. Giessibl, PNAS 115, 4571 (2018). [2] A. Peronio, N. Okabayashi, F. Griesbeck, and F. J. Giessibl, Rev. Sci. Instrum. (in press)

O 105.4 Thu 11:15 WIL C107

Nonequilibrium Bond Forces in Single-Molecule Junctions — Jonathan Brand[1], Susanne Leitherer[2], Nick R. Papior[3], •Nicolas Néel[1], Yong Lei[1], Mads Brandbyge[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [2]Center for Nanostructured Graphene, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark — [3]Department of Applied Mathematics and Computer Science, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Passing a current across two touching C_{60} molecules imposes a nonequilibrium population of bonding and antibonding molecular orbitals, which changes the equilibrium bond character and strength. A current-induced bond force therefore contributes to the total force at chemical-bond distances. First-principles calculations and scanning probe experiments exploring currents and forces in a wide C_{60}–C_{60} distance range consistently evidences the presence of current-induced attraction that occurs when the two molecules are on the verge of forming a chemical bond. The unique opportunity to arrange matter at the atomic scale with the atomic force and scanning tunneling microscope tip has enabled closely matching molecular junctions in theory and experiment. The findings consequently represent the first report of current-induced bond forces at the single-molecule level and further elucidate the intimate relation between charge transport and force.

O 105.5 Thu 11:30 WIL C107

Electrostatic Force Separation in Electrochemical Strain Microscopy — •Sebastian Badur[1], Diemo Renz[2], Thomas Göddenhenrich[1], Bernhard Roling[2], and André Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig University Gießen, Germany — [2]Philipps-University Marburg, Germany

In electrochemical strain microscopy an AC voltage is applied to a conductive SPM tip in contact to a mixed conductor. Detection of a few picometer of Vegard-strain allows characterization of electrochemical processes on the nanoscale. However, electrostatic contributions conceal the small displacements and thus are the major challenge to be overcome. Here, we present a novel compensation method, where the frequency dependence of Vegard-strain is utilized in a low and a high frequency regime in order to separate the electrostatic contribution and quantify electrochemical strain on mixed conducting $Cu_2Mo_6S_8$ under ultra high vacuum conditions.

O 105.6 Thu 11:45 WIL C107

Sensing with an ultra-sensitive cantilever — •Marc-Dominik Krass, Urs Grob, Raphael Pachlatko, Alexander Eichler, and Christian Degen — ETH Zürich, Solid State Physics, Switzerland

Magnetic resonance force microscopy (*MRFM*) is a scanning probe technique capable of detecting nuclear magnetic resonance (*NMR*) signals from nanoscale sample volumes. The sample is attached to the cantilever tip and is brought in close proximity to a sub-micrometer sized magnet which provides a magnetic field gradient. Periodic spin inversions synchronized with the cantilever frequency generate an oscillatory force at the tip apex.

The forces generated by nuclear spins in a nanometer-sized volume are on the order of 10 aN and detection requires very compliant cantilevers (spring constant below 10^{-4} N/m). Though mounted in pendulum geometry, strong interactions between the magnet and the cantilever lead to snap-in distances of tens of nanometers, resonance frequency shifts over one order of magnitude, and significant changes of the effective spring constant even for small scan ranges.

We present our latest setup improvements in order to obtain an artifact-free 3D magnetic resonance image on nanometer scale. This includes the correction of static cantilever deflections as well as the determination of the instantaneous dynamic spring constant, and real-time adjustments of feedback damping parameters.

O 105.7 Thu 12:00 WIL C107

Coupling broadband single-cycle THz pulses from a spintronic emitter to an STM junction — •Melanie Müller[1], Natalia Martín Sabanés[1,2], Sarojini Mahajan[1], and Martin Wolf[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]Freie Universität Berlin, Berlin, Germany

THz-gated Scanning Tunneling Microscopy (THz-STM) combines submolecular spatial with femtosecond temporal resolution, as first impressively demonstrated in 2016 [1]. Combined with plasmonic enhanced optical excitation THz-STM provides a powerful platform to study the atomically-resolved dynamics of photoexcited surfaces. We have developed an ultrahigh-vacuum STM for broadband excitation from the VIS through the THz spectral range. In particular, we employ an ultra-broadband (1-30 THz) spintronic THz emitter (STE) as source of single-cycle THz pulses to modulate the junction bias. To characterize the bandwidth, phase and voltage amplitude of the THz near-field, we sample the tip-enhanced THz waveform via THz-induced modulation of photocurrents [2]. Careful comparison to the far-field waveform allows us to investigate the antenna properties of the STM tip. Considering strong tip-induced low pass filtering, frequencies up to 10 THz can be detected in the near-field. We further demonstrate versatile phase and polarity control of the THz waveform via the STE excitation conditions, and show that THz transients with a half-cycle period of 115 fs and several Volts amplitude can be achieved in the current setup. References: [1] Cocker T., el at, Nature 539, 263-267 (2016); [2] Yoshida S., et al, ACS Phot. 6, 1356-1364 (2019)

O 105.8 Thu 12:15 WIL C107

Single Asperity Sliding Friction across the Superconducting Phase Transition — Wen Wang, •Dirk Dietzel, and Andre Schirmeisen — Instititute of Applied Physics, Justus Libieg Universtity Giessen, 35392 Giessen, Germany

In sliding friction, different energy dissipation channels have been proposed, including phonon and electron systems, plastic deformation, and crack formation. However, the details of how energy is coupled into these channels is heavily debated, and especially the relevance of the electron system for energy dissipation often remains elusive. Here, we present contact mode AFM friction experiments of a single asperity sliding on a high T_c BSCCO-superconductor in a wide temperature range from 40 K to 300 K. Overall, friction decreases with temperature as expected based on thermally activated friction models, but we find an unexpected large peak around T_c of 95 K. We model these results by a superposition of different energy dissipation channels, where the influence of electronic contributions vanishes when cool- ing below the superconducting phase transition T_c. Our experiments thereby unambiguously link electronic friction effects to the number of normal state electrons in the superconducting phase below T_c, allowing us to quantify the relative importance of the electron system to overall friction.

O 105.9 Thu 12:30 WIL C107

Non-contact heat transfer between metallic surfaces — •Paul Philip Schmidt and Carsten Henkel — Universität Potsdam, Institut für Physik und Astronomie

The heat transfer at distances beyond contact can be described by fluctuating electrodynamics developed by Rytov [1]. Recent experiments provide deviations from the theoretical predictions. In the measurements, a flat gold surface was approached by a gold-coated probe tip, the distance between the two being less than 10nm [2,3]. In this work we model the measured data in a phenomenological way. The basic assumption is that at a critical distance, the heat flow between flat surface elements saturates, proportional to the number of transport channels. When combined with the proximity force (Deryagin) approximation, this “snap-in model” is in good agreement with the experimental data [4].

[1] D.V.H.M. Polder and M. Van Hove, PRB **4** (1971) 3303.

[2] K. Kloppstech, N. Könne, S.-A. Biehs, A. W. Rodriguez, L. Worbes, D. Hellmann, and A. Kittel, Nature Commun. **8** (2017) 14457.

[3] L. Cui, W. Jeong, V. Fernández-Hurtado, J. Feist, F. J. García-Vidal, J. C. Cuevas, E. Meyhofer, and P. Reddy, Nature Commun. **8** (2017) 14479.

[4] C. Henkel and P. P. Schmidt, JOSA B **36** (2019) C10.

O 106: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions V (joint session O/HL/DS/CPP)

Time: Thursday 15:00–17:30 Location: GER 38

Invited Talk O 106.1 Thu 15:00 GER 38

Huge quantum effects on the 250 K superconducting lanthanum hydride — •Ion Errea — University of the Basque Country, Donostia/San Sebastián, Spain

The discovery of superconductivity at 200 K in the hydrogen sulfide system at large pressures was a clear demonstration that hydrogen-rich materials can be high-temperature superconductors. The recent synthesis of LaH10 with a superconducting critical temperature (Tc) of 250 K place these materials at the verge of reaching the long-dreamed room-temperature superconductivity. Here we show that quantum atomic fluctuations stabilize in the superconducting pressure range a high-symmetry Fm-3m crystal structure consistent with experiments, which has a colossal electron-phonon coupling of 3.5. Even if ab initio classical calculations predict this structure to distort below 230 GPa yielding a complex energy landscape, the inclusion of quantum effects evidences the Fm-3m as the true ground state. The agreement between the calculated and experimental Tc values further supports this phase as responsible for the 250 K superconductivity. The relevance of quantum fluctuations questions many of the crystal structure predictions made for hydrides within a classical approach that at the moment guide the experimental quest for room-temperature superconductivity. Furthermore, quantum effects are revealed to be crucial to stabilize solids with extraordinary electron-phonon coupling, which may otherwise be destabilized by the large electron-phonon interaction, reducing the pressures needed for their synthesis.

O 106.2 Thu 15:30 GER 38

Self-Interaction Corrected SCAN for Solids: All-Electron Implementation with Numeric Atom-Centered Basis Functions — •Sheng Bi[1], Igor Ying Zhang[2], Christian Carbogno[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Fudan University, Shanghai, China

For all semi-local density-functional approximations (DFAs), electronic self-interaction errors lead to an erroneous description of charge-transfer processes, a systematic underestimation of band gaps in semiconductors, and incorrect total energies [1]. These errors can be alleviated via localized-orbital scaling corrections [2] or via self-interaction corrections (SIC) [3]. In this work, we have implemented a reciprocal-space formulation of self-consistent SIC in the all-electron, numeric atomic-orbitals code *FHI-aims*, which is applicable for all semi-local DFAs, including the promising meta-GGA “strongly constrained and appropriately normed” (SCAN) functional [4]. We validate our implementation by inspecting charge transfer, cohesive energies, and band gaps for a test set of molecules and solids, showing that SIC considerably improves SCAN calculations and yields results on par with standard *GW* calculations at a fraction of the computational cost. This allows us to use SCAN-SIC for studying the adsorption of organic molecules on the H-Si(111) surface.

[1] A. J. Cohen *et al.*, *Chem. Rev.* **112**, 289 (2011).
[2] N. Q. Su *et al.*, *Proc. Natl. Acad. Sci.* **115**, 9678 (2018).
[3] Z. Yan *et al.*, *Phys. Rev. A* **95**, 052505 (2017).
[4] J. Sun *et al.*, *Phys. Rev. Lett.* **115**, 036402 (2015).

O 106.3 Thu 15:45 GER 38

Understanding the lattice dynamics of 3D hexagonal boron nitride (h-BN): beyond the LDA approach — •Luigi Cigarini, Michal Novotný, and František Karlický — Department of Physics, Faculty of Science, University of Ostrava, Czech Republic

It is fundamental to achieve a clear depiction of the lattice dynamics of 3D h-BN in order to understand the experimental outcomes. Five different stacking conformations are possible for 3D h-BN and at least two or three of them are systematically present in samples in variable amounts [1-2], resulting as a source of irreproducibility for experiments, such as the infrared optical response [3-4].

The lattice dynamics of h-BN is particularly tough to describe, stated the different nature of the forces participating in it: covalent bonds and Van der Waals interactions. The LDA approach seemed to be the most effective compromise, at the DFT level [1,5-6].

In this work we explain the surprisingly good performance of LDA. We also show that it is possible to achieve better results, in comparison with experimental IR spectra, by using, instead, the GGA approach to DFT and treating separately the two parts of the dynamical matrix. Besides, we found that IR spectroscopy is able to give some information about stacking composition. [1]. Liu, L. et al., Phys. Rev. B, 68(10), 104102 (2003). [2]. Constantinescu, G. et al., Phys. Rev. Lett., 111(3), 036104 (2013). [3]. Çamurlu, H.E. et al., Ceram. Int., 42(5), 6312-6318 (2016). [4]. Mukheem, A. et al., Nanomaterials, 9(4), 645 (2019). [5]. Cuscó, R. et al., Phys. Rev. B, 97(15), 155435 (2018). [6]. Serrano, J. et al., Phys. rev. lett., 98(9), 095503 (2007).

O 106.4 Thu 16:00 GER 38

Error Estimation of Energy-per-Atom of Semiconductor Compounds Using Statistical Learning — •Daniel T. Speckhard[1,2], Sven Lubeck[2], Christian Carbogno[1], Luca Ghiringhelli[1], Claudia Draxl[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

Material databases such as NOMAD give researchers the ability to work with millions of material simulation results [1]. However, it is typically unclear to which extent calculations performed with different numerical settings and computer codes can be trusted and related to each other. This project presents statistical learning strategies to model errors in energies for two all-electron DFT codes, *FHI-aims* and `exciting`, for different basis-set sizes and **k**-point densities. Specifically, we use mutual information scores to select features that are able to capture the energy-per-atom errors. With respect to several metrics, random forest regression on the selected features shows the most promising results. This work lays the foundation for estimating errors in DFT data in NOMAD and helps to save computing resources by *a priori* predicting the DFT simulation settings required to achieve a desired level of precision. This also enables us to estimate the basis-set and **k**-point converged results of not fully converged calculations.

[1] C. Draxl and M. Scheffler, *J. Phys. Mat.*, **2** 036001 (2019). https://nomad-coe.eu

O 106.5 Thu 16:15 GER 38

Force balance approach for advanced approximations in density functional theories — •Mary Leena Tchenkoue[1], Markus Penz[1], Iris Theophilou[1], Michael Ruggenthaler[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, New York NY 10010, USA

We propose a systematic and constructive way to determine the exchange-correlation potentials of density-functional theories including vector potentials. The approach does not rely on energy or action functionals. Instead it is based on equations of motion of current quantities (force balance equations) and is feasible both in the ground-state and the time-dependent setting. This avoids, besides differentiability and causality issues, the optimized-effective-potential procedure of orbital-dependent functionals. We provide straightforward exchange-type approximations for different density functional theories that for a homogeneous system and no external vector potential reduce to the exchange-only local-density and Slater Xα approximations.

O 106.6 Thu 16:30 GER 38

Combining embedded mean field theory with linear-scaling density functional theory — •Joseph Prentice[1,2], Robert Charlton[2], Arash Mostofi[2], and Peter Haynes[2] — [1]St Edmund Hall and Department of Materials, University of Oxford, Oxford, UK — [2]Department of Materials, Department of Physics and the Thomas Young Centre, Imperial College London, London, UK

We demonstrate the capability of embedded mean field theory (EMFT) within the linear-scaling density-functional theory code ONETEP, which enables DFT-in-DFT quantum embedding calculations on systems containing thousands of atoms at a fraction of the cost of a full calculation. We perform simulations on a wide range of systems from molecules to complex nanostructures to demonstrate the performance of our implementation with respect to accuracy and efficiency. This work paves the way for the application of this class of quantum embedding method to large-scale systems that are beyond the reach of existing implementations.

O 106.7 Thu 16:45 GER 38

Topological semimetallic phase in PbO$_2$ promoted by temperature — •Bo Peng[1], Ivona Bravić[1], Judith L. MacManus-Driscoll[2], and Bartomeu Monserrat[1] — [1]Cavendish Laboratory, University of Cambridge, United Kingdom — [2]Department of Materials Science and Metallurgy, University of Cambridge, United Kingdom

Materials exhibiting topological order host exotic phenomena that could form the basis for novel developments in areas ranging from low-power electronics to quantum computers. The past decade has witnessed multiple experimental realization and thousands of predictions of topological materials. However, it has been determined that increasing temperature destroys topological order, restricting many topological materials to very low temperatures and thus hampering practical applications. Here, we propose the first material realization of temperature promoted topological order. We show that a semiconducting oxide that has been widely used in lead-acid batteries, β-PbO$_2$, hosts a topological semimetallic phase driven by both thermal expansion and electron-phonon coupling upon increasing temperature. We identify the interplay between the quasi-two-dimensional nature of the charge distribution of the valence band with the three-dimensional nature of the charge distribution of the conduction band as the microscopic mechanism driving this unconventional temperature dependence. Thus, we propose a general principle to search for and design novel topological materials whose topological order is stabilized by increasing temperature. This provides a clear roadmap for taking topological materials from the laboratory to technological devices.

O 106.8 Thu 17:00 GER 38

How Electric Fields Affect Intermolecular van der Waals Interactions — •Mohammad Reza Karimpour, Dmitry Fedorov, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

van der Waals (vdW) dispersion interactions between atoms or molecules originate from electromagnetic forces caused by the zero-point quantum-mechanical fluctuations of electronic charge densities. They are ubiquitous in nature and present in many areas of physics, chemistry, biology, and nanotechnology. Recently, it has been shown that the strength of vdW interactions can be controlled and tailored by external electric charges [1]. In addition, an external field strongly modifies the dispersion interaction between two hydrogen atoms and can change both its spatial dependence and its attractive or repulsive character [2]. To describe such important phenomena in large molecular systems, we employ the Many-Body Dispersion (MBD) method [3] based on the quantum Drude oscillator model. Since the conventional MBD method includes only dipole-dipole coupling, it does not capture the effects of external fields on vdW interactions. Therefore, we first extend the approach to dipole-quadrupole and quadrupole-quadrupole couplings. Then, the developed formalism is applied to calculate the MBD energy in the presence of an external electric field for low-dimensional systems including bilayer graphene.

[1] Kleshchonok and Tkatchenko, Nat. Commun. **9**, 3017 (2018)
[2] Fiscelli *et al.* arXiv:1909.03517 (2019)
[3] Tkatchenko *et al.* Phys. Rev. Lett. **108**, 236402 (2012)

O 106.9 Thu 17:15 GER 38

Electronic structure of β-SiAlON: effect of Al/O doping and of finite temperature — •Saleem Ayaz Khan[1], Ondrej Sipr[2], Jiří Vackář[2], Robin Niklaus[3], Wolfgang Schnick[3], and Jan Minár[1] — [1]University of West Bohemia, Plzen, Czech Republic —

[2]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [3]LMU Munich, Germany

Electronic structure of a series of ordered and disordered β-Si_{6-z}Al_{z}O_{z}N_{8-z} systems is investigated by means of ab initio calculations, using the FLAPW method as implemented in the wien2k code and Green function KKR method as implemented in the SPR-KKR code. Finite temperature effects are included within the alloy analogy model. We found that the trends with the Al/O doping are similar for ordered and disordered structures. The electronic band gap decreases with increasing z by about 1 eV when going from z=0 to z=2. The optical gap decreases analogously as the electronic band gap. The changes in the density of states (DOS) at Si and N atoms introduced by doping β-Si_{3}N_{4} with Al and O are comparable to the DOS at Al and O atoms themselves. The bottom of the conduction band in β-Si_{6-z}Al_{z}O_{z}N_{8-z} is formed by extended states residing on all atomic types. Increasing the temperature leads to a shift of the bottom of the conduction band to lower energies. The amount of this shift increases with increasing doping z.

O 107: Semiconductor Surfaces (joint session O/HL)

Time: Thursday 15:00–17:30 Location: REC C 213

O 107.1 Thu 15:00 REC C 213

Time-resolved reflection anisotropy spectroscopy reveals the impact of surface non-idealities for water adsorption on GaP

— •Matthias M. May[1], Helena Stange[1], Jonas Weinrich[2], Thomas Hannappel[3], and Oliver Supplie[3,4] — [1]Helmholtz-Zentrum Berlin, Germany — [2]Ferdinand-Braun-Institut, Berlin, Germany — [3]Technische Universität Ilmenau, Germany — [4]Humboldt-Universität zu Berlin, Germany

The initial interaction of water with semiconductor surfaces typically leads to surface chemical reactions, which determine the electronic structure of the solid–liquid interface as well as stability against corrosion. Access to this interface to reveal the nature of the interaction is, however, challenging. Here, we study gallium phosphide-based (100) surfaces exposed to H_2O by means of time-resolved reflection anisotropy spectroscopy during water adsorption in vacuum [1]. We show that the introduction of imperfections in the form of surface steps via substrate off-cut variation or trace contaminants not only changes the dynamics of the interaction, but also its qualitative nature. While the clean surface without steps does not show any presence of oxygen after several 10 kL of exposure at room temperature, this changes with the introduction of trace carbon or a substrate off-cut. The decay rate of the surface optical anisotropy allows us to estimate activation energies of the surface reactions. Our findings emphasise the challenges for the comparability of experiments with idealised electronic structure models.

[1] May et al., *SciPost Physics* **6**, 058 (2019).

O 107.2 Thu 15:15 REC C 213

Ion-Induced Surface Nanostructures of Germanium(001)

— •Ricardo de Schultz, Denise Erb, and Stefan Facsko — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden, Germany

Ion beam irradiation can lead to various self-organized surface nanopatterns depending on the irradiation conditions and the sample material. In this case, the surface patterns of Ge(001), which evolve during high-fluence 1 keV ion irradiation with Ar^+ ions at elevated temperatures, have been studied. Whereas at room temperature the semiconductor surface would become amorphous during ion irradiation, high temperatures enhance the diffusion so that bulk vacancies and interstitials can recombine before the next ion hits the same surface region. Thus the surface stays crystalline. This results in a biased surface diffusion because of the Ehrlich-Schwoebel barrier at step edges and kinks.

The periodic surface patterns that emerge on Ge(001) reflect the four-fold symmetry of the crystalline surface. These patterns consist of a checkerboard of inward and outward oriented pyramids. For normal ion incidence their bases are square and oriented along the <100> crystal direction. For two different azimuthal ion incidence angles - along <110> and <100> - the emerging patterns have been examined for different polar incidence angles and compared to simulations. These indicate that the height gradient dependent sputter erosion plays an important role during pattern formation.

O 107.3 Thu 15:30 REC C 213

Structural and Electronic Properties of the FeSi(110) Surface

— •Biao Yang[1], Martin Uphoff[1], Yi-Qi Zhang[1], Joachim Reichert[1], Ari P. Seitsonen[2], Andreas Bauer[3], Christian Pfleiderer[3], and Johannes V. Barth[1] — [1]Physics Department E20, Technical University of Munich, D-85748 Garching, Germany — [2]Département de Chimie, École Normale Supréieure, 24 rue Lhomond, F-75005 Paris, France — [3]Physics Department E51, Technical University of Munich, D-85748 Garching, Germany

Iron silicide (FeSi) is a fascinating material which has attracted numerous research efforts for decades.[1] It has B20 crystal structure featuring cubic unit cell without an inversion center. To gain insight into the unusual surface properties of this system, we successfully prepare the atomically flat FeSi(110) surface with the Ar ion sputtering and annealing treatment. By scanning tunneling microscopy (STM), we clearly resolve a step-terrace topography and the details of the atomic lattice. The atomically resolved STM images and DFT calculations give strong indications for the surface termination, where the topmost comprises of one Fe and one Si atom. Furthermore, a small energy gap of 80 meV close to the Fermi level is derived by scanning tunneling spectroscopy (STS). Intriguingly, two in-gap states are identified for the first time. References 1. V. Jaccarino, G. K. Wertheim, J. H. Wernick, L. R. Walker, S. Arajs. Phys. Rev. 1967, 160, 476.

O 107.4 Thu 15:45 REC C 213

Detection of stress hormone cortisol in saliva using silicon nanowire field effect transistors with a portable measurement system

— •Stephanie Klinghammer[1], Nadia Licciardello[1], Tetiana Voitsekhivska[2], Clemens Kirschbaum[3], Larysa Baraban[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [3]3Department of Psychology, TU Dresden, 01062 Dresden Germany

The accurate and rapid detection of various targets from patients on portable point-of-care devices is attracting great attention in bio- and nanotechnology for more than a decade [1]. Here, we demonstrate a portable, label-free and real-time sensing platform based on silicon nanowire field effect transistors which is capable for detection of several small molecules [2]. We particularly focus on the sensitive recognition of the stress hormone cortisol by using aptamers as receptors in order to allow high sensitive screenings in physiological conditions. We show the working principle by determination of cortisol levels in saliva of volunteers and compared to levels obtained with conventional ELISA method.

References: [1] Patolsky F, Zheng G, Lieber CM. 2006. Nanomed. 1(1):51*65 [2] Voitsekhivska T, Suthau E, Wolter K-J. 2014. in IEEE. 173-178

Invited Talk O 107.5 Thu 16:00 REC C 213

Coupling of electronic and atomic degrees of freedom in surface-stabilized quasi-1D systems

— •Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn

Minute structural changes may lead to drastic modifications of the electronic properties of quasi-1D systems, while, on the other hand, an electronic charge redistribution, induced, e.g., by optical excitations or surface vibrations may induce pronounced structural modifications in such systems. This is illustrated in my talk using two prominent examples: (i) Localized photoholes at the Brillouin zone boundary of the In/Si(111)(8x2) nanowire system are shown to drive an ultrafast (8x2) $\longrightarrow$ (4x1) phase transitions that is accompanied by the formation of metallic In-In bonds along the wire direction [1,2]. (ii) A Si $sp^3 \longrightarrow sp^2+p$ rehybridization accompanied by a lateral surface charge transfer is demonstrated to destabilize the Si(553)-Au spin chains [3] with respect to a diamagnetic surface ground state that complies with electron counting heuristics [4]. Thermal excitation leads to soft Au chain vibrations that alter transiently the Au electron affinity and eventually the hybridization of the Si step edge atoms.

[1] T Frigge et al., Nature 544, 207 (2017).
[2] CW Nicholson et al., Science 362, 821 (2018).
[3] SC Erwin, FJ Himpsel, Nat. Commun. 1, 58 (2010).
[4] C Braun et al., PRB 98, 121402(R) (2018).

O 107.6 Thu 16:30 REC C 213

Determining surface phase diagrams including anharmonic effects — •Yuanyuan Zhou, Matthias Scheffler, and Luca M. Ghringhelli — Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin-Dahlem, Germany

A prerequisite for analyzing and understanding the electronic properties and the function of surfaces is the detailed knowledge of their structure under realistic conditions. We have developed a replica-exchange grand-canonical (REGC) algorithm that enables the unbiased calculation of pressure-temperature phase diagrams of surfaces or clusters in reactive atmospheres including anharmonic effects. [1] Moreover, the multi-canonical sampling yields the temperature-pressure dependence (map) of all equilibrium observables that can be measured within the given model Hamiltonian. For instance, structural parameters such as the radial distribution function, or the HOMO-LUMO gap. This allows for rational design, where *operando* condition are taking fully into account. Our approach is demonstrated by studying Si clusters and the Si(100) surface in a hydrogen atmosphere, by coupling REGC with *ab initio* molecular dynamics. All interactions are described at the density-functional-theory level, with the Perdew-Burke-Ernzerhof gradient-corrected exchange-correlation functional. In particular, we show how to determine *observable structures* at finite temperature and pressure, i.e., obtained by ensemble averaging the sampled structures. [1] Y. Zhou, M. Scheffler, and L. M. Ghringhelli, Phys. Rev. B. 100, 174106 (2019).

O 107.7 Thu 16:45 REC C 213

Doping-induced metal-insulator transition in Au atomic wires — •Zamin Mamiyev[1], Simone Sanna[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Appelstrasse 2 Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — [2]Institut für Theoretische Physik, Justus-Liebig- Universität Gießen

Close coupling between structural and electronic parameters has been demonstrated in the past for arrays of quasi one-dimensional Au chains on Si surfaces. Here we employ plasmon spectroscopy and LEED to study electronic and structural modifications as a result of surplus Au concentrations, x, starting at 0.48 ML on Si(553) and at 0.65 ML on Si(111). For the Si(111)-Au surface an abrupt metal-insulator transition (MIT) was observed by adding more than 0.05 ML Au. In contrast, the Si(553)-Au surface shows a rather gradual decrease of plasmon frequency up to x= 0.1 ML. Moreover, self-doping with Au on Si(553)-Au improves the chain quality up to x=0.03 ML, resulting also in an increase of plasmon intensity. Further addition of Au at room temperature leads to a vanishing plasmon frequency, coupled with the disappearance of the $\times 2$ periodicity. By annealing the doped samples at 630°C the Au atoms form small clusters with ($\sqrt{3}\times\sqrt{3}$)R30° symmetry, while the metallicity of the Au chains is fully recovered, but the structural imperfections in the chains as well. The appearance of $\sqrt{3}$-order indicates local restructuring into larger terraces and their spatial separation from the Au-chains. This proves that not only the amount of dopant but also its distribution is important for reversible MIT on such surfaces. These findings were corroborated by DFT calculations.

O 107.8 Thu 17:00 REC C 213

Selective Excitation of Amplitude Modes Driving the In/Si(111) Peierls Transition — •Hannes Böckmann-Clemens, Jan Gerrit Horstmann, and Claus Ropers — 4th Physical Institute, Solids and Nanostructures, University of Göttingen, Göttingen 37077,Germany

The use of laser pulses to actively steer a system along the transition pathway from a reactant towards a desired product state is a fundamental scheme in the field of femtochemistry. Transferring this concept to solid-state surface systems requires the ultrafast manipulation of coherent phonons, associated with the reaction coordinate. Here, we demonstrate the mode-selective vibrational control over the Peierls metal-to-insulator phase transition of In/Si(111) by means of tailored pulse sequences. We explore the potential energy surface spanned by the amplitude modes of the system via selection of specific pathways along the transition path. We identify two essential modes, identify their separate roles in controlling the transition, and carry out experiments with mode-selective excitation.

O 107.9 Thu 17:15 REC C 213

Novel electronic junctions in an atomic wire array: metallic states, charge density waves and solitonic excitations — •Abdus Samad Razzaq[1], Sun Kyu Song[2], Han Woong Yeom[2], and Stefan Wippermann[1] — [1]Max-Planck-Institut für Eisenforschung, Germany — [2]Pohang University, South Korea

The Si(111)-(4x1)In atomic wire array is an extremely popular model for one-dimensional (1D) electronic systems. It features a reversible, temperature-induced metal insulator transition into a charge density wave (CDW) ordered ground state with (8x2) translational symmetry. Close to the phase transition temperature, both phases can coexist and form novel types of electronic junctions between the metallic (4x1) phase and the insulating CDW-ordered (8x2) phase. Furthermore, the CDW phase is 4-fold degenerate, giving rise to solitonic excitations of the CDW, that take the form of phase boundaries between different CDW ground states. Combining scanning tunnelling microscopy (STM) and ab initio molecular dynamics (AIMD) calculations, we explore the microscopic structures of interfaces between distinct electronic phases at the atomic scale. These models enable insights into soliton propagation and soliton-mediated charge transport. Financial support from the German Research Foundation (DFG), grant no. FOR1700, and BMBF NanoMatFutur, grant no. 13N12972, is gratefully acknowledged.

O 108: Electron-Driven Processes at Surfaces and Interfaces

Time: Thursday 15:00–17:45 Location: TRE Ma

O 108.1 Thu 15:00 TRE Ma

Probing Optical Modes of Gold Tapers Using Electron Beams — •Nahid Talebi[1], Surong Guo[1], Martin Esmann[2], Mathieu Kociak[3], Christoph Lienau[2], and Peter van Aken[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Birkenweg 20 — [3]Laboratoire de Physique des Solides, Universitet Paris Sud, Orsay 91400, France

Three-dimensional gold tapers have fabulous applications in adiabatic nanofocusing (ACS Nano 6 (7), 6040-6048 (2012)), tailoring photoemission processes (ACS Photonics 5 (9), 3584-3593 (2018)), and optical microscopy (Rev. Sci. Inst. 75, 837 (2004)). Recently, it has been also demonstrated that through a combination of adiabatic nanofocusing and scanning-near-field optical microscopy, weak and strong interactions between nanostructures and gold tips can be nicely probed (Nature Nanotechnology 14, 698*704(2019)). Here, we investigate the interaction of optical gold tapers with electron beams. Using electron-energy loss spectroscopy (Nano letters 16 (10), 6137-6144 (2016)) and cathodoluminescence (ACS photonics 6 (10), 2509-2516 (2019)), optical modes of gold tapers are thoroughly investigated, covering both radiating and nonradiating modes. Moreover, we will show that the synchronization of the electron beams with the launched plasmons with high angular momentum orders lead to pronounced resonances in the electron-energy-loss spectra.

O 108.2 Thu 15:15 TRE Ma

Metastable Configurations of a Molecule on a Scanning Probe Tip — •hadi arefi[1,2], marvin knol[1,2], daniel corken[3], frank s. tautz[1,2], reinhard maurer[3], and chrisitan wagner[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]Department of Chemistry, University of Warwick, Gibbet Hill, Coventry, CV4 7AL, United Kingdom

For scanning probe based molecular nanorobotics and tip-attached single molecule devices, the tip-molecule bonding scheme plays an important role, determining for example, the effective geometric degrees of freedom of the molecule. Exploring various bonding geometries of a PTCDA (3,4,9,10-perylene-tetracarboxylic acid dianhydride) molecule to a pyramid-shaped silver tip, we have studied the potential energy landscape of the molecule using density functional theory. Furthermore, we investigated the effect of the tip shape on the potential energy landscape. Our simulations as well as recent experiments indicate coherently that a bonding scheme different from the originally assumed single tip-molecule bond is present for the PTCDA / Ag-tip system and that the planar PTCDA with carbonyl groups forms two covalent bonds with the tip at sufficiently large tip-surface separations, in similarity to the upright standing PTCDA molecules on a pedestal of two addatoms on the surface [T. Esat, N. Friedrich, F. S. Tautz, and R. Temirov. Nature 558, 573 (2018)].

O 108.3 Thu 15:30 TRE Ma

Two-color coherent control in photoemission from a metal needle tip — •Ang Li[1], Yiming Pan[2], Philip Dienstbier[1], and Peter Hommelhoff[1] — [1]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen — [2]Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 7610001, Israel

Nanotips are routinely used as electron sources in high-resolution electron microscopes [1] and as a basis for studying strong-field phenomena at the surface of solids [2]. Two-color laser-induced photoemission from these nanotips shows high visibility in photoemission with femtosecond coherent control [3,4]. Here, we report electron emission studied as a function of the laser wavelength. High visibilities of up to 95.8% in the photoemission has been observed. Further, the photoemission is studied as a function of the ratio of two laser intensities and for a large range of laser intensities. We present an exact quantum mechanical solution based on quantum-pathway interference. Supported by the measured results, this analysis delivers a general explanation to the two-color coherent control in photoemission on a metal nanotip.

[1] A. V. Crewe et al., Rev. Sci. Instrum. 39, 576 (1968).
[2] M. Krüger et al., J. Phys. B. 51, 172001 (2018).
[3] M. Förster et al., Phys. Rev. Lett. 117, 217601 (2016).
[4] T. Paschen et al., J. Mod. Opt. 64, 1054-1060 (2017).

O 108.4 Thu 15:45 TRE Ma

Mechanism of ultrafast, spin-dependent electron transfer on ferromagnetic interfaces: an ab initio study — •Simiam Ghan, Karsten Reuter, and Harald Oberhofer — Chair of Theoretical Chemistry, Technical University of Munich, Garching, Germany.

Using ab-initio calculations, we explore the mechanism behind an observed spin-dependent electron transfer from photoexcited Argon monolayers into ferromagnetic substrates Fe(110), Ni(111) and Co(0001). A generalized Fermi golden rule is used to calculate transfer rates for majority and minority electrons from donor to acceptor-localized diabatic states. The diabatic states are created through partial diagonalization of the Kohn-Sham Hamiltonian, which also yields inter-state couplings. A faster transfer of minority (down) spins is predicted for Fe and Co substrates, as well as nonpreferential transfer for Ni - all in excellent agreement with ultrafast core-hole clock spectroscopic measurements.

The scheme allows us to compare the roles of donor-acceptor couplings and acceptor density of states in determining a final preferential spin transfer, and highlights the importance of the spacial character of participating states for spin transport on interfaces. Initial applications to self-assembled monolayers of organic molecules are discussed, with the prospect of predicting tunable electron (spin) transport behavior for e.g. organic spintronic devices.

O 108.5 Thu 16:00 TRE Ma

A trip down memory lane: non-Markovian electronic friction effects in ultrafast dynamics at metal surfaces — •Connor Box and Reinhard J. Maurer — Department of Chemistry, University of Warwick, United Kingdom

Electronic friction theory describes how nuclear motion, in the vicinity of a metallic surface, becomes coupled to electron-hole pair excitations. An efficient and practical DFT implementation based on time-dependent perturbation theory [1] has previously been developed, allowing simulation of vibrational decay [2] as well as molecular beam-like surface scattering. [3] In this work; we investigate the importance of memory effects in nonadiabatic energy loss during vibrational decay and molecular scattering. We propose an efficient and robust approach to calculate memory dependent electronic friction and study its effects on a number of well-studied systems including carbon-monoxide adsorbed at Cu(100) and Pt(111). Finally, we explore different approaches to incorporate memory-dependent electronic friction into on-the-fly ab-initio molecular dynamics simulations to achieve a description of nonadiabatic effects beyond the quasi-static limit. [1] PRB 94, 115432 (2016) [2] PRL 116, 217601 (2016) [3] PRL 118, 256001 (2017)

O 108.6 Thu 16:15 TRE Ma

Photocarrier dynamics in CsPbBr3 perovskite single crystals — •Serhii Polishchuk[1], Michele Puppin[1], Alberto Crepaldi[2], Dmitry Dirin[3], Olga Nazarenko[3], Maksym Kovalenko[3], Marco Grioni[2], and Majed Chergui[1] — [1]LSU and LACUS, EPFL, Lausanne, Switzerland — [2]IoP and LACUS, EPFL, Lausanne, Switzerland — [3]LAC, ETHZ, Zurich, Switzerland

The ability to harvest hot carrier energy can elevate the power conversion efficiency of modern single junction solar cells by up to 25%. In conventional solar materials the photogenerated charge carriers loose the excess electronic energy before the charge collection happens. The understanding of the energy dissipation mechanisms is the fundamental step towards the emergence of hot carrier photovoltaics. The time- and angle-resolved photoelectron spectroscopy (TR-ARPES) is a direct probe of the electronic structure and carrier dynamics of solar materials. The photogenerated electron cooling to the conduction band minimum has been visualized and tracked by TR-ARPES in fully-inorganic CsPbBr3 perovskite single crystals. The results yield the cooling timescale of approximately 250 fs, and the sub-ps population decay. While hot phonon bottleneck and Auger heating are considered to govern electron cooling dynamics, the surface and Auger recombination, and the diffusion into the bulk supposedly define the apparent population decay. These findings showcase the capabilities of this experimental approach and constitute an important milestone in understanding the processes controlling the ultrafast photocarrier dynamics in CsPbBr3 semiconductor.

O 108.7 Thu 16:30 TRE Ma

Simulating Electromigration in Metallic Atomic Contacts — •Markus Ring[1], Fabian Pauly[1,2], and Peter Nielaba[1] — [1]Universität Konstanz, Konstanz, Deutschland — [2]Okinawa Institute of Science and Technology, Okinawa, Japan

This talk presents the results of ab-initio simulations of metallic contacts with the aim to understand current-induced structure changes and switching. To do this the effect of the electronic motion is integrated into a Langevin equation for the atoms.

The metallic contacts are investigated with density functional theory (DFT) for the atomic and electronic structure as well as the interaction between the two. All of these properties are calculated perturbatively with nonequilibrium Green's function methods to determine transport properties. Among those properties are current-induced forces acting on the atoms. Those forces are modeled in a Langevin equation for the atoms, whose dynamics and kinetics are analyzed.

The primary results are threshold voltages at which vibration modes of the system turn unstable in the presence of non-equilibrium transport. These threshold voltages are investigated for a significant sample of contact realisation changing distance an lead structure for four metals (Pb, Au, Al, Cu) and compared with experimental switching voltages. Finally the unstable vibration modes are used to search and find additional stable conductance states. Overall this is an approach to bridging the time-scale gap between electronic and atomic motion and simulating switching and electromigration of atomic contacts from first principles.

O 108.8 Thu 16:45 TRE Ma

Superoxide formation near DMSO/Cu(111) interfaces — •Angelika Demling[1], Sarah B. King[2], and Julia Stähler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14169 Berlin — [2]Department of Chemistry and James Franck Institute, University of Chicago, 929 E 57th St Chicago, IL 60637

DMSO is a common non-aqueous solvent with the potential to be used in lithium-oxygen batteries due to its ability to catalyze the superoxide formation [1]. In this study we investigate the electron dynamics in DMSO films on Cu(111) using time- and angle-resolved two-photon photoemission and disentangle the individual steps of charge transfer leading to superoxide formation:

Electrons are injected from the metal to the DMSO, where they form small polarons on sub-picosecond time scales. The subsequent trapping extends the electronic lifetimes to several seconds [2]. Co-adsorption of molecular oxygen quenches the trapped electron signal and leads to

the appearance of an occupied state whose binding energy is in good agreement with electrochemical data of superoxide [3]. These results may contribute to a basic understanding of charge transfer processes in novel battery systems.
[1] K. M. Abraham, J. Electrochem. 162, A3021, (2015)
[2] S. B. King et al., J. Chem. Phys., 150, 041702 (2019)
[3] D. T. Sawyer et al., J. Electroanal. Chem. 12, 90 (1966)

O 108.9 Thu 17:00 TRE Ma

Structural Dynamics in the Si(111)-In Atomic Wire System Studied by femtosecond-RHEED: Excitation, Metastable State and Relaxation — •Christian Brand[1], Bernd Hafke[1], Tobias Witte[1], David Janoschka[1], Pascal Dreher[1], Frank-J. Meyer zu Heringdorf[1,2], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen and CENIDE, Germany — [2]ICAN, Duisburg, Germany

The prototypical atomic wire system, i. e. the (4×1) reconstructed In atomic wires on Si(111) undergoes a first order phase transition to a Peierls distorted (8×2) reconstructed ground state at $T_c = 130\,\mathrm{K}$. The structural dynamics of these wires upon impulsive excitation by intense fs-IR laser pulses is probed through time resolved electron diffraction and proceeds via an accelerated displacive structural transition to the (4×1) state in only 700 fs [Nature **544**, 207 (2017)]. An energy barrier for the atoms collective motion from the excited (4×1) state to the (8×2) state hinders the immediate recovery of the ground state: the In wires remain for many nanoseconds in a super cooled metastable (4×1) state. The relaxation happens through the nucleation of the (8×2) ground state at step edges which then trigger a recrystallization front. This front propagates 1-dimensionally at a speed of $\sim 100\,\mathrm{m/s}$ as determined from a correlation of the step morphology (as obtained by PEEM) to the recovery time constant [Struc. Dyn. **6**, 045101 (2019)].

O 108.10 Thu 17:15 TRE Ma

Excitation of a CDW Amplitudon Mode in Indium Atomic Wires on Si(111) studied by Femtosecond Surface Electron Diffraction — Bernd Hafke[1], Tobias WItte[1], Christian Brand[1], and •Michael Horn-von Hoegen[1,2] — [1]Fakultät Physik, Universität Duisburg-Essen — [2]Center for Nanointegration Duisburg-Essen, CENIDE

The ground state of the Indium atomic wire system on Si(111) is Peierls distorted with periodicity doubling along and perpendicular to the wires, thus resulting in a (8×2) reconstruction. This low-temperature state comes with a metal to insulator transition, opening of a bandgap, and formation of a CDW and exhibits a by 0.1 eV lower energy than the metallic high-symmetry (4×1) state. Here, we report on the excitation of an amplitudon mode of the CDW system by impulsive optical excitation through an IR fs laser pulse under conditions of weak laser fluence $< 1\,\mathrm{mJ/cm^2}$. The observed intensity oscillation in ultra-fast time resolved electron diffraction at a period of 1.4 ps can be described by a superposition of the two characteristic phonon modes, namely the soft rotational and soft shear mode at frequencies of 0.82 THz and 0.54 THz, respectively, which at laser fluences $> 2\,\mathrm{mJ/cm^2}$ facilitate the systems non-thermally driven transition to the excited (4×1) state [Nature **544** (2017) 207].

O 108.11 Thu 17:30 TRE Ma

Coherent vibrational control of the Peierls transition in atomic Indium wires on Si(111) — •Jan Gerrit Horstmann, Hannes Böckmann, Bareld Wit, Felix Kurtz, Gero Storeck, and Claus Ropers — IV. Physical Institute, University of Göttingen, Friedrich-Hund-Platz 1, Germany

Exerting active optical control over solids by harnessing the energy stored in the electronic, lattice or spin degrees of freedom is a key objective of ultrafast science. In femtochemistry, the coherences in the electronic and vibrational states of molecules are already employed to steer reactions towards states or products far from equilibrium. However, a transfer of this concept to solids is complicated, e.g. due to a high electronic and vibrational density of states. In this respect, low-dimensional and strongly correlated systems represent a promising intermediate between molecules and solids, with phase transitions assuming the role of a "reaction". Here, we report coherent vibrational control over the phase transition in a quasi-one-dimensional Peierls insulator by manipulating the vibrational amplitudes of decisive lattice modes. Specifically, we employ an optical double-pulse excitation scheme and monitor the structural transformation between the insulating (8×2) and the metallic (4×1) phase of atomic indium wires on Si(111) by ultrafast low-energy electron diffraction (ULEED). An analysis of the delay-dependent phase transition efficiency proves the distinct roles of specific phonon modes for the transition and provides insight into the underlying control mechanisms and structural pathways.

O 109: Heterogeneous Catalysis on Metal Oxides

Time: Thursday 15:00–17:30 Location: TRE Phy

O 109.1 Thu 15:00 TRE Phy

Photoinduced CO Oxidation on N-doped $\mathbf{TiO_2}$ — •Helena Gleissner[1], Michael Wagstaffe[1], Heshmat Noei[1], and Andreas Stierle[1,2] — [1]DESY NanoLab, Deutsches Elektronen-Synchrotron, Hamburg — [2]Fachbereich Physik, Universität Hamburg

Modification of the electronic structure in TiO_2 is a crucial factor for developing more efficient and visible light sensitive photocatalysts [1]. We studied the effect of nitrogen doping on the photoactivity of the rutile (110) and anatase (101) surfaces for the CO oxidation to CO_2 under UV illumination. Rutile (110) and anatase (101) single crystals were doped with nitrogen via ion implantation and their surfaces were characterized using low energy electron diffraction (LEED). The low energy electron diffraction patterns of the doped surfaces reveal no reconstruction. The nitrogen incorporation and CO oxidation were examined by X-ray Photoelectron Spectroscopy (XPS). The CO oxidation was performed at 97 K under UV illumination of 365 nm and the O 1s and C 1s core levels were measured to monitor CO and CO_2 species. On rutile (110), the CO oxidation rate was slightly enhanced compared to the undoped surface, while on anatase (110) the inhibition of the reaction increased with the dopant concentration.

References

[1] Ulrike Diebold, *The surface science of titanium dioxide*, U. Surf. Sci. Rep. 48, 53-229 (2003).

O 109.2 Thu 15:15 TRE Phy

Adsorption of $\mathbf{O_2}$ on the rutile $\mathbf{TiO_2}$(110) surface revisited by nc-AFM — •Igor Sokolović[1], Michele Reticcioli[2], Martin Čalkovský[1], Margareta Wagner[1], Michael Schmid[1], Cesare Franchini[2], Ulrike Diebold[1], and Martin Setvin[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Center for Computational Materials Science, Faculty of Physics, University of Vienna, Vienna, Austria

Rutile TiO_2(110) surface is extensively studied and it is considered a model transition-metal oxide surface [1]. The adsorption of molecular O_2 has been long investigated with various techniques [2], but still even the basic adsorption configurations remain unclear. In this research, we used non-contact atomic force microscopy (nc-AFM) to directly observe the adsorption configurations of molecular O_2 dosed at low sample temperatures. We demonstrate that an oxygen-terminated AFM tip provides excellent lateral resolution, and that it does not perturb the adsorbates. Using density functional theory (DFT) we simulated the observed adsorption configurations and determined the charge state of the adsorbed molecules, which is 2- (peroxo) in all cases. We performed experiments of thermal annealing, charge injection/removal, and ultraviolet light irradiation of the O_2 covered surface. By directly observing the reactants of such experiments, we explain that the rich behavior of O_2 on this surface stems from the differences in the types of the adsorbed molecules, thus answering several long-standing questions. [1] U. Diebold, Surface science reports 48, 53 (2003). [2] J. T. Yates Jr, Surface Science 603, 1605 (2009).

O 109.3 Thu 15:30 TRE Phy

Computational Scheme for Preparing Realistic Structural Models of Amorphous Metal Oxide Surfaces — •Hannah Schlott and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Surfaces of metal oxides are often amorphous. The variation in the local environment of the surface sites, which gives rise to a distribution of their chemical and electronic properties, is not captured by using single crystal surface structure models in atomistic simulations. For studying the interaction of real metal oxide surfaces with a liquid or gas phase surrounding, it is therefore of great interest to have a computational scheme for generating amorphous surface structures with accurate and realistic distributions of atomic coordinations and bonding environments. Here we propose a new technique which allows the direct preparation of amorphous surface structures by the melt–quench technique without requiring to cleave amorphous bulk structures. The method also allows a seamless incorporation of other species such as hydroxyl groups into the amorphous surfaces. Using Car-Parrinello molecular dynamics (CPMD) we prepared amorphous ZnO, TiO_2 and Al_2O_3 bulk and surface structures. The reliability of our approach will be demonstrated by a detailed analysis of their structural features such as radial and angular distribution functions, coordination numbers and binding motifs.

O 109.4 Thu 15:45 TRE Phy

Poisoning by Hydroxylation: Photoreforming of Primary Alcohols on Rutile Titania — •Martin Tschurl, Carla Courtois, Moritz Eder, Constantin Walenta, and Ueli Heiz — Chair of Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

Some years ago, we reported the catalyst poisoning during the photoreaction of ethanol on a titania(110) single crystal in an ultra-high vacuum atmosphere. In this work, we now focus on the origins of this peculiar reaction property. The comparison of different alcohols enables a closer look into the reaction mechanism, in order to determine the decisive factors for the inhibition of the reaction. For this purpose all steps of the reaction sequence, the alcohol adsorption, the migration of photon-generated charges, the photochemical reaction and the desorption of the oxidized products, are discussed to finally reveal the reason for the poisoning.

O 109.5 Thu 16:00 TRE Phy

Photocatalytic Conversion of Tertiary Alcohols on Rutile Titania — •Carla Courtois, Moritz Eder, Kordula Schnabl, Constantin Walenta, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

While tertiary alcohols are usually inert towards oxidation, photocatalysis of tertiary alcohols on a bare single crystal rutile titania show new and unexpected reaction pathways. Tertiary alcohols are selectively photo-oxidized on titania at room temperature by a C-C bond cleavage leading to a ketone and the respective alkane. Studies under highly defined vacuum conditions allow elucidating the reaction mechanism and the impact of adding a metal co-catalyst on the product spectrum.

O 109.6 Thu 16:15 TRE Phy

Sum frequency spectroscopy on the surface of semiconductors — •Denise Franziska Bullert, Anupam Bera, and Eckart Hasselbrink — Universität Duisburg-Essen, Universitätsstr. 5, 45117 Essen, Germany

Titanium dioxide (TiO_2) is a versatile material with important applications in environmental purification. Therefore it gained much attention over the last decades. Recently the understanding of adsorbed organic molecules on TiO_2 has made much progress. But little is known about catalytic processes under near-ambient conditions. With a home-made compact cell and the application of sum frequency generation vibrational spectroscopy (SFG-VS) it was possible to address this problem for the first step of a catalytic process. SFG-VS is a powerful method to investigate the chemical identity and structure of adsorbates. Vibrational spectra of adsorbed short-chained alcohols such as methanol (MeOH), ethanol (EtOH) and isopropanol (iPrOH) could be recorded under room temperature and low vacuum conditions. For MeOH and EtOH it was revealed that the molecular species as well as dissociated species are present. In contrast for iPrOH the related spectra show only the molecular species on the surface of the catalyst. The next promising step would be to follow the reaction pathway of catalytically transferred short-chained alcohols under near-ambient conditions. Those kind of studies are also covered by applying SFG-VS because it allows for in-situ spectroscopy.

O 109.7 Thu 16:30 TRE Phy

Low-dimensional projections of high-dimensional kinetic phase diagrams — •Sina Dortaj and Sebastian Matera — Faculty of Mathematics and Computer Science, Freie Universität Berlin

Microkinetic models of heterogeneous catalysis depend on often dozens of kinetic parameters, each showing some degree of uncertainty. This high dimensional parameter space complicates the interpretation phase behaviour if we, ideally, want to take the uncertainty of these parameters into account. Using a first-principles kinetic Monte Carlo model for the CO oxidation on $RuO_2(110)$, we demonstrate how methods from classification can be used to obtain low-dimensional projections of the original high-dimensional phase diagram on the whole parameter space. For the problem at hand, we find that the original 22-dimensional space can efficiently be mapped onto only two effective dimensions. This then allows for a global picture of the phase behaviour.

O 109.8 Thu 16:45 TRE Phy

Trends in Oxidation of Transition-Metal Surfaces at Realistic Temperature and Pressure Conditions — •Zhong-Kang Han[1,2], Santiago Rigamoni[3], Maria Troppenz[3], Claudia Draxl[3], Matthias Scheffler[2], and Sergey V. Levchenko[1,2] — [1]Skolkovo Institute of Science and Technology, Moscow, RU — [2]Fritz-Haber-Institut der MPG, Berlin, DE — [3]Humboldt Universität zu Berlin, Berlin, DE

Oxidation of transition-metal surfaces is a ubiquitous phenomenon, but its thermodynamics is still not fully understood. Using the all-electron FHI-aims code, we present a systematic DFT study (comparing various xc approximations) of the adsorption of oxygen at different elemental and alloyed metal surfaces. The effects of configurational entropy are evaluated by combining a cluster expansion (CE) model with Monte Carlo sampling and the Wang-Landau algorithm, as implemented in our python package CELL [1]. Configurational disorder for both alloy components and adsorbates within several atomic layers of the surface is explicitly taken into account. We show that long-range repulsive interactions between the negatively charged oxygen anions are essential to explain the stability of ordered structures of adsorbed O atoms at (110) and (111) surfaces of elemental metals. The stronger the repulsive interaction is, the higher is the temperature of order-disorder phase transitions. The structures of adsorbed O at the Pd- or Pt-alloyed Cu surfaces exhibit a larger variety of patterns depending on coverage, with Pd/Pt segregating to the surface at low oxygen coverages. 1. http://sol.physik.hu-berlin.de/cell

O 109.9 Thu 17:00 TRE Phy

Revisiting the high temperature oxidation of $Ni_3Al(111)$ by in situ STM — •Tim Kratky[1], Xinzhou Ma[1,2], and Sebastian Günther[1] — [1]TUM, Dept. Chemie, Lichtenbergstr. 4, D-85748 Garching — [2]Foshan University, Materials Science and Energy Engineering, CN-528000 Guangdong

The $Ni_3Al(111)$ surface was characterized during oxidation within the temperature range of 690-800 K by in situ scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and auger electron spectroscopy (AES). Surface aluminum oxide formation is observed. Above 790 K, the known $(\sqrt{67} \times \sqrt{67})R12.2^\circ$ double layer oxide grows, which consists of two Al–O layers. Oxygen dosing at the lower temperature of 740±10 K leads to a single layer oxide showing a (7×7) moiré pattern. Surprisingly, when lowering the temperature below 720 K during oxygen exposure, a so far unknown bilayer oxide arises. At temperatures close to 720 K, the 2nd layer is ordered and a novel diffraction pattern with a $(4\sqrt{3} \times 4\sqrt{3})R30^\circ$ unit cell is observed with its hexagonal O lattice aligned to the support. Below 700 K, the 2nd oxide layer is still formed ontop of the single layer oxide but in a disordered state so that the LEED pattern of the single layer oxide with a (7×7) moiré unit cell is observed again. Thus, the confusing fact arises that the (7×7) LEED pattern may originate from both, a single- or a low temperature double layer oxide.

O 109.10 Thu 17:15 TRE Phy

X-ray standing waves reveal lack of OH-termination at hydroxylated ZnO(0001) surfaces — •Jens Niederhausen[1,2], Antoni Franco-Cañellas[3], Simon Erker[4], Thorsten Schultz[1,2], Katharina Broch[3], Alexander Hinderhofer[3], Steffen Duhm[5], Pardeep K. Thakur[6], David A. Duncan[6], Alexander Gerlach[3], Tien-Lin Lee[6], Oliver T. Hofmann[4], Frank Schreiber[3], and Norbert Koch[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany — [2]Humboldt-Universität zu Berlin, Germany — [3]Universität Tübingen, Germany — [4]Graz University of

Technology, Austria — [5]Soochow University, China — [6]Diamond Light Source, UK

The vertical adsorption distances of the planar conjugated organic molecule 3,4,9,10-perylenetetracarboxylicdiimide (PTCDI) on hydroxylated ZnO(0001), determined with the X-ray standing wave technique (XSW), are at variance with adsorption geometries simulated with density functional theory for surface-structure models that employ terminating hydroxyl groups (OH). In contrast, good agreement is found for PTCDI in direct contact with the topmost Zn layer. The consequential assignment of OH to subsurface sites is supported by additional XSW and energy scanned photoelectron diffraction data and calls for a reconsideration of the prevalent surface models with important implications for the understanding of ZnO(0001) surfaces.

O 110: Surface Magnetism I (joint session O/MA)

Time: Thursday 15:00–18:00 Location: WIL A317

O 110.1 Thu 15:00 WIL A317

Magnetic properties of multilayer vanadyl phthalocyanine on Pb(111) — •Piotr Kot, Maximillian Uhl, Robert Drost, and Christian R. Ast — Max Planck Insitute for Solid State Research

Single-molecule magnets have been of great interest to the condensed matter community due to their potential applications in memory storage and quantum computing [1], and their inherent usefulness in studying fundamental quantum mechanics [2]. Here we present a study of vanadyl phthalocyanine (VOPc) molecules which, when deposited in the correct conditions, form multilayer nano-crystals on the surface of Pb(111) with two possible molecular orientations at each layer. Only one of the VOPc orientations on the first layer shows a spin excitation with energy splitting consistent with a spin half system, which agrees with recent findings [3]. The magnetic properties found on the second layer of molecules is also only observed in one of the molecular orientations, and shows strong zero-field splitting. This suggests that the way the first and second layer molecules interact with their environments varies significantly.

1. Leuenberger, Michael N., and Daniel Loss. "Quantum computing in molecular magnets." *Nature* 410.6830 (2001): 789.
2. Gatteschi, Dante, and Roberta Sessoli. "Quantum tunneling of magnetization and related phenomena in molecular materials." *Angewandte Chemie International Edition* 42.3 (2003): 268-297.
3. Malavolti, Luigi, et al. "Tunable Spin*Superconductor Coupling of Spin 1/2 Vanadyl Phthalocyanine Molecules." *Nano letters* 18.12 (2018): 7955-7961.

O 110.2 Thu 15:15 WIL A317

Influence of the Molecular Arrangement on the Magnetic Properties of FePc and FePcF$_{16}$ thin films — •Katharina Greulich[1], Axel Belser[1], Sven Bölke[1], Reimer Karstens[1], Peter Nagel[2], Stefan Schuppler[2], Michael Merz[2], Thomas Chassé[1], and Heiko Peisert[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen — [2]Institute for Solid-State Physics, Karlsruhe Institute of Technology

The electronic configuration and thus the magnetic properties of the central metal atom of some transition metal phthalocyanines are not fully understood and have been intensely debated over the last years. A particularly broad complexity of the electronic structure is expected for Fe(II) phthalocyanines and porphyrins. In our XPS, XAS and XMCD studies, we compare thin films of FePc with their perfluorinated counterpart FePcF$_{16}$. The results indicate that the magnetic and electronic properties of the central Fe atom depend distinctly on the arrangement of the molecules in thin films. Compared to FePcF$_{16}$, FePc shows an unusually large XMCD signal at the Fe L$_{3,2}$-edge pointing to collective magnetic properties that do not seem possible in FePcF$_{16}$ due to a different molecular arrangement.

O 110.3 Thu 15:30 WIL A317

Kondo effect of a singly occupied molecular orbital in bis(phthalocyaninato)-dysprosium double decker molecules — •Timo Frauhammer[1], Timofey Balashov[1,2], Gabriel Derenbach[1], Svetlana Klyatskaya[3], Eufemio Moreno-Pineda[3], Mario Ruben[3], and Wulf Wulfhekel[1,3] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Germany — [2]II. Physikalisches Institut, RWTH Aachen, Germany — [3]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany

Double decker bis(phthalocyaninato)-dysprosium single molecule magnets adsorbed on Au(111) have been investigated using low temperature STM. No direct magnetic signal by the 4f electrons could be detected in STS. However, a clear Kondo resonance located on the ligands of the molecules can be observed. This indicates an odd number of electrons residing in the molecular orbitals of the ligands. Interestingly, a splitting of this Kondo resonance has been observed even in the absence of external magnetic fields, which can be attributed to a ferromagnetic exchange coupling between the unpaired spin on the ligands and the 4f angular momentum of the Dy central ion. Using spin-polarized tips, this might enable the readout of the 4f spin of Dy.

O 110.4 Thu 15:45 WIL A317

Real-time susceptibility measurements of CoTMPP on magnetic Ni/Cu(110)-(2x1)O thin films — •Gizem Mendirek[1], Aleksander Brozyniak[1], Michael Hohage[1], Mariella Denk[1], Andrea Navarro-Quezada[1,2], and Peter Zeppenfeld[1] — [1]Institut für Experimentalphysik, Johannes Kepler Universität Linz, Altenberger Str. 69, 4040 Linz, Österreich — [2]Institut für Halbleiter und Festkörperphysik, Johannes Kepler Universität Linz, Altenberger Str. 69, 4040 Linz, Österreich

The magneto-optic signal of organic molecular thin films is expected to be rather small. Therefore, a high sensitivity is required to measure the magnetic susceptibility of thin molecular layers. In this work we present the implementation of a sinusoidal modulation of the magnetic field to a Reflectance Difference Magneto-Optical Kerr Effect (RD-MOKE) setup with increased sensitivity that allows detecting of variations of the Kerr rotation angle below 1 μrad/mT at applied fields of a few mT. We illustrate the capabilities of the setup for Ni thin films grown on Cu(110)-(2x1)O surfaces, which exhibit a sharp spin reorientation transition (SRT) of the magnetic easy axis from in-plane to out-of-plane at a coverage of 9 ML. Subsequent deposition of cobalt tetramethoxyphenylporphyrin (CoTMPP) on Ni/Cu(110)-(2x1)O surface induces characteristic changes in the magnetic properties that can be monitored in real-time during the growth of the organic layer. Our results demonstrate the potential of the setup for studying ultrathin organic/ferromagnetic interfaces.

O 110.5 Thu 16:00 WIL A317

Emergence of on-surface molecular magnetism by non-magnetic impurity doping — •Roberto Robles[1], We-Hyo Soe[2], Carlos Manzano[3], Nicolás Lorente[1,4], and Christian Joachim[2] — [1]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), San Sebastián, Spain — [2]Centre d'Elaboration de Matériaux et d'Études Structurales (CEMES), CNRS, Université de Toulouse, Toulouse, France — [3]Institute of Material Research and Engineering (IMRE), Agency for Science, Technology and Engineering (A*STAR), Singapore — [4]Donostia International Physics Center (DIPC), San Sebastián, Spain

Using a low-temperature scanning tunneling microscope (LT-STM) combined with density functional theory (DFT) calculations we show how non-magnetic organic molecules on a metallic surface can become magnetic by doping them with light metal atoms. By single atom/molecule manipulation we construct a complex formed by two aluminum atoms doping a phenanthrazine molecule on an Au(111) surface. We use the Kondo effect to characterize the magnetic moment and confirm the emergence of a localized magnetic moment in the 2(Al)-phenanthrazine complex. DFT calculations allow us to describe the electronic and magnetic properties of the new system. This procedure opens a new way to design light magnetic molecular complexes without the need of transition metal atoms.

O 110.6 Thu 16:15 WIL A317

Probing intramolecular metal-ligand spin coupling by STM — •yuqi wang[1], soroush arabi[1], klaus kern[1,2], and markus ternes[3,4] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — [3]RWTH Aachen University, Institute of Physics, D-52074 Aachen, Germany — [4]Peter-Grünberg-Institute, Forschungszentrum Jülich, D-52425 Jülich, Germany

The bonding of metal-organic molecules to a substrate induces molecular ligand spin states, which lead to an intramolecular conductance and spin dynamics [1]. However, the intramolecular spin coupling has not been studied in detail at molecular scale yet. Here we use a low-temperature scanning tunneling microscope (STM) to study cobalt phthalocyanine (CoPc) molecules on a 2H-NbSe$_2$ substrate. We observe that there are two kinds of adsorbed CoPc molecules due to two slightly different adsorption geometries. While one behaves like a $S = 1/2$ system which introduces Yu-Shiba-Rusinov states in the superconducting gap of the substrate [2], the other behaves like an effective $S = 0$ system which shows a singlet-triplet transition at about 23 meV due to the antiferromagnetic coupling between the central Co atom of the metal-organic complex and its ligands. [1] A. Mugarza, *et al., Nat. Comm.* **2**, 490 (2011). [2] S. Kezilebieke, *et al., Nano Lett.* **18**, 2311 (2018).

O 110.7 Thu 16:30 WIL A317

Mapping magnetic anisotropies in molecular junctions — •Cristina Mier[1], Leonard Garnier[2], Benjamin Verlhac[2], Roberto Robles[1], Laurent Limot[2], Nicolás Lorente[1], and Deung-Jang Choi[1] — [1]Centro de Física de Materiales (MPC) CSIC-EHU, San Sebastián, Spain — [2]Université de Strasbourg, CNRS, IPCMS, UMR 7504, Strasbourg, France

The ability to control the spin of single molecules is of great interest for the development of quantum technologies. Nickelocene ((Ni(C$_5$H$_5$)$_2$,NiCp$_2$) is a magnetic molecule with spin S=1, which shows a big electronic inelastic signal due to the excitation of its spin state [1]. We studied this molecule on a superconducting surface and used a superconducting tip which allows us having a higher energy resolution than the one with normal metallic tips. We found peaks in the differential conductance due to the spin excitations, permitting us to determine the magnetic anisotropy energy (MAE) of the system. The energy position of peaks is slightly shifted at different molecules, which indicates differences in magnetic anisotropy energies for each molecules. This study gives us more parameters to tune the MAE in a molecular junction.

[1] M. Ormaza, N. Bachellier, M. N. Faraggi, B. Verlhac, P. Abufager, P. Ohresser, L. Joly, M. Romeo, F. Scheurer, M.-L. Bocquet, N. Lorente, and L. Limot. Efficient spin-flip exci- tation of a nickelocene molecule. Nano Letters, 17(3):1877*1882, 2017. PMID: 28199115.

O 110.8 Thu 16:45 WIL A317

Organic radical functionalisation of a gold surface — •Tobias Junghöfer, Ewa Malgorzata Nowik-Boltyk, and Maria Benedetta Casu — Eberhard Karls Universität Tübingen, Institut für Physikalische und Theoretische Chemie, 72076 Tübingen, Germany

Organic radical thin films are of great interest for organic electronics such as spin filtering devices, data storage devices, and as quantum bits for quantum computing devices. Here we present the functionalisation of a gold substrate by using a derivative of the perchlorotriphenylmethyl (PTM) radical. PTM is a very chemically and thermally stable radical. We investigate the gold/PTM derivative interface by using soft X-ray techniques, such as X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS) spectroscopy. Our results show that the functionalisation is successful under specific preparation conditions. The radical is still intact and keeps its magnetic character at the interface. Our findings are a significant step forward on the implementation of organic radicals in molecular-based devices with different properties and applications as energy, sensing, imaging, memories, and spintronics.

O 110.9 Thu 17:00 WIL A317

Spin-polarized photoelectron emission from chiral cupric oxide layers — •Paul Möllers[1], Daniel Nürenberg[1], Koyel Banerjee Ghosh[2], Wenyan Zhang[2], Francesco Tassinari[2], Yitzhak Mastai[2], Ortal Lidor-Shalev[2], Simon Wei[3], Emil Wierzbinski[3], David Waldeck[3], Ron Naaman[2], and Helmut Zacharias[1] — [1]Center for Soft Nanoscience, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Department of Chemical and Biological Physics, Weizmann Institute of Science, 76100 Rehovot, Israel — [3]Chemistry Department, University of Pittsburgh, Pittsburgh, PA 15260, United States

The chirality-induced spin selectivity (CISS) effect introduces a coupling between the linear and the spin angular momentum of electrons moving through a chiral molecule [1]. Chiral cupric oxide (CuO) layers can be grown by electrodeposition from a solution containing chiral precursor molecules such as tartaric acid [2]. The choice of the enantiomer of this precursor determines the chiral crystal structure and the preferential crystallographic orientation.

Here, we present results from spin-resolved photoemission experiments performed with chiral CuO layers to investigate the presence of CISS. We demonstrate that the spin polarization observed in these layers can be exploited to enhance the chemical selectivity of an electrocatalytic water splitting reaction [3].

[1] R. Naaman et al., Nat Rev Chem 3, 250 (2019) [2] Kothari et al., Chem. Mater. 16, 4232 (2004) [3] K. B Gosh et al., J. Phys. Chem. C 123, 3024 (2019)

O 110.10 Thu 17:15 WIL A317

Quantifying exchange forces of a spin spiral on the atomic scale — Nadine Hauptmann[1], Soumyajyoti Haldar[2], Tzu-Chao Hung[1], •Wouter Jolie[1], Lorena Niggli[1,3], Mara Gutzeit[2], Daniel Wegner[1], Stefan Heinze[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität, Kiel, Germany — [3]Physik Institut, University of Zurich, Switzerland

Chiral magnetic structures are stabilized by an interplay between competing exchange interactions at the atomic scale. Spin-polarized scanning tunneling microscopy (SP-STM) has achieved great success in investigating the magnetization of such structures, but faces a number of limitations in being able to directly detect the underlying exchange forces, as well as delineate between structural and electronic contributions. To go beyond these limitations, we have developed a new method, which combines SP-STM and magnetic exchange force microscopy (SPEX) based on nc-AFM. Here, we utilize SPEX to investigate a monolayer of Mn on W(110), which exhibits an antiferromagnetic cycloidal spin-spiral ground state driven by the Dzyaloshinskii-Moriya interaction. We show that our force measurements are more sensitive to atomic-scale variations of the exchange force field and the local chemical environment than the current [1]. First-principles calculations explain our observations and reveal the magnetic exchange force mechanisms.

[1] N. Hauptmann et al., arXiv:1908.00959

O 110.11 Thu 17:30 WIL A317

Magnetism of valence electrons in lanthanide atoms on metallic substrates and lanthanide thin films — •Daria Sostina[1,2], Aparajita Singha[1,2], Christoph Wolf[1,2], Safa Ahmed[1,2], Denis Krylov[1,2], Pierluigi Gargiani[3], Alessandro Barla[4], Woosuk Noh[5], Marina Pivetta[6], Stefano Rusponi[6], Harald Brune[6], Andreas Heinrich[1,2], and Fabio Donati[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul, Republic of Korea — [2]Department of Physics, Ewha Womans University, Seoul, Republic of Korea — [3]ALBA Synchrotron Light Source, Cerdanyola del Vallès, Catalonia, Spain — [4]Istituto di Struttura della Materia (ISM), Consiglio Nazionale delle Ricerche (CNR), Trieste, Italy — [5]Pohang University of Science and Technology, Pohang, Republic of Korea — [6]Institute of Physics, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Valence electrons in rare earth single atoms play a fundamental role in determining their magnetic stability and energy level structure [Phys. Rev. Lett. 121, 027201 (2018)]. Here, we investigate the occupation and magnetic moments of 5d and 6p electrons of Gd in the metallic state using X-ray magnetic circular dichroism. We observe charge transfer to occur when Gd atoms and clusters are deposited on Ag(100) surface and negligible occupation of Gd 5d orbital. Additional measurements performed on Gd films and related comparison with density functional theory allow us to understand the contribution of electron-electron correlations and hybridization of the Gd 5d orbitals to the magnetism of rare earths atomic-scale structures.

O 110.12 Thu 17:45 WIL A317

Magnetism of surface-embedded lanthanide single atoms with room temperature structural stability — •Safa Lamia Ahmed[1,2], Aparajita Singha[1], Denis Krylov[1], Stefano Rusponi[3], Marina Pivetta[3], Christoph Wolf[1], Alessandro Lodesani[4], Andrea Picone[4], Alberto Brambilla[4], Alessandro Barla[5], Harald Brune[3], Andreas Joachim Heinrich[1,2], and Fabio Donati[1,2] — [1]Center for Quantum Nanoscience, Institute for

Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea — [3]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [4]Dipartimento di Fisica, Politecnico di Milano, 20133 Milano, Italy — [5]Istituto di Struttura della Materia (ISM), Consiglio Nazionale delle Ricerche (CNR), I-34149 Trieste, Italy

We investigate surface embedded lanthanide atoms in ultra-thin MgO film on Ag(100) as a potential solution towards realizing single atom magnets [Science 352, 318 (2016)] with room-temperature (RT) structural stability. RT scanning tunneling microscopy images show negligible surface diffusion and nucleation of the embedded atoms. Using X-ray magnetic circular dichroism, we reveal out-of-plane anisotropy for Tm and Sm; in-plane anisotropy for Ho and Dy and negligible anisotropy for Er and Gd. All systems show paramagnetic loops at 2.5 K. Using density functional theory and multiplet calculations, we model the interaction between the 4f electrons and their ligand environment, and determine the atom's magnetic level structure.

O 111: Nanostructured Surfaces and Thin Films II: 1D and 2D Systems (joint session O/CPP)

Time: Thursday 15:00–17:15 Location: WIL B321

O 111.1 Thu 15:00 WIL B321

Edges in group-IV monochalcogenides: stability and electronic properties — •Mahdi Ghorbani-Asl and Arkady V. Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany.

The group-IV monochalcogenides including tin sulfide (SnS) and germanium sulfide (GeS) are layered semiconductors with an anisotropic crystal structure giving rise to several unusual physical properties. In this study, based on density functional theory combined with different dispersion corrections, we systematically investigated the structure, stability and electronic properties of monolayer and multilayer SnS and GeS with various possible stoichiometric and nonstoichiometric terminations of the edges. It was found that the (110) facet has the lowest energy and it is thus expected to be the most stable edge. We further demonstrated that nonstoichiometric edges can exist as they provide reconstructed structure or covalent interlayer coupling between layers, which lowers the formation energies of the edges. The results indicate that the stability of the edges generally decreases for higher facet indices. The electronic structure calculations showed that most of the studied compounds are semiconductors with a band gap in the range of 0.2 - 1.6 eV, depending on the crystallographic direction of the edge and its chemical termination. For both GeS and SnS nanoribbons, the band gap is smallest in the case of the (010) edge and largest for the (110) edge. The edge states are more pronounced in multilayer than monolayer nanoribbons.

O 111.2 Thu 15:15 WIL B321

MoS2 monolayers under cluster ion irradiation: a molecular dynamics study — •Sadegh Ghaderzadeh, Vladimir Ladygin, Mahdi Ghorbani-Asl, and Arkady V. Krasheninnikov — Institue of Ion beam Physics and Materials Research Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

Ion irradiation is a powerful method to tailor the properties of low-dimensional materials, and is thought to be particularly promising for patterning two-dimensional (2D) materials through tuning the energy, type, charge state of the incident particles and the supporting substrate. This tool is recently employed to tackle the important issue of controlled pore creation in 2D materials to be performed as filters for water desalination, gas sensing, etc. This aim requires a clear insight into the microscopic process which is yet to be fully understood. In this work, we use classical Molecular Dynamics (MD) simulations to shed light on the behavior of 2D materials under cluster ion irradiation, and specifically focous on the production and characterization of defects. To a great extent, the properties of the induced defects depend on the size and energy of the clusters, which has not been studied beyond graphene so far. In particular, we are focused on the response of MoS2 monolayers, which have shown various exciting properties complementary to graphene, under cluster irradiation. Furthermore, we show that depending on the incident angle and energy of the clusters, sulfur atoms can be sputtered mainly from the top layer, creating unique opportunities for patterning MoS2 monolayers.

O 111.3 Thu 15:30 WIL B321

One-dimensional molecular chains of Quinacridone on Ag(100) and Cu(111): STM- and SPA-LEED-investigations — •Niklas Humberg[1], Rémi Bretel[2], Alexander Eslam[1], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany — [2]University of Paris-Saclay, Institut des Sciences Moléculaires D'Orsay, France

One-dimensional molecular aggregates are of high interest because they often show specific and pronounced coupling effects for electronic excitations, e.g. in optical spectra. Here, we report a structural analysis of two such systems, quinacridone (QA) on Ag(100) and Cu(111), by STM and SPA-LEED.

On Ag(100) QA grows in homochiral domains of parallel one-dimensional chains at room temperature (RT), forming a metastable structure. Within these chains the molecules are parallel and linked pairwise via two hydrogen bonds. The distance between chains varies with coverage. After annealing at 500 K, a 2D commensurate heterochiral structure is formed. It consists of homochiral dimers forming periodically indented and closely packed chains. On Cu(111), QA grows in similar fashion at RT, but compared to QA/Ag(100) the structure shows stronger disorder in form of kink-like defects in the chains. Annealing at different temperatures between RT and 600 K leads to different chain-like structures, that are stable at RT. The comparison to the similar system QA/Ag(111) [1] indicates that the structures of QA/Cu(111) at RT are determined by kinetic limitations.

[1] Wagner et al, J. Phys. Chem. C 2014, 118, 20, 10911-10920.

O 111.4 Thu 15:45 WIL B321

Fabrication of highly regular Moth-Eye inspired Nanostructures to generate Anti-Reflective Surfaces — •Louise Kaeswurm, Zhaolu Diao, Johannes Hirte, Klaus Weishaupt, and Joachim Spatz — Max-Planck-Institute for Medical Research, Jahnstr. 29, 69120 Heidelberg, Germany

We developed a possibility to create highly regular moth-eye inspired anti-reflective (AR) nanostructures on different substrates such as silica glass, sapphire, diamond and silicon. Although thin-film technology can solve reflection related problems to a certain extent, AR moth-eye nanostructures have many advantages.

The method proposed is based on block copolymer micellar lithography to apply an etching mask and reactive ion etching to nanostructure the surface. Compared to other fabrication methods, this approach is fast and easily scalable. The method is based on the principle of index matching: the generated nanostructures lead to the reported reduction of the reflectivity. For transparent substrates the transmission is severely increased, for non-transparent the absorption. Since nanopillars and bulk are the same material, mechanical stress is reduced enabling applications in the high-energy regime. I.e. laser systems and EUV technology can profit from such an AR treatment. Additionally, AR sapphire windows for endoscopes can improve the imaging quality and AR silicon enhances the efficiency of different electronic devices. Further developing the processes will enable the use of the full potential of such AR surfaces for a variety of applications ranging from electronics to medical and optical applications.

O 111.5 Thu 16:00 WIL B321

Length dependent symmetry in narrow chevron-like graphene nanoribbons — •Koen Houtsma[1], Mihaela Enache[1], Remco Havenith[1,2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Groningen, the Netherlands — [2]Stratingh Institute for Chemistry, University of Groningen, Groningen, the Netherlands

Graphene nanoribbons (GNRs) are an exciting material that has aroused much interest due to their excellent and tunable electronic properties. Using on-surface synthesis, narrow chevron-like GNRs, which host a mixture of armchair and zigzag edge terminations, were synthesized from the prochiral molecular building block 6,12-dibromochrysene on a Au(111) substrate [1]. An interesting property of these ribbons is the changing structural symmetry depending on the number of monomer units incorporated in the ribbon, where ribbons consisting of an odd and even number of monomers are point and mirror symmetric, respectively. In our research, we characterized the electronic properties of these GNRs using scanning tunneling spectroscopy, also in dependence of their length and parity.

[1] T.A. Pham et al., Small 13 (2017) 1603675.

O 111.6 Thu 16:15 WIL B321

Chirality transfer to supported metal particles and within organic dye films — •Natalie Fehn, Alexander von Weber, Matthias Jakob, Philip Stanley, Aras Kartouzian, and Ueli Heiz — Chair of Physical Chemistry, Department of Chemistry and Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

Chirality - the absence of improper rotation axes within a structure or molecule - is a phenomenon known since the early 19th century and leads to optical activity of the substance such as optical rotatory dispersion and circular dichroism. The phenomenon plays an important role in medication, biochemistry, and fine chemicals and still opens many questions such as the origin of life. We are especially interested in the transfer of chirality from chiral surfaces to small metal particles and adsorbates, which is addressed via circular dichroism spectroscopy and second harmonic generation-circular dichroism spectroscopy. We already observed induced circular dichroism in silver nanoparticles [1] and organic dye thin films [2]. Now, the question arises whether chirality can be introduced into metal clusters which may serve as catalysts in asymmetric heterogeneous catalysis [3].

[1] M. Jakob, A. von Weber, A. Kartouzian, U. Heiz *PCCP* **31** (2018), 20347-20351, DOI: 10.1039/c8cp02970a. [2] A. von Weber, P. Stanley, M., Jakob, A. Kartouzian, U. Heiz *J. Phys. Chem. C* **14** (2019), 9255-9261, DOI: 10.1021/acs.jpcc.9b01323. [3] A. Kartouzian *Chirality* **31** (2019), 641-657, DOI: 10.1002/chir.23113.

O 111.7 Thu 16:30 WIL B321

Enhanced efficiency of graphene-silicon Schottky junction solar cell through inverted pyramid arrays texturation — •Jiajia Qiu[1], Huaping Zhao[1], Long Liu[1], Wenhui Ma[2], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano* (ZIK), Technische Universität Ilmenau, Ilmenau, Germany — [2]State Key Laboratory of Complex Nonferrous Metal Resources Clean Utilization, Kunming University of Science and Technology, Kunming 650093, China

Nanostructures of silicon are gradually becoming hot candidate due to outstanding capability for trapping light and improving conversion efficiency of solar cell. In this paper, silicon nanowires (SiNWs) and silicon inverted pyramid arrays (SiIPs) were introduced on surface of Gr-Si solar cell through silver and copper-catalyzed chemical etching, respectively. The effects of SiNWs and SiIPs on carrier lifetime, optical properties and efficiency of Gr-SiNWs and Gr-SiIPs solar cells were systematically analyzed. The results show that the inverted pyramid arrays have more excellent ability for balancing antireflectance loss and surface area enlargement. The power conversion efficiency (PCE) and carrier lifetime of Gr-SiIPs devices respectively increase by 62% and 34% by comparing with that of Gr-SiNWs solar cells. Finally, the Gr-SiIPs cell with PCE of 5.63% was successfully achieved through nitric acid doping. This work proposes a new strategy to introduce the inverted pyramid arrays for improving the performance of Gr-Si solar cells.

O 111.8 Thu 16:45 WIL B321

Spatial Extent of Surface Photovoltage in the Vicinity of Individual Plasmon Excited Nanoparticles — •Katharina Engster, Kevin Oldenburg, Karl-Heinz Meiwes-Broer, Sylvia Speller, and Ingo Barke — Institute of Physics, University of Rostock

The investigation of photophysical processes of heterogeneous systems largely relies on local probing techniques [1]. For plasmon assisted electron-hole generation a key property is the size of the region that is affected by enhanced charge carrier density which is accessible via the local surface photovoltage (SPV). Here we present SPV studies of single resonantly excited Ag clusters [2] on Si(100)-(2x1) measured by energy-resolved two-photon photoemission electron microscopy (2PP-PEEM). Analysis of the distance dependence from the particles reveals an enhanced plasmon induced charge carrier density which decays on the scale of 1 μm. This observation is corroborated by comparing spatially averaged SPV for different particle densities. We envision opportunities in the context of plasmon enhanced solar cells, particularly regarding the choice of optimal particle concentrations.

[1] K. Sell *et al.*, Phys. Stat. Sol. (b) **247**, 1087 (2010).

[2] K. Oldenburg *et al.*, J. Phys. Chem. C **123**, 1379 (2019).

O 111.9 Thu 17:00 WIL B321

Supramolecular nanopatterns of arylenes and arylene-alkynylenes: Addressing the third dimension — Georgiy Poluektov, Tristan J. Keller, Joshua Bahr, David A. Hofmeister, Anna Krönert, Anna Jochemich, Dirk Laux, Daniel Kalle, Sebastian Henzel, Steven Becker, •Stefan-Sven Jester, and Sigurd Höger — Kekulé-Institut für Organische Chemie und Biochemie der Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Arylenes and arylene-alkynylenes that carry long alkoxy side chains physisorb at the solid/liquid interface on graphite (HOPG). The resulting two-dimensional (2D) supramolecular nanopatterns have periodicities in the order of 3 nm to 10 nm and are *in situ* imaged by scanning tunneling microscopy (STM) with submolecular resolution. The electronic and mechanic decoupling of the active units in such systems from (i) the substrate surface and (ii) adjacent species within the nanopatterns is essential for a single-molecule functionality similar to systems in a solution. Here, we report on bicyclophanes as well as shape-persistent stars and macrocycles, all carrying anchor groups that point along the surface normal.

O 112: Development of Novel Methods I

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

Invited Talk O 112.1 Thu 15:00 WIL C107

Positron Beams for Elemental and Structure Analysis of Surfaces — •Christoph Hugenschmidt — MLZ and Physics Department E21, Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany

With the advent of bright low-energy positron beams novel analysis tools have been developed exploiting the unique properties of positron matter interaction such as repulsive crystal potential or positron trapping in surface states [1]. Positron annihilation is established for defect spectroscopy and the characterization of the free volume in amorphous matter. By applying a slow positron beam, however, defects near the surface can be specifically addressed, e.g. for the determination of the O vacancy concentration in YBa2Cu3O7-x [2]. The positron counterparts of reflection high-energy electron diffraction (RHEED) and electron induced Auger-electron spectroscopy (AES) intrinsically exhibit superior surface sensitivity. In contrast to electrons, positrons show total reflection for small glancing angles. It was demonstrated that with reflection high-energy positron diffraction the structure of the topmost and the immediate subsurface atomic layer of surfaces can be revealed with outstanding accuracy. The main advantages of positron annihilation induced AES are the missing secondary electron background and its topmost layer sensitivity for elemental analysis, e.g. for the in situ observation of the Ni adatom migration from the Pd surface into the bulk [3]. [1] C. H.; Surf. Sci. Reports 71 (2016) 547 [2] M. Reiner et. al.; Phys. Rev. B 97 (2018) 144503 [3] S. Zimnik et. al.; Surf. Sci. 664 (2017) 61

O 112.2 Thu 15:30 WIL C107

X-Ray Absorption Spectroscopy at Free-Electron Lasers using a Split-Beam Referencing Scheme — •Robin Y. Engel[1,3], Günter Brenner[1], Siarhei Dziarzhytski[1], Piter S. Miedema[1], Jan Schunck[1,3], Florian Döring[2], Benedikt Rösner[2], Christian David[2], and Martin Beye[1] — [1]Deutsches Elektronen Synchrotron DESY, Germany — [2]Paul Scherrer Institut, Switzerland — [3]Universität Hamburg, Germany

Any absorption spectroscopy is based on the exact measurement of the ratio between incident and transmitted intensity. If the used lightsource provides a constant incident intensity, measuring only the transmitted light can be sufficient. In order to measure X-ray Absorption Spectra (XAS) with a time-resolution on the fs-scale, X-ray sources with high brilliance and short pulse duration are required. Modern Free Electron Lasers (FEL) deliver such pulses, but most exhibit a strongly fluctuating spectral content, so that an exact measurement of both incident and transmitted intensities becomes necessary. This can be achieved using a diffraction grating in transmission that splits the FEL beam into two identical copies (+/- 1. diffraction order) which are used as probe- and reference-beams. For ideal comparability, both beams are measured on the same CCD-detector after one of them has interacted with the sample. This concept was implemented at the Free Electron LASer in Hamburg (FLASH) both in transmission and reflection geometries. X-ray absorption spectra can be recorded either in monochromatic mode, or by directly normalizing two copies of an energy-dispersed beam on the same CCD.

O 112.3 Thu 15:45 WIL C107

Two-dimensional spin detection with high-resolution laser ARPES based on hemispherical analyzer and exchange scattering spin detector — •Tristan Heider, Claus M. Schneider, and Lukasz Plucinski — FZ Jülich PGI-6, Jülich, Germany

Two existing approaches for measuring 2D spin maps in angle-resolved photoemission are single k-point detectors behind the hemispherical analyzer [1], and 2D spin detectors in combination with momentum microscopes, either with hemispherical [2] or time-of-flight energy filtering (other related concepts exist). Here we describe the setup of the first type based on the *A*1 hemispherical analyzer with the lens deflection system (MBS AB) with the *Ferrum* spin detector (Focus GmbH) mounted on a 90-deg deflector. The point-by-point spin scanning is efficient when using the 6eV *cw* laser excitation (LEOS Solutions), and a typical 50 × 50 pixel 2D spin map can be collected within 10-20 min. The unique advantages are the access to both in-plane and out-of-plane spin components using *Ferrum*, the negligible instrumental asymmetries, and the access to the energy resolution down to 5 meV in spin. We will discuss several applications, including the high resolution spin-integrated laser-ARPES from Fe-based superconductor, and spin-resolved in-plane and out-of-plane 2D spin-texture from the Bi_2Se_3-family material. The challenges in data collection of our large 3D ARPES maps will be discussed in a separate talk [3].

[1] L. Plucinski et al. J. Electron Spectroscopy Rel. Phen. 181, 215 (2010) [2] C. Tusche et al., Ultramicroscopy 159, 520 (2015) [3] L. Plucinski et al., this conference

O 112.4 Thu 16:00 WIL C107

The TensErLEED Management Package: A new environment for analysis and calculation of IV-LEED data — •Florian Kraushofer[1], Michael Schmid[1], Ulrike Diebold[1], Lutz Hammer[2], and Michele Riva[1] — [1]TU Wien, Vienna, Austria — [2]FAU Erlangen-Nürnberg, Erlangen, Germany

Low Energy Electron Diffraction (LEED) is a structure sensitive technique commonly available in most surface science laboratories. Beyond the usual application as a tool to determine periodicity and degree of order of a surface phase, quantitative analysis of the modulation of beam intensities as a function of voltage (IV-LEED) allows direct comparison to theoretically predicted structural models. This, however, requires complex full-dynamical intensity calculations as well as a time-consuming optimization of structural parameters minimizing the deviation between experimental and calculated $I(V)$ curves. The Erlangen program package TensErLEED [1] readily performs this task, but its required user input is almost prohibitively complex.

We show that for most cases, the necessary TensErLEED input can be generated automatically by combining a handful of user parameters, a set a default values, and a structure file in a standard format. Based on this, we introduce a new package that greatly simplifies the use of TensErLEED and substantially reduces the amount of work and potential for errors, even for experienced users. The package is completed by a versatile utility for extracting experimental $I(V)$ spectra from a LEED video or a stack of LEED images.

[1] V. Blum, K. Heinz, Comput. Phys. Commun., 2001. 134(3)

O 112.5 Thu 16:15 WIL C107

Photoelectron Momentum Imaging Using a Combination of Single Hemispherical Analyzer and Time-of-Flight Recording — •Katerina Medjanik, Sergey Babenkov, Dmitry Vasilyev, Hans-Joachim Elmers, and Gerd Schönhense — JGU, Institut für Physik, Mainz, Germany

Extensive work of Tusche et al. [1] uncovered principal advantages of the "non-inverted" operation of a double-hemispherical analyser, a concept that can be simplified to a large single hemispherical dispersive analyser (HDA). We implemented an additional time-of-flight (ToF) section behind the HDA as "booster" improving resolution. The time spread of the electrons passing the HDA is detrimental in standard operation [2] but is strictly deterministic in our instrument, because the momentum image is encoded as angular pattern in the analyzer. First data taken with laboratory sources show that the time spread (1-2 ns at typical settings) varies linearly with coordinate ky (dispersive direction) but does not affect kx. Combining the flexibility of the HDA with the advantage of 3D ToF-recording, the hybrid instrument increases detection efficiency by 1-2 orders of magnitude. It does not require special filling patterns of Synchrotron- and FEL-sources and will be most relevant for high-resolution and spin-resolved work in the soft- and hard-X-ray range, where ToF-recording has proven superior [3].

[1] Tusche et al., Ultramicr. 206, 112815 (2019); [2] Sise & Zouros, J. Spectroscopy 153513 (2015); [3] Medjanik et al., J. Synchr. Rad. 26, 1996 (2019).

O 112.6 Thu 16:30 WIL C107

Adsorption controlled permeation as a new approach in surface science — •Petr Dementyev — Bielefeld University, Bielefeld 33615, Germany

Molecular adsorption on solids and interfacial diffusion are of paramount importance in heterogeneous chemistry and membrane separation. Recently, two-dimensional (2D) materials have been employed as ultrathin windows for probing related surface phenomena. In particular, X-ray photoelectron spectroscopy with radiation transparent films has been significantly advanced to be applied under realistic reaction conditions. Herein, we introduce another methodology based on the ultimate thickness of free-standing 2D membranes - Adsorption Controlled Permeation (ACP). As there is no much internal volume, mass transfer across porous planar nanomaterials is expected to be dominated by entrance kinetics. We demonstrate experimentally that studying transport rates in 2D layers yields unprecedented information on physicochemical processes ranging from condensation to solvation. The ACP measurements are carried out in an originally designed vacuum system with a mass-spectrometric detector. Vapor permeation studies with carbon nanomembranes (CNMs) reveal that adsorbed species are able to promote transmembrane diffusion of noncondensable gases. Furthermore, concentration-induced disruption of single-file water was discovered to take place in narrow nanochannels.

The author is grateful to the "Fonds der Chemischen Industrie" for a Liebig Fellowship.

O 112.7 Thu 16:45 WIL C107

Optimization of a UHV-compatible electrochemical flow cell combined with IRAS and DEMS for single crystal experiments — •Claus Kovacs, Jiri Pavelec, Michael Schmid, Ulrike Diebold, and Gareth S. Parkinson — Institute of Applied Physics, Vienna University of Technology, Austria

Electrochemical reactions involving metal-oxide catalysts are increasingly important in energy conversion technologies, but the mechanisms involved remain shrouded in mystery. Electrochemical surface science is relatively well established, but studies involving metal-oxide single crystals remain rare, and best practices for UHV-to-electrolyte transfer are still being established. Here, we will discuss the development of a UHV-compatible electrochemical flow cell, which is to be combined with in-situ differential electrochemical mass spectroscopy (DEMS) and infrared reflection absorption spectroscopy (IRAS) measurements. Crucially, the transfer must be made without exposure to air. To speed up the design process and optimize cell performance, we have performed numerical simulations utilizing the program COMSOL Multiphysics®. In particular, the simulations allow us to optimize the thickness of the flow cell, which has a major impact on IRAS and the electrochemical cell performance. Further, the residence time in the cell is also optimized to improve DEMS detection. The simulations focus on mass transport through the cell, as well as the reaction at the catalytic interface. Finally, charge transport is studied to optimize the position and shape of the counter and reference electrodes.

O 112.8 Thu 17:00 WIL C107

shear flow-driven dewetting for wrinkle-free transfer of centimeter-scale ultrathin alumina membrane onto arbitrary substrates — •Huanming Zhang, Min Zhou, Rui Xu, and Yong

Lei — Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693 Ilmenau

The transfer of ultrathin membrane (UTM) onto arbitrary substrates is important in different practical fields. The polymer-supported transfer of UTM keeps the structure of membrane intact, but suffers from organic residual. Wet transfer is applicable to the UTM without a polymer support, where the liquid surface serves as an underlying support. However, conventional wet transfer methods inevitably induce wrinkle defects as a result of the large contact angle of the trapped droplet between UTM and substrate. To solve this problem, the target substrates always need either hydrophilic treatments or organic liquid wetting. However, they are not applicable to all the substrates. Here we demonstrate a shear flow-driven dewetting method to transfer centimeter-scale membrane onto arbitrary substrates without wrinkle. Compared with hydrophilic treatments or organic liquid wetting, this method is fast, simple, cheap, convenient and safe. Taking widely-used ultrathin anodic aluminum oxide membrane (UTAM) as an example, we investigate the microscale details of these macroscale wrinkles and successfully demonstrate the application of large-area wrinkle-free UTAM to defect-free ordered nanostructure arrays fabrication. Corresponding superiority over the defective counterpart is further studied in optical sensing.

O 112.9 Thu 17:15 WIL C107

Preparative mass spectrometry using electrospray controlled-ion-beam-deposition device — •Andreas Walz, Karolina Stoiber, Wei Ran, Annette Hüttig, Joachim Reichert, Hartmut Schlichting, and Johannes V. Barth — Physics Department E20, Technical University of Munich, Germany

Designing novel nanostructures of organic and anorganic compounds requires precise and controlled growth of atomically clean films of clusters or molecules on well-defined surfaces. Our home-build Electrospray Controlled Ion Beam Deposition device (ES-CIBD) opens access to the large, reactive and thermolabile species including biomolecules like proteins or DNA which had been excluded form investigation with standard deposition devices. The implemented Quadrupole Mass Spectrometer (QMS) allows for the characterization of the molecules as well as their purification prior to deposition. It is operated in a digital technique, allowing for very high m/z ratios and adaption of the resolution thereto. The innovative Radio Frequency (RF) controlled ion guides preserve the beam intensity of up to 1nA through the subsequent vacuum chambers from ambient conditions to ultrahigh vacuum (UHV). This allows for precise, short-time depositions, soft-landing conditions with 1-2 eV kinetic energy may be adjusted as well as reactive-landing conditions with some 100 eV. Simulations with SIMION assisted the design. Scanning tunneling microscopy (STM) investigations of large plasmid DNA molecules (1,7 MDa) and N-doped graphene nanoribbons proof quality and versatility of the depositions performed with the instrument.

O 113: Annual General Meeting of the Surface Science Division

Report of the chairperson; election of a new vice-chair; miscalleneous; award ceremony – Gerhard Ertl Young Investigator Award

Time: Thursday 19:00–19:30 Location: HSZ 01

Duration: 30 min.

O 114: Post-Deadline Talks

Contributed post-deadline talks, TBD

Time: Thursday 19:30–20:30 Location: HSZ 01

Duration: 60 min.

O 115: Overview Talk: Susan Stipp

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

Topical Talk O 115.1 Fri 9:30 TRE Phy

Natural Material Surfaces: How they behave and why we care — •Susan L. Svane Stipp — Physics, Technical University of Denmark

The ultrahigh resolution techniques of physics and materials engineering can equally be used to investigate the solid-fluid interfaces that we find in nature. Although natural systems are extremely complex, molecular level understanding about the interactions between mineral surfaces and the gases and liquids in contact allows us to tackle the challenges that society and industry face in health, energy and the environment. Using techniques such as atomic force microscopy, X-ray photoelectron spectroscopy, micro and nanotomography and many others, we have discovered some of the reasons that natural solid-fluid systems often do not behave as thermodynamic and kinetic models suggest that they should. Mineral surfaces are never a simple termination of the bulk so models with such assumptions are bound to fall short. Surfaces are restructured, hydrated and sometimes hydrolysed. Adsorbed species, even at fractions of a monolayer, change surface free energy dramatically. The secondary minerals produced as reaction products are often too small to identify using traditional techniques but they control chemical reactivity and often affect flow of fluids through porous media. Current examples are conversion of CO2 back to rock, where it is stable for millennia, and the role of organic compounds in controlling biomineral growth.

O 116: Wetting and Liquids at Interfaces and Surfaces II (joint session CPP/DY/O)

Time: Friday 9:30–12:15 Location: ZEU 260

Invited Talk O 116.1 Fri 9:30 ZEU 260

Slide electrification: charging of surfaces by moving water drops — •Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Mainz, Germany

Water drops sliding over insulating surfaces can lead to surface charging. In contrast to charging caused by friction between two solids, drop slide electrification is largely unexplored. Slide electrification has been consistently reported, but results are difficult to reproduce. One reason for the lack of quantitative understanding is that the deposition of charge is a non-equilibrium effect and depends essentially on microscopic processes at the contact line. We address both the experimental and theoretical sides of this problem. We reproducibly measure the charge gained by water drops sliding down hydrophobic surfaces. To explain these results, we theorize that some fraction of the charge in the Debye layer is transferred to the surface rather than being neutralized as the drop passes. Given that nearly every surface in our lives comes in contact with water, this water-dependent surface charging may be a ubiquitous process that we are only beginning to understand.

O 116.2 Fri 10:00 ZEU 260

Spreading on viscoelastic solids: Are contact angles selected by Neumann's law? — Mathijs van Gorcum[1], •Stefan Karpitschka[2], Bruno Andreotti[3], and Jacco H. Snoeijer[1] — [1]Physics of Fluid Group, University of Twente, Enschede, Netherlands — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [3]Laboratoire de Physique Statistique, Univ. Paris-Diderot, Paris, France

The spreading of liquid drops on soft substrates is extremely slow, owing to strong viscoelastic dissipation inside the solid. A detailed understanding of the spreading dynamics has remained elusive, partly owing to the difficulty in quantifying the strong viscoelastic deformations below the contact line that determine the shape of moving wetting ridges. Here we present direct experimental visualizations of the dynamic wetting ridge, complemented with measurements of the liquid contact angle. It is observed that the wetting ridge exhibits a rotation that follows exactly the liquid angle, as was previously hypothesized [Karpitschka et al., Nat. Commun. (2015)]. This experimentally proves that, despite the contact line motion, the wetting ridge is still governed by Neumann's law. Furthermore, our experiments suggest that moving contact lines lead to a variable surface tension of the substrate. We set up a new theory that incorporates the influence of surface strain, the so-called Shuttleworth effect, for soft wetting. It includes a detailed analysis of the boundary conditions at the contact line, complemented by a dissipation analysis, which shows, again, the validity of Neumann's balance.

O 116.3 Fri 10:15 ZEU 260

Formation of a thin film during drop merging leads to fingering instability — •Peyman Rostami[1,2] and Günter Auernhammer[1,2] — [1]Max Planck Institute for Polymer Research, 55128, Mainz, Germany — [2]Leibniz Institute of Polymer Research, 01069, Dresden, Germany

The coalescence and interaction between two drops have been the subject of intensive studies in recent years [1], due to its wide range of application and the presence in the nature.

Here, we study the merging of partially miscible drop. We deposit drops of different liquids on a substrate. Under appropriate conditions, the merging process generates an instability which resembles the Rayleigh-Plateau instability. If the liquid with higher surface activity is deposited as a second droplet. Its vapor can diffuse through the air and induce a Marangoni flow inside the already deposited droplet. This induced flow can pull a thin liquid layer over the surface , which decays into drops by a Rayleigh-Plateau instability.

We present a detailed study of this instability analyzing the onset of the instability and its characteristic length scales. Finally, a model is presented to explain the Marangoni flow induced by the gas phase. This model is validated by particle tracking.

References [1] S. Karpitschka, C. Hanske, A. Fery, and H. Riegler, Langmuir, vol. 30, no. 23, pp. 6826*6830, 2014.

O 116.4 Fri 10:30 ZEU 260

Condensation frosting on lubricant impregnated surfaces — •Lukas Hauer[1], Lou Kondic[2], and Doris Vollmer[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Department of Mathematical Sciences, NJIT, Newark, USA

In many technical applications the formation of frost and ice displays a hazard to the steady functionality of devices. This motivates the development of new materials to tackle the reduction of icing on surfaces. Understanding the nature of frosting and icing is indispensable to this effort. While icing on surfaces is commonly studied by localized nucleation mechanisms, the formation of frost is comparable more complicated. Condensation frost is characterized by multi-step and multi-physical phenomenon. The formation of condensate droplets, percolation, and frost front propagation is an inherently stochastic process. Despite its ubiquitous nature, a quantitative model for frost growth on surfaces remains elusive. Lubricant impregnated surfaces are known for improved anti-icing properties. They experience lower ice drop adhesion and allegedly delayed surface frosting. We show that frost formation can induce immensely strong capillary forces that could result in surface damage, lubricant depletion and the loss of anti-icing properties. Laser scanning confocal microscopy enabled us to monitor the dynamic lubricant migration during condensation frosting on micro-structured surfaces. We present a model of the lubricant migration, utilizing lubrication theory. This work serves to improve understanding of lubricant dynamic during condensation frosting, providing future roadmaps towards the future design of anti-icing surfaces.

O 116.5 Fri 10:45 ZEU 260

Dynamics of liquid droplets on switchable prestructured substrates — •Moritz Stieneker[1] and Svetlana Gurevich[1,2] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, D-48149 Münster, Germany — [2]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstrasse 2, D-48149 Münster, Germany

A mesoscopic continuum model is employed to model a thin, liquid film on a substrate with a spatio-temporal wettability. In particular, the effect of a switchable wettability pattern on the structure formation is analyzed for a one-dimensional case with the help of path-continuation techniques and direct numerical time simulations. It is found that if the periodic switching is introduced, the system reaction depends on the ratio between the time scale given by switching and the reaction time of the liquid. The behaviour of the contact angle during the slow and fast switching is investigated in details. Furthermore it is demonstrated that in the case of the slow switching the droplet solutions corresponding to the local minima of the free energy can be stabilized.

O 116.6 Fri 11:00 ZEU 260

Liquid-liquid phase separation in contact with deformable surfaces — •Hansol Jeon[1,2] and Stefan Karpitschka[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Georg-August-Universität Göttingen

The capillary forces of droplets on top of soft solids deform the solid surface into sharp wetting ridges. The amplitude of the wetting ridge is governed by elasto-capillary length, the ratio of liquid surface tension to the solid's shear modulus. Previous experiments on soft wetting used large liquid-vapour surface tensions and thus were in a highly nonlinear regime regarding the response of the solid. This led to debates in the literature regarding the effects of strain dependent solid surface tensions or the dynamics of soft wetting. Liquid interfaces with small surface tensions could instead probe the linear regime of soft wetting and shed new light onto the static and dynamic behaviours of solid surface tension. Thus we investigate the liquid-immersed case of soft wetting, aiming for a control of the liquid and solid surface tensions. We tested various liquid combinations and explored a wide range of surface tensions and substrate shear moduli, finding valid Neumann constructions in all cases.

15 min. break

O 116.7 Fri 11:30 ZEU 260

Droplets fighting contamination — •Abhinav Naga, William Wong, Anke Kaltbeitzel, Maria D'Acunzi, Hans-Jürgen Butt, and Doris Vollmer — Max Planck Institute for Polymer Research, Mainz, Germany

Lubricated surfaces are prone to accumulating contaminants due to their sticky yet slippery nature. The presence of contaminants, such as dust and dirt particles, alters their performance. An understanding of the effect of contaminated particles on the friction of surfaces is important not only from a fundamental perspective whereby further insight can be gained of the underlying mechanisms, but also from an applied perspective to predict the effectiveness of lubricated surfaces in the presence of contaminants.

In this study, we systematically contaminate lubricated silicone surfaces (Sylgard 184) and non-lubricated surfaces with spherical glass microparticles. We place a droplet on each surface and measure the force needed to push the droplet at different speeds towards an individual microparticle. We visualise this process with laser scanning confocal microscopy, focusing on the deformation inflicted by the microparticle on the droplet and its lubricant ridge. We combine these visualisations with our force measurements to suggest a mechanism for the removal of contaminated particles from surfaces using droplets, and we outline the differences between the outcomes on the lubricated and the non-lubricated surfaces. This work will help to understand droplet dynamics on imperfect or dirty lubricated surfaces.

O 116.8 Fri 11:45 ZEU 260

Memory effects in polymer brushes showing co-nonsolvency effects — •Simon Schubotz[1,2], Petra Uhlmann[1], Andreas Fery[1,2], Jens-Uwe Sommer[1,2], and Günter K. Auernhammer[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden, Germany — [3]Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany

Some polymer brushes show a co-nonsolvency effect: They collapse in a mixture of two good solvents at some specific mixing ratio. Previous studies focused on the response of brushes which are entirely covered by a liquid. Here, we concentrate on partial wetting of co-nonsolvent polymer brushes, i.e., on the dynamics of a three-phase contact line moving over such brushes. We demonstrate that the wetting behavior depends on the wetting history of the polymer brush.

We use Poly(N-isopropylacrylamide) (PNiPAAm) brushes and water and ethanol as good solvents. In water/ethanol mixtures, the brush thickness is a non-monotonous function of the ethanol concentration. The memory of brushes is tested by consecutively depositing drops of increasing size at the same position. Previously deposited drops induce changes in the brush that modifies the wetting behavior (advancing contact angle) of subsequent drops.

We believe that the change in the contact angels is induced by adaptation like swelling of or liquid exchange in the brush due to the drop on top.

O 116.9 Fri 12:00 ZEU 260

Gradient dynamics model for drops spreading on polymer brushes — •Simon Hartmann and Uwe Thiele — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Deutschland

When a liquid drop spreads on an adaptive substrate the latter changes its properties what may result in an intricate coupled dynamics of drop and substrate. We present a generic mesoscale hydrodynamic model for such processes that is written as a gradient dynamics on an underlying energy functional. We specify the model details for the example of a drop spreading on a dry polymer brush. There, liquid absorption into the brush results in swelling of the brush causing changes in the brush topography and wettability. The liquid may also advance within the brush via diffusion (or wicking) resulting in coupled drop and brush dynamics. The specific model accounts for coupled spreading, absorption and wicking dynamics when the underlying energy functional incorporates capillarity, wettability and brush energy. We employ a simple version of such a model to numerically simulate a droplet spreading on a swelling brush and provide an in-depth analysis of the simulation results and some interesting quantities.

O 117: Graphene II: Adsorption, Intercalation and Doping (joint session O/TT)

Time: Friday 10:30–12:30 Location: GER 37

O 117.1 Fri 10:30 GER 37

Ab initio thermodynamics of hydrocarbons relevant to graphene growth at solid and liquid Cu surfaces — •Mie Andersen, Juan Santiago Cingolani, and Karsten Reuter — Theoretical Chemistry, Technische Universität München, Germany

High quality graphene can be synthesized through chemical vapor deposition (CVD) at liquid Cu [1]. However, the role of the liquid catalyst surface is not yet well understood, and the role of hydrogen in the reactant mixture is still debated [2]. Here [3], we use *ab initio* thermodynamics to study the stability of a wide range of hydrocarbons under various CVD conditions (temperature, methane and hydrogen pressures) used in experimental growth protocols at solid and liquid Cu surfaces. We compare various low-index Cu facets and make use of hindered translator/rotator or ideal 2D gas models [4] to describe the adsorbate free energies. We find that smaller hydrocarbons will completely dehydrogenate under most CVD conditions. For larger graphene-like clusters, metal-terminated and hydrogen-terminated edges have very similar stabilities. While both cluster types might thus form during the experiment, we show that the low binding strength of clusters with hydrogen-terminated edges could result in instability towards desorption.

[1] D. Geng *et al.*, PNAS **109**, 7992 (2012)
[2] X. Zhang *et al.*, JACS **136**, 3040 (2014)
[3] M. Andersen, J.S. Cingolani, K. Reuter, J. Phys. Chem. C **123**, 22299 (2019)
[4] L.H. Sprowl *et al.*, J. Phys. Chem. C **120**, 9719 (2016)

O 117.2 Fri 10:45 GER 37

Graphene on liquid Cu, a multiscale model rationalizing mesoscale flake alignment — •Juan Santiago Cingolani, Karsten Reuter, and Mie Andersen — Chair of Theoretical Chemistry, Technical University of Munich, Germany

In recent years the use of liquid Cu as a catalyst during chemical vapor deposition (CVD) has emerged as a promising method for the continuous production of high-quality single layer graphene. The processes involved, such as carbon nucleation, defect healing, or flake alignment, remain largely unexplored or lack convincing atomic-scale rationalization. Of particular interest is the reported meso-scale interaction between growing flakes that leads to an ordering into 2D lattices.

To address the latter, we engage in a multiscale modeling study, hierarchically combining molecular dynamics (MD) simulations with continuum theory. Using a third-generation charge optimized many body potential (COMB3), the MD simulations reveal a strong interaction of graphene flakes with the liquid substrate, leading even to their partial immersion. On the basis of thus determined material parameters like surface energy, charge transfer or average flake height above the surface, we then set up a simple continuum model assuming the flakes to be spherically charged particles. Within an order of magnitude, this model rationalizes the experimental observation of a coalescence of the growing hexagonal flakes into a close-packed structure with well-defined inter-flake separation in terms of long-range capillary and electrostatic interactions.

O 117.3 Fri 11:00 GER 37

Experimental access to thermodynamics and kinetics predicting the CVD growth of graphene on Cu — •Paul Leidinger, Jürgen Kraus, and Sebastian Günther — TUM, Dept. Chemie, Lichtenbergstr. 4, D-85748 Garching

Most Graphene growth recipes by chemical vapor deposition (CVD) on copper in a reactive CH_4/H_2 atmosphere are results of parameter variations optimized by trial and error. Many existing growth models described in the literature are qualitative or contain phenomenological parameters to describe the growth process. In our study, we aim at analyzing the key processes during CVD at 900-1050 °C while maintaining the defined geometry of a growing graphene flake surrounded by graphene free copper. For this purpose, it is essential to control the flake nucleation before and, more importantly, during the entire CVD growth. Systematic variation of the CVD parameters provides the experimental data used to formulate a kinetic model which predicts the graphene growth velocity as function of the chosen mass action constant Q. Determining experimentally the thermodynamic equilibrium of the CH_4 decomposition reaction enables us to use the equilibrium as reference point to which any chosen CVD parameter set can be related quantitatively. With experimental validation of our growth model we can understand both, the thermodynamics and kinetics of graphene growth on copper. Furthermore, we can also predict the growth rate of single graphene flakes formed during any CVD experiment on copper at high precision.

O 117.4 Fri 11:15 GER 37

Stacking Relations and Substrate Interaction of Graphene on Copper Foil — •Philip Schädlich[1], Florian Speck[1], Stiven Forti[2], Camilla Coletti[2], and Thomas Seyller[1] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Istituto Italiano di Tecnologia, Pisa, Italy

Graphene-based device production requires graphene sheets of perfect crystallinity and low defect density on a large scale. Beyond mechanical exfoliation, where the flake size is uncontrollable, there are two promising approaches for high-quality wafer-scale graphene growth: (i) the sublimation growth on silicon carbide (SiC) by thermal decomposition of the substrate [1] and (ii) the chemical vapour deposition (CVD) on metal substrates such as copper [2].

In the present study we investigate the crystallinity of CVD grown graphene and the orientation with respect to the underlying copper foil by means of low-energy electron microscopy (LEEM) and diffraction (LEED). We find a lattice match within ± 1° between the graphene and the Cu(111) surface, which shows a surface facetting depending on the graphene thickness on top. Recently, stress-induced stacking domains in bi- and multilayer graphene were found for epitaxial graphene on SiC [3], revealing a much less homogeneous system than believed. Our LEEM dark field images and reflectivity spectra suggest a similar decomposition into domains of different stacking order for the CVD grown graphene flakes. [1] K. V. Emtsev et al., Nature Mater. 8, 203 (2009). [2] X. S. Li et al., Science 324, 1312 (2009). [3] T. A. de Jong et al., Physical Review Materials 2, 104005 (2018).

O 117.5 Fri 11:30 GER 37

Sidewall epigraphene investigated by STEM — •Markus Gruschwitz, Steffen Schulze, and Christoph Tegenkamp — TU Chemnitz, Chemnitz, Germany

Epitaxial graphene nanoribbons (GNR) grown on SiC facets reveal ballistic transport channels. The structure and growth were studied intensively by STM, LEED and LEEM [1]. Spatially resolved transport measurements and tight-binding calculations suggest that the bonding of the ribbons to the SiC substrate plays an important role [2]. In this study, cross-section STEM on similar structures were performed in order to characterize the interface and bonding between graphene and SiC in more detail.

Indeed, the zig-zag GNRs, grown along the [1100] direction, are delaminated from the SiC facet as seen by high resolution C$_S$ corrected STEM. Mini steps at the top and the bottom of the sidewalls define the edges of the GNRs. Atomically resolved EELS and EDX confirm that the top part of the freestanding GNR merges into a bufferlayer. The SiC facet reveals a silicon deficiency in the three topmost substrate layers. These SiC imperfections were found already for epitaxial graphene on SiC(0001) and result from the sublimation processes [3]. The lower edge merges into SiC and shows a sp^3-hybridization. Moreover, differential phase contrast measurements allow the calculation of charge density maps and therefore the visualization of space charge distributions in the substrate. References: [1] Zakharov et al., ACS Appl Nano Mat., 2, 156 (2019) [2] Aprojanz et al., Nat. Comm. 9, 4426, (2018). [3] Gruschwitz et al., PRM 3, 094004 (2019).

O 117.6 Fri 11:45 GER 37

Epitaxial growth of high-quality armchair graphene nanoribbons — •H. Karakachian[1], J. Aprojanz[2], T. T. N. Nguyen[2], A. A. Zakharov[3], R. Yakimova[4], P. Rosenzweig[1], C. M. Polley[3], T. Balasubramanian[3], C. Tegenkamp[2], and U. Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]Institut für Physik, Technische Universität Chemnitz — [3]MAX IV laboratory, Lund — [4]IFM, Linköping University

Graphene nanoribbons (GNRs) are considered to be the fundamental building blocks for future carbon-based nanoelectronics. The functionality of GNRs is governed by the detailed atomic structure of their edges. Namely, a GNR terminated by armchair edges develops a bandgap in its electronic structure driven by quantum confinement effects, where the size of the bandgap scales with the width of the ribbon itself. Thus, the controlled growth of armchair GNRs (AC-GNRs) may solve the long-lasting problem of graphene, which is its inability to be embedded in modern quantum integrated circuitry. Here, we grow high-quality AC-GNRs on the sidewalls of 6H-SiC mesa structures. Using angle-resolved photoelectron spectroscopy we study the electronic structure of the one-dimensionally (1D) confined AC-GNRs which truly reveals a width-dependent bandgap formation. We observe a set of well-resolved sub-bands and a Fermi surface that consists strictly of a straight line which are characteristic features of 1D confined systems. Our findings provide a solid ground for further theoretical assessment and a deeper understanding of quantum confinement phenomena.

O 117.7 Fri 12:00 GER 37

Monodispersed graphene nanoribbons on Ag(111) by electrospray controlled ion beam deposition: their self-assembly and on-surface extension visited by STM — •Wei Ran[1], Andreas Walz[1], Karolina Stoiber[1], Peter Knecht[1], Anthoula C. Papageorgiou[1], Annette Huettig[1], Diego Cortizo-Lacalle[2], Juan P. Mora-Fuentes[2], Aurelio Mateo-Alonso[2,3], Hartmut Schlichting[1], Joachim Reichert[1], and Johannes V. Barth[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]POLYMAT, University of the Basque Country UPV/EHU, Spain — [3]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

Graphene nanoribbons (GNRs) are of interest due to their potential in electronics, energy conversion, and storage. For atomically precise GNRs, elaborate bottom-up fabrication protocols have been developed, utilising the reactivity of a metallic support.[1] However this approach often results in GNR arrays with a variety of lengths. Here we employ a different approach for the preparation and study of GNRs on surfaces: chemical synthesis and purification of well-defined nanoribbons[2] followed by processing with electrospray controlled ion beam deposition (ES-CIBD). With this method, we can deposit well-defined GNRs on any solid support under ultra-high vacuum conditions. The quality of the films produced is exemplified for a ~ 3 nm GNR on Ag(111). We explore their self-assembly and thermally activated polymerisation reactions by means of scanning tunnelling microscopy.

1) Fasel et al. *Adv. Mater.* **2016**, *28*, 6222.
2) Mateo-Alonso et al. *Angew. Chem., Int. Ed.* **2018**, *57*, 703.

O 117.8 Fri 12:15 GER 37

Understanding trends in lithium binding at 2D materials — •Zeljko Sljivancanin[1,2], Srdjan Stavric[2], and Zoran S. Popovic[2] — [1]Serbian Academy of Sciences and Arts, Belgrade, Serbia — [2]Vinca Institute of Nuclear Sciences, Belgrade, Serbia

Employing density functional theory we studied microscopic mechanisms governing binding of metal atoms and their nanostructures at selected 2D materials. We considered the interaction of a Li adatom with monolayers of several transition metal oxides and dichalcogenides, carbides of group XIV elements, functionalized graphene, silicene and germanene, as well as black phosphorus and Ti$_2$C MXene. We found that the general trend in Li binding can be estimated from positions of conduction band minima of 2D materials, since the the energy of the lowest empty electronic states shows a nice correlation with the strength of Li adsorption [1]. At variance to the majority of studied surfaces where occurs a simple electron transfer from Li to the substrate, in monolayers of carbides of group XIV elements Li adsorbates profoundly modify substrates, creating well-localized mid-gap states. This gives rise to their capability to accommodate Li structures with the nearly constant binding energy of alkaline atoms over Li coverages ranging from well-separated adatoms to a full monolayer.

O 118: Surface Magnetism II (joint session O/MA)

Time: Friday 10:30–13:45 Location: GER 38

O 118.1 Fri 10:30 GER 38

Observation of tunable single-atom Yu-Shiba-Rusinov states — •Artem B. Odobesko[1], Domenico DiSante[2], Alexander Kowalski[2], Felix Friedrich[1], Ronny Thomale[2], Giorgio Sangiovanni[2], and Matthias Bode[1] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, Würzburg, Germany — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, Würzburg, Germany

Through scanning tunneling spectroscopy, we analyze the interdependence of Kondo screening and superconductivity. Our data obtained on single Fe adatoms on Nb(110) show that the coupling and the resulting Yu-Shiba-Rusinov (YSR) bound states are strongly adsorption site-dependent and exhibit a quantum phase transition, where two YSR resonances cross at zero bias. By sweeping the external magnetic field to turn off and on superconductivity in the Nb substrate, we were able to study the interaction of individual magnetic adatoms with the normal-metallic or superconducting substrate in two consecutive experiments. The data show that the in-gap position of YSR states scales with the Kondo temperature and exhibits a cross-over at 0.7Δ, in good agreement with theoretically predicted value. The observed experimental signatures are rationalized by combined density functional theory and continuous-time quantum Monte-Carlo calculations. This treatment shows that the size of the magnetic moment and the hybridization of the impurity orbitals with the substrate are key parameters for understanding the interaction between magnetic adatoms and superconductors.

O 118.2 Fri 10:45 GER 38

YSR states in manually assembled clusters of molecules on a superconducting surface — •Jan Homberg, Manuel Gruber, Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24118 Kiel, Germany

The interaction between magnetic adsorbates and Cooper pairs of a superconducting substrate leads to Yu-Shiba-Rusinov (YSR) resonances. This effect has so far been investigated with low-temperature scanning tunneling microscopy (STM) on adsorbates containing a metal atom, which provides the magnetic moment. We show that non-magnetic molecules without any metal ion can acquire a net magnetic moment upon assembly into clusters as evidenced by YSR resonances. The magnetic moment is due to a partial filling of the lowest unoccupied molecular orbital of the adsorbed molecules. We show that the filling and the corresponding magnetic moment depend on the number of neighboring molecules, on their relative orientations, and on the positions of hydrogen atoms in neighboring molecules. The YSR resonances are due to fractional charges that we analyze using an Anderson-like model.

Support via the European Union's Horizon 2020 research and innovation programme (766726) is acknowledged.

O 118.3 Fri 11:00 GER 38

Tunneling of Cooper pairs through a molecular junction — Cristina Mier[1], Rose Reina[1], Leonard Garnier[2], Benjamin Verlhac[2], Laurent Limot[2], Nicolas Lorente[1], and •Deung-Jang Choi[1] — [1]Centro de Física de Materiales (MPC) CSIC-EHU San Sebastián, Spain — [2]Université de Strasbourg, CNRS, IPCMS, UMR 7504 Strasbourg, France

The tunneling of Cooper pairs between two superconductors connected through a weak link is called Josephson effect. Cooper pairs tunnel through Andreev bound states (ABS) which is localized to the weak link. The dependence of the ABS on the phase difference between the two superconductors fixes the way the Cooper pairs tunnel. ABS are a characteristic of the junction and they cannot be probed by varying the bias between the two superconductors since they take place at zero bias. This is very different from Yu-Shiba-Rusinov (YSR) in-gap state that can take place already for one superconductor and are due to the weakening of Cooper pairs produced by a magnetic impurity [1]. We will present experimental data and theoretical analysis characterizing the ABS of a reproducible Scanning Tunneling Microscope molecular junction giving us access to the elusive phase difference in an STM setup.

[1] Choi, D.-J. et al. Mapping the orbital structure of impurity bound states in a superconductor. Nat. Commun. 8, 15175 (2017).

O 118.4 Fri 11:15 GER 38

Charge transport between discrete superconducting bound states at the atomic scale — •Haonan Huang[1], Ciprian Padurariu[2], Jacob Senkpiel[1], Robert Drost[1], Björn Kubala[2], Juan Carlos Cuevas[3], Alfredo Levy Yeyati[3], Joachim Ankerhold[2], Klaus Kern[1,4], and Christian R. Ast[1] — [1]MPI für Festkörperforschung, Stuttgart, Germany — [2]Institut für komplexe Quantensysteme, Universität Ulm, Ulm, Germany — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain — [4]EPFL, Switzerland

A Yu-Shiba-Rusinov (YSR) state is a pair of in-gap states resulting from the interaction of magnetic atoms with a superconductor. While YSR states have received intensifying attention especially in the field of scanning tunneling microscopy (STM) due to its capability to resolve and measure the transport through single atom, the tunneling processes between YSR states still remain elusive. We are now able to controllably introduce YSR state of desired properties to the apex of the STM tip and measure the tunneling between the tip YSR state and a sample YSR state, which we call *Shiba-Shiba tunneling*. This results in a current peak at the sum of the two YSR energies. We observe a blockade in Shiba-Shiba peak when increasing conductance, which renders YSR tip a general probe of the single level lifetime at the atomic scale.

O 118.5 Fri 11:30 GER 38

Theory of Shiba-Shiba tunneling at the edge of a Majorana chain — •Ciprian Padurariu[1], Haonan Huang[2], Björn Kubala[1], Christian R. Ast[2], and Joachim Ankerhold[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

The realization of the Majorana chain [1], a 1D-chain of Yu-Shiba-Rusinov (YSR) states created by magnetic impurities on the surface of a superconductor, suggests that Majorana states emerging at the edges can be probed by the STM.

Recently, we have developed an ideal tool to probe and manipulate the edge states of a Majorana chain. It consists of a superconducting STM tip with its own in-gap YSR state created by a magnetic impurity on the tip. With this device we have studied the sharp resonant transport between the YSR state on the tip and another one on the superconducting sample, and have developed its theory.

This talk will expand on the theory of Shiba-Shiba tunneling and present the possible opportunities to manipulate edge states of the Majorana chain. We discuss the effects of spin-orbit coupling on tunneling, that may be relevant to the experimental realization. In certain parameter regimes theory predicts that the edge state will transfer from the chain to the tip. This may provide a first step towards realizing braiding of edge states using the STM.

[1] S. Nadj-Perge, I. K. Drozdov, J. Li, H. Chen, S. Jeon, J. Seo, A.H. MacDonald, B.A. Bernevig, A. Yazdani, Science **346**, 602 (2014).

O 118.6 Fri 11:45 GER 38

Bloch-type spin helix in bilayer Fe islands on Ir(110) by spin polarized STM — Jeison A. Fischer[1], •Timo Knispel[1], Mahasweta Bagchi[1], Jens Brede[1], Vasily Tseplyaev[2], Markus Hoffmann[2], Stefan Blügel[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, 50937 Cologne, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Most work on interfacial chiral spin textures focused on films exhibiting C3v symmetry and isotropic Dzyaloshinskii-Moriya interaction (DMI), known to only support Néel-type spin helices and skyrmions [1]. In contrast, C2v symmetry systems such as the (110) surface of an fcc crystal, are predicted to show anisotropic DMI leading to various scenarios of topological pattern formation [2]. Fully unexpectedly, our spin-polarized STM/STS study reveals a magnetic stripe phase, due to a spin helix with a period of 1.2 nm along the [-1 1 0] direction in bilayer Fe islands on unreconstructed Ir(110). Based on detailed field dependent measurements with a vector magnet, we conclude that the chirality of the spin helix is of Bloch-type, where the rotation is perpendicular with the propagation direction. This contradicts the assumption of the spin helix being induced by an interface in-plane DMI vector. Combined with theoretical insights, we discuss our findings in terms of the formation energy in systems with C2v symmetry. Funding: CRC1238 and the Jülich Supercomputing Center project CJIAS1F

[1] S. Heinze et al. Nat. Phys. Vol.7, p.713 (2011).

[2] M. Hoffmann et al. Nat. Commun. Vol.8, p.308 (2017).

O 118.7 Fri 12:00 GER 38

Study of the skyrmion formation on Co monolayers deposited on superconducting Ru(0001) substrate — •Loic Mougel[1], Julian Skolaut[1], Marie Hervé[1,2], Timofey Balashov[1], Jasmin Jandke[1], Bertrand Dupé[3], and Wulf Wulfhekel[1] — [1]Physikalisches Institut ,KIT, Karlsruhe, Germany — [2]Institut des Nanosciences de Paris, CNRS, Sorbonne université, Paris, France — [3]Institute of Physics, Johannes Gutenberg-Universität (JGU), Mainz, Allemagne

It has been theoretically proposed in the last years that magnetic skyrmions, when positioned in proximity to a superconductor might host Majorana bound states. These states are predicted to appear in pair of entangled states, as a zero-energy excitation in a superconducting gap. Such states are of great interest for the realization of Topological Quantum Computation.

Recently we demonstrated that it was possible to stabilize skyrmions using low magnetic field, on monolayers of Co deposited on a Ru(0001) surface. By submitting the system to a magnetic field one can create skyrmions that will remain meta-stable in the remanent state. In this communication we report on the preliminary experiments realized on the Co monolayers deposited on the superconducting Ru(0001) surface. We will present the measurements of Ruthenium superconducting gap, as well as the study of the proximity effect that arise at the Ferromagnetic/Superconductor interface, and how the superconducting state can influence the spin-spiral structure.

O 118.8 Fri 12:15 GER 38

Theoretical description of single-Co Kondo effect in atomic Cu wires on Cu(111) — Nicolas Néel[1], Markus Bohn[1], Jörg Kröger[1], •Malte Schüler[2,3], Bin Shao[2,3], Tim Wehling[2,3], Alexander Kowalski[4], and Giorgio Sangiovanni[4] — [1]Institute for Physics, Technical University of Ilmenau — [2]Bremen Center for Computational Materials Science, University Bremen, — [3]Institute for Theoretical Physics, University Bremen — [4]Institute for Theoretical Physics and Astrophysics and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg

Linear atomic chains containing a single Kondo atom, Co, and several nonmagnetic atoms, Cu, assembled atom by atom on Cu(111) with the tip of a scanning tunneling microscope show a peculiar evolution of the Kondo resonance. The evolution of this resonance can be inferred from changes in the line shape of the Abrikosov-Suhl-Kondo resonance. Strikingly, for two geometries no Kondo resonance at all is observed. We perform state-of-the-art first-principles calculations to describe the resonance and unravel possible microscopic origins of the remarkable experimental observations. We focus on the fact that the theoretical results are in line with experimental findings for all but two geometries which show no resonance and draw conclusions on the current state of theoretical description of many-body phenomena in real materials.

O 118.9 Fri 12:30 GER 38

Ensembles of Orbital Memories on Black Phosphorus — •Elze Knol[1], Brian Kiraly[1], Hilbert Kappen[2], and Alexander Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Donders Institute for Neuroscience, Radboud University, Nijmegen, The Netherlands

Cobalt atoms at the surface of black phosphorus (BP) have demonstrated bistable valencies [1], which can be utilized to store digital information. According to density functional theory calculations, each valency hosts a unique magnetic moment. The calculations further reveal that the bistable valencies arise due to a vertical atom displacement which modifies the screening from the underlying BP. In order to study the role of this screening, we take advantage of the tip-induced band bending occurring at the tip-sample junction of a scanning tunneling microscope to probe the energy landscape governing the valency stability. We find, both in single atom memories and ensembles of atomic memories, that the effects of local band bending are depending on the black phosphorus surface. We visualize this dependency directly with a scanning tunneling microscope by carefully studying the position dependence of the stochastic current noise. The inherent properties of this system [2] provide a unique opportunity for atomic ensembles in solids.

[1] Kiraly, et. al., Nature Commun. 9, 3904, (2018). [2] Kiraly, et. al., Phys. Rev. Lett. 123, 216403, (2019).

O 118.10 Fri 12:45 GER 38

Efficient Ab-initio Multiplet Calculations for Magnetic Adatoms on MgO — •Christoph Wolf[1], Fernando Delgado[2], Jose Reina[3], and Nicolas Lorente[3] — [1]Center for Quantum Nanoscience, Seoul, Korea — [2]Universidad de La Laguna, Spain — [3]Centro de Fisica de Materiales CFM/MPC, Spain

Scanning probe microscopy and spectroscopy, and more recently in combination with electron spin resonance, have allowed the direct observation of electron dynamics on the single-atom limit. The interpretation of data is strongly depending on model Hamiltonians. However, fitting effective spin Hamiltonians to experimental data lacks the ability to explore a vast number of potential systems of interest.

By using plane-wave density functional theory (DFT) as starting point, we build a multiplet Hamiltonian making use of maximally-localized Wannier functions. The Hamiltonian contains spinorbit and electron-electron interactions needed to obtain the relevant spin dynamics. The resulting reduced Hamiltonian is solved by exact diagonalization. We compare three prototypical cases of 3d transition metals Mn (total spin S=5/2), Fe (S=2) and Co (S=3/2) on MgO with experimental data and find that our calculations can accurately predict the spin orientation and anisotropy of the magnetic adatom. Our method does not rely on experimental input and permits us to explore and predict the fundamental magnetic properties of adatoms on surfaces.

O 118.11 Fri 13:00 GER 38

Probing the magnetism of single atoms with orbital sensitivity — Aparajita Singha[1,2], Daria Sostina[1,2], Christoph Wolf[1,2], Safa Ahmed[1,2], Denis Krylov[1,2], Luciano Colazzo[1,2], Alessandro Barla[3], Pierluigi Gargiani[4], Stefano Agrestini[4], Woo-suk Noh[5], Marina Pivetta[6], Stefano Rusponi[6], Harald Brune[6], Andreas J. Heinrich[1,2], and •Fabio Donati[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul, Republic of Korea — [2]Department of Physics, Ewha Womans University, Seoul, Republic of Korea — [3]Istituto di Struttura della Materia (ISM), Consiglio Nazionale delle Ricerche (CNR), Trieste, Italy — [4]ALBA Synchrotron Light Source, Cerdanyola del Vallès, Catalonia, Spain — [5]Pohang University of Science and Technology, Pohang, Republic of Korea — [6]Institute of Physics, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Individual Ho atoms adsorbed on MgO/Ag(100) show large magnetic anisotropy and long magnetic lifetime up to 40 K [Science 352, 318 (2016)]. Investigating the distribution of the electron spins among the valence orbitals is crucial to understand the quantum level structure and the origin of magnetic stability in these atoms. Here, we use the orbital sensitivity of x-ray absorption spectroscopy to investigate the valence magnetism of rare earth atoms and clusters on MgO/Ag(100). We find both Gd and Ho atoms in a monovalent state, with one electron transferred to the underneath substrate. Combining our findings with density functional theory, we clarify the controversy on the ground state of Ho single atom magnets [Phys. Rev. Lett. 121, 027201 (2018)].

O 118.12 Fri 13:15 GER 38

Quantum stochastic resonance of single Fe atoms — •Max Hänze[1,2], Gregory McMurtrie[1], Luigi Malavolti[1,2], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Stochastic resonance [1] can be observed in a variety of different systems, ranging from the periodicity of glacial periods in paleontology [2] to the time-dependent behavior of individual neurons [3] in the field of neuroscience. All such systems exhibit stochastic behavior which, because of a strong nonlinear response, can be synchronized to a small harmonic excitation. We observe quantum stochastic resonance in a single Fe atom deposited on the copper nitride surface [4] using scanning tunneling microscopy. Unlike in standard stochastic resonance, the atomic-scale process is dominated by quantum fluctuations where the magnetic state of the Fe atom is driven resonantly between two states in a classically forbidden regime. This phenomenon enables the direct observation of spin dynamics in open quantum system.

[1] R. Benzi, J. Phys. A: Math. Gen 14, L453 (1981) [2] P. N. Pearson et al. Paleontological Society Papers 18, 1-38 (2012) [3] A. J. Bulsara et al. Theor. Biol. 152, 531-555 (1991) [4] C. F. Hirjibehedin et al. Science 317, 1199-1203 (2007)

O 118.13 Fri 13:30 GER 38

Electronic transport properties in bidimensional ferromagnet GdAu2 with atomic scale resolution — •Alberto Moya[1,2,3], David Serrate[1,2], M. Ricardo Ibarra[1,2], and Matthias Bode[3] — [1]Instituto de Ciencia de Materiales de Aragón, CSIC-Universidad de Zaragoza, E-50009 Zaragoza, Spain — [2]Instituto de Nanociencia de Aragón, Universidad de Zaragoza, E-50018 Zaragoza, Spain — [3]Physikalisches Institut, Lehrstuhl für Experimentelle Physik 2, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Electronic properties of atomic scale motifs are difficult to measure because of complexity associated to patterning such small electrical probe contacts. In this work, we measure the electrical resistance of an antiphase boundary of a GdAu2 surface alloy. The GdAu2 monolayer is prepared on a Au(111) substrate and is known to be in-plane ferromagnetically ordered at low temperatures. It exhibits occasional antiphase boundaries which separate structurally identical but phase shifted domains by an atomically sharp 1D lattice defect. Here we measure the magnetotransport response across the boundary.

The measurements were performed by means of the recently developed Molecular Nanoprobe (MONA) technique. In this technique charge carriers (electrons or holes) are injected from the tip of a scanning tunneling microscope (STM) and detected by conformational switching processes excited inelastically by hot electrons reaching dehydrogenated phthalocyanine molecules. By statistically analyzing thousands of injection sequences the charge transport between two surface spots can be evaluated.

O 119: Oxides III: Single-Atom Catalysis, Iron Oxides

Time: Friday 10:30–12:45 Location: REC C 213

Invited Talk O 119.1 Fri 10:30 REC C 213

theoretical studies on the state and fate of single atom catalysts: from hydroformylation to CO oxidation — •Felix Studt — Karlsruhe Institute of Technology, Institute of Catalysis Research and Technology, Eggenstein-Leopoldshafen, Germany

Single atom catalysts (SAC) are attracting widespread attention as they promise the highest achievable atom efficiency in heterogeneously catalyzed reactions. Herein, we show theoretical calculations of the state, stability and activity of SAC supported on different oxide surfaces for the hydroformylation reaction and evaluate differences between the homogeneous catalysts that are used nowadays. Additionally, we use quantum chemical calculations to reveal the reaction mechanism of SAC for a highly selective tandem olefin isomerization-hydrosilylation process. Finally, we will show how the stability of Pt single atoms supported on ceria depend on reaction conditions and how their state relates to CO oxidation activity.

O 119.2 Fri 11:00 REC C 213

Probing structural changes upon carbon monoxide coordination to single metal adatoms — •Paul T. P. Ryan[1,2], Matthias Meier[3,4], Zedenek Jakub[3], Jan Balajka[4], Jan Hulva[3], David J. Payne[2], Tien-Lin Lee[1], Cesare Franchini[4], Francesco Allegretti[5], Gareth S. Parkinson[3], and David A. Duncan[1] — [1]Diamond Light Source, Didcot, OX11 0QX UK — [2]Department of Materials, Imperial College London, SW7 2AZ UK — [3]Institute of Applied Physics, TU Wien, Austria — [4]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Austria — [5]Physics Department E20, Technical University of Munich, 85748 Garching, Germany

The application of highly accurate, but yet computationally cheap, density functional theory (DFT) calculations allows for the fine tuning of catalyst development. However, it is necessary to have stringent benchmarks against which these calculations are tested. In this work, the adsorption height of Ag adatoms on the Fe_3O_4(001) surface after exposure to CO was determined using normal incidence X-ray standing waves. The Ag adatoms bound to CO (Ag^{CO}) are found to be pulled out of the surface to an adsorption height of 1.15 ± 0.08 Å, compared to the previously measured height of 0.96 ± 0.03 Å for bare Ag adatoms[1]. Utilising DFT+vdW+U calculations with the substrate unit cell dimension fixed to the experimental value, the predicted adsorption height for Ag^{CO} was 1.16 Å, in remarkably good agreement with the experimental results. [1] M. Meier et. al., Nanoscale 10, 2226 (2018)

O 119.3 Fri 11:15 REC C 213

Atomic-Scale Studies of Hydroformylation on Rh_1/Fe_3O_4(001) — •Manuel Ulreich[1], Zdeněk Jakub[1], Florian Kraushofer[1], Matthias Meier[1,2], Michael Schmid[1], Ulrike Diebold[1], Cesare Franchini[2], and Gareth S. Parkinson[1] — [1]Institute of Applied Physics, TU Wien, 1040 Vienna, Austria — [2]Center for Computational Materials Science, University of Vienna, 1090 Vienna, Austria

Hydroformylation (alkene + CO + $H_2 \rightarrow$ aldehyde) is an important industrial reaction typically performed in solution using highly-selective mononuclear complexes. Recently, Rh-based “single-atom” catalysts (SACs) have been shown to catalyze this reaction heterogeneously with similar levels of selectivity, suggesting SAC can be a strategy to heterogenize problematic reactions. The main advantage of heterogeneous catalysis is easy separation of the catalyst from the products. SAC is intended to unify this advantage with the high selectivity and activity of homogeneous catalysis. In this talk, TPD and XPS are used to study the coadsorption of ethylene and carbon monoxide on isolated Rh_1 adatoms on Fe_3O_4(001), a critical first step in the hydroformylation reaction. Our results show that 2-fold coordinated Rh_1 adatoms on Fe_3O_4(001) are able to coadsorb C_2H_4 and CO, but 5-fold coordinated Rh_1 adatoms cannot. We conclude that gaining control of the active site geometry is key to the development of highly-selective single-atom catalysis.

O 119.4 Fri 11:30 REC C 213

Influence of Surface Dynamics on Oxidation Processes: Case Study of H_2O_{surf} Desorption on Fe_3O_4(001) — •Matthias Meier[1,2], Jan Hulva[1], Zdeněk Jakub[1], Florian Kraushofer[1], Manuel Ulreich[1], Michael Schmid[1], Ulrike Diebold[1], Cesare Franchini[2], and Gareth S. Parkinson[1] — [1]Institute of Applied Physics, TU Wien — [2]Center for Computational Materials Science, Faculty of Physics, University of Vienna

Experiments performed under UHV, on so called "model systems", where surfaces are well defined and controlled, are combined with DFT calculations to propose reaction mechanisms and determine activation barriers of relevant chemical processes.

Fe_3O_4(001) is such a model system. It is debatable whether the observed surface in UHV is also maintained under real catalytic conditions, such as high pressure, or electrochemical environments. Our results indicate that the surface undergoes modifications, already in UHV and in some cases even below room temperature. O distortions and Fe displacements can occur for any given transition state along a reaction path, if energetically favored. So if their costs are at least compensated by the gain in adsorption energies of present adsorbates or the reduction of activation barriers.

We show here an example of how these surface dynamics influence H mobility, the formation and extraction of H_2O_{surf} and their consequences on experimental observations.

O 119.5 Fri 11:45 REC C 213

Formic acid adsorption and dissociation on magnetite (111) — •Kai Sellschopp[1], Marcus Creutzburg[2,3], Björn Arndt[2,3], Heshmat Noei[2], Andreas Stierle[2,3], Stefan Müller[1], and Gregor Vonbun-Feldbauer[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology — [2]DESY NanoLab, Deutsches Elektronen-Synchrotron, Hamburg — [3]Fachbereich Physik, Universität Hamburg

Magnetite (Fe_3O_4) nanoparticles are utilized in different fields like waste water treatment, single-atom catalysis or hybrid materials. Formic acid molecules are usually present in atmospheric conditions. Further, they can be seen as the smallest representative of the carboxylic acid family. Therefore, studying the interaction of formic acid with the major facets of magnetite nanoparticles, namely the {111} and {001} facets, is highly interesting for their various applications. Here, we present results on the adsorption of formic acid on magnetite (111) studied through calculations based on Density Functional Theory (DFT). In agreement with surface science experiments, the formation of a $(\sqrt{3} \times \sqrt{3})R30^\circ$ superstructure and two different binding modes, a quasi-bidentate and a chelating mode, are found. Independent of the binding mode, the formic acid dissociates on the surface into formate and hydrogen. Calculated surface phase diagrams give further insights in the processes involved under experimental conditions and indicate a separation of the formate and the residual hydrogen originating from the formic acid dissociation.

O 119.6 Fri 12:00 REC C 213

Formic acid induced superstructure formation on magnetite (111) — •Marcus Creutzburg[1,2], Heshmat Noei[1], Björn Arndt[1,2], Vedran Vonk[1], Elin Grånäs[1], Kai Sellschopp[3], Gregor Vonbun-Feldbauer[3], and Andreas Stierle[1,2] — [1]DESY NanoLab, Deutsches Elektronen-Synchrotron, Hamburg — [2]Fachbereich Physik, Universität Hamburg — [3]Institute of Advanced Ceramics, Hamburg University of Technology

Magnetite (Fe_3O_4) is an important and diverse transition metal oxide with applications as a catalyst in various industrial processes such as the water-gas shift reaction [1]. In material science magnetite nanoparticles are linked by oleic acid to form supercrystals with exceptional mechanical properties [2]. However, the oxide/carboxylic acid interface is not fully understood. In this contribution the adsorption of formic acid on the magnetite (111) single crystal surface is studied under UHV conditions at room temperature. Formic acid dissociates upon adsorption and forms a $(\sqrt{3} \times \sqrt{3})\,R\,30^\circ$ superstructure, which is investigated using low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). Fourier transform infrared reflection-absorption spectroscopy (FT-IRRAS) results indicate two different formic acid adsorption sites. Density functional theory (DFT) calculations of the two adsorption structures prove that both configurations form the superstructure and are the most stable under our experimental working conditions.

[1] M. Zhu *et al.*, ACS Catalysis. **6**, 722-732 (2016).

[2] A. Dreyer *et al.*, Nature Materials **15**, 522-528 (2016)

O 119.7 Fri 12:15 REC C 213

Atomistic modelling of the structural and dynamical behaviour of interfaces between biomolecules and magnetite — Mine Konuk[1], Kai Sellschopp[2], Gregor Vonbun-Feldbauer[2], and •Robert Horst Meissner[1,3] — [1]Institute of Polymer and Composites, Hamburg University of Technology — [2]Institute of Advanced Ceramics, Hamburg University of Technology — [3]MagIC Magnesium Innovation Centre, Institute of Materials Research, Helmholtz Zentrum Geesthacht

Based on a newly developed force field for magnetite surfaces that mimics the charge migration of a Bader charge analysis, results of atomic-level calculations on the stability of (001) and (111) magnetite surfaces are presented. The recently proposed subsurface cation vacancy (SCV) termination on Fe_3O_4(001) or the distorted bulk truncation (DBT) are now stable configurations in MD simulations using typical experimental conditions. Within this formalism, the electrostatic interactions between magnetite surfaces and organic molecules with a bidental or quasi-bidental binding motif are also optimized. The results for formic acid adsorption on the (111) or (001) magnetite surface are well in line with the latest experimental findings and *ab initio* calculations. The stability of molecular and dissociated water clusters on SCV and DBT surfaces is additionally investigated and it is further shown that on a DBT surface model a layer of ordered water rows, forming a network of hydrogen bonds, is thermodynamically more stable at room temperature than the same amount of water adsorbed on a SCV termination.

O 119.8 Fri 12:30 REC C 213

Near-surface diffusion of Fe_3O_4 (001) observed by nuclear forward scattering — •Steffen Tober[1,2], Jan-Christian Schober[1,2], Esko Erik Beck[1,2], Guilherme Dalla Lana Semione[1,2], Simon Chung[1,2], Kai Schlage[1], Olaf Leupold[1], Ilya Sergeev[1], René Steinbrügge[1], Hans-Christian Wille[1], Heshmat Noei[1], Vedran Vonk[1], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchrotron, Hamburg — [2]Universität Hamburg, Fachbereich Physik

The near surface defect structure is of key importance to tune the performance of magnetite (Fe_3O_4) in catalysts and spintronic devices. Recent observations of the formation and lifting of the subsurface cation vacancy reconstruction on the (001) surface indicate the presence of a near surface transport process influencing surface phenomena [1,2]. The near surface cation transport between a homoepitaxially grown ${}^{57}Fe_3O_4$ layer and a (001) oriented Fe_3O_4 single crystalline substrate was studied by nuclear forward scattering at the P01 Beamline of PETRAIII. A smearing of the isotope distribution at the film/substrate interface was observed by nuclear resonant reflectivity [3] as a function of temperature in vacuum or oxygen, indicating interfacial cation transport. The sample's chemical state was monitored by time spectra. These results allow to quantify the mobility of near surface cations in magnetite.

[1] Arndt, B. et al. Chem. Comm. 1, 92 (2019)
[2] Arndt, B. et al. Surf. Sci. 653, 76 (2016)
[3] Andreeva et al., Mosc. Univ. Phys. Bull. 63, 132 (2008)

O 120: Focus Session: Nonequilibrium Electron Transfer Across Interfaces in Real Time

(Photo)electrocatalytic devices, 2D material heterostructures and much interesting biophysics all require transferring electrons across interfaces between condensed phases. Despite this motivation, and much effort, gaining experimental insight into *how* electrons move across such interfaces has proven extremely challenging. Part of the challenge lies in the difficulty of experimentally characterising molecular level structure at such buried interfaces. More profoundly, however, even if an appropriate experimental approach is available, characterisation of an interfacial system held at a, nonequilibrium, steady-state is not generally useful in providing mechanistic insight into electron transfer (one cannot distinguish the relationship of minority species). Overcoming this challenge requires perturbation/relaxation techniques: one creates a temporally short non-equilibrium condition in which electron transfer is initiated and characterises the interface as the system relaxes to steady-state conditions over timescales from femto to milliseconds. Within the last several years work along these lines has appeared in a variety of usually disconnected communities. This Focus Session aims to bring together electrochemists approaching electron transfer using all-electrical relaxation techniques, chemical physicists studying (photo)electrocatalysis by initiating electron transfer using femtosecond optical pulses and probing using photons or photoelectrons and solid state physicists conducting similar experiments investigating charge transfer in solid heterostructures.

Organizers: Andrea Eschenlohr, R. Kramer Campen, Uwe Bovensiepen, U. Duisburg-Essen

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

Invited Talk O 120.1 Fri 10:30 TRE Ma

Ultrafast charge transfer dynamics in 2D heterostructures — •Giulio Cerullo, Stefano Dal Conte, Zilong Wang, and Chiara Trovatello — Dipartimento di Fisica, Politecnico di Milano, 20133 Milano, Italy

In the last few years, the research on 2D materials has developed towards the engineering and realization of new heterostructures (HS) based on stacking two or more 2D crystals on top of each other. In such HSs, the electronic structure of the single layers is well retained because of the weak interlayer van der Waals coupling. Nevertheless, new physical properties and functionalities, depending on the type and the stacking sequence of layers, arise beyond their constituent blocks. These new HS have high potential in the field of flexible optoelectronics because they combine strong light matter interaction, high flexibility and high charge carrier mobility. The experimental study of the interlayer charge scattering process in such HS is of paramount importance for developing 2D HS-based optoelectronic devices. In this work we use optical pump-probe spectroscopy to study photoinduced charge transfer dynamics in two different 2D HS: a TMDs heterobilayer (WSe2/MoSe2) and a graphene/WS2 HS. We resolve interlayer exciton formation (200-fs) and decay dynamics in WSe2/MoSe2. We also monitor photothermoionic charge transfer dynamics from graphene to WS2 when pumped well below the semiconductor bandgap, due to hot carriers injection across the HS Schottky barrier.

O 120.2 Fri 11:00 TRE Ma

Ultrafast charge transfer and vibronic coupling in donor/acceptor interfaces — •Matheus Jacobs, Jannis Krumland, Ana M. Valencia, and Caterina Cocchi — Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Donor-acceptor (DA) interfaces are ubiquitous in materials for optoelectronic applications and strongly characterize their intrinsic properties. Interfacial charge transfer, in particular, plays a crucial role in the electronic structure and optical response of these systems. For this reason, it is essential to gain insight on the fundamental processes involved at the interface also beyond the static picture. In the framework of real-time time-dependent density-functional theory coupled to

Ehrenfest molecular dynamics, we investigate the microscopic mechanisms driving ultrafast charge transfer at DA interfaces. Specifically, we address the role of vibronic coupling in systems perturbed by an external laser pulse. For this purpose, we consider prototypical inorganic/organic and all-organic interfaces formed by the acceptor 2,3,5,6-tetrafluoro-7,7,8,8-tetracyano-quinodimethane (F4TCNQ) by doping a hydrogenated silicon cluster and an oligothiophene molecule. From the analysis of charge distribution across the interface, of the induced electron density, and of the bond length dynamics, we demonstrate that the nature and amount of charge transfer results from a complex interplay between coupled electronic and vibrational degrees of freedom, which is crucially dependent on the material composition.

Invited Talk O 120.3 Fri 11:15 TRE Ma

Dynamic non-linear multi-frequency analysis: investigating the electron-transfer theory — •Fabio La Mantia — Universität Bremen, Energiespeicher- und Energiewandlersysteme, Bibliothekstr. 1, 28359 Bremen, Germany

The possibility to study and analyze the frequency response of electrochemical systems in dynamic conditions has shown the powerful advantage over classic electrochemical impedance spectroscopy (EIS) to be not limited only to stable systems. This is achieved by superimposing to a slow changing perturbation (dc) a broadband multi-sine perturbation (ac), which can cover several decades of frequency. However, typically the design of the multi-sine allows recovering and collecting only the first order frequency responses, typically named dynamic impedance spectra, for example through fast Fourier-transform EIS (FFT-EIS) or dynamic multi-frequency analysis (DMFA). In doing so, the information on the temporal asymmetry of the electrochemical reaction, carried by the intermodulation between any two frequencies of the multi-sine, is lost and cannot be recovered. In this work, after defining the concept of dynamic intermodulation, the multi-sine perturbation signal is redesigned in order to allow recovering and analyzing it. Non-linear dynamic multi-frequency analysis (NL-DMFA) will be used for investigating the electron transfer reaction to a redox couple in solution. The dynamic impedance and intermodulation spectra will be used in order to extract information on the dependence of the symmetry coefficient on the electrode's potential and its correlation to the Marcus theory of electron transfer.

O 120.4 Fri 11:45 TRE Ma

New spectroscopical tools for single-molecule junctions — •Albert Aragonès[1], Ismael Díez-Pérez[2], and Katrin Domke[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Department of Chemistry, Faculty of Natural & Mathematical Sciences, London, UK

Biological charge transport (CT) is the key step in many basic cellular processes such as respiration or photosynthesis and nature has developed highly specialized molecular building blocks to achieve it with unprecedented efficiency. Understanding the mechanisms behind biological CT is key to elucidate the changes in its regimes caused by specific structural variations of the associated molecular machinery. Such knowledge will ultimately lead us to tailor its electrical properties and exploit them as high performance bioelectronic devices with a wide variety of applications in organic electronics, sensing, biomanufacturing etc.

To investigate CT in single-molecule bioelectronic devices, we exploit Scanning Tunnelling Microscopy-based approaches in the break-junction mode (STM-BJ) under electrochemical control (EC-STM). It allows the trapping of individual molecules in a junction to characterize their main electrical signatures. This contribution will present novel light-induced tunneling transport studies carried out with Azurines molecules (blue copper proteins) under electrochemical control. Evident effects over the electron transport mechanism have been demonstrated due employing laser illumination in resonance with the "Ligand-to-Metal Charge Transfer" transition of the Azurine.

O 120.5 Fri 12:00 TRE Ma

Charge transfer and the hydrogen evolution reaction on Pt: bridging timescales from femto- to milliseconds by ultrafast electrochemical and optical measurements — •Gregor Zwaschka[1], Yujin Tong[1,2], Martin Wolf[1], and Kramer Campen[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin — [2]Universität Duisburg-Essen, Fakultät für Physik, Lotharstr. 1, 47057 Duisburg

Despite decades of study, the mechanism of the hydrogen evolution reaction (HER) on the best available catalyst, Pt, remains controversial. At least in part, understanding is complicated by the necessity to describe processes with timescales ranging from femtoseconds (interfacial charge transfer) to milliseconds (mass transport). We approach this problem by performing perturbation experiments with ultrashort laser pulses that drive the HER close to its reversible potential and induce charge transfer along the Pt-H bond in the underpotential deposition region. We disentangle the involved timescales by performing both i) time averaged electrochemical measurements under femtosecond laser irradiation and ii) time resolved sum frequency generation spectroscopy (SFS) of Pt-H after laser excitation. Ultrafast charge transfer is found to be a function of interfacial structure (electrode and electrolyte). Trends on single crystals and a microelectrode correlate with HER activity and allow insight into the reactions rate determining step. SFS provides information on Pt-H as a function of potential, electrolyte composition and temporal evolution during and after ultrafast charge transfer. Implications for the HER are discussed.

O 120.6 Fri 12:15 TRE Ma

Real-time first-principles simulations of excitation dynamics in organic systems — •Jannis Krumland[1], Ana M. Valencia[1], Stefano Pittalis[2], Carlo A. Rozzi[2], and Caterina Cocchi[1] — [1]Humboldt-Universität zu Berlin, Germany — [2]CNR-NANO Modena, Italy

Recently, the importance of vibronic coupling in the ultrafast dynamics following a photo-excitation in organic molecules has become more and more appreciated, e.g. in the context of charge transfer in photovoltaics. Gaining a deeper understanding of these processes is paramount to fully exploit their technological potential.

Towards a comprehensive description of the excitation dynamics in organic light-absorbing systems, we employ real-time time-dependent density functional theory, which provides a quantum-mechanical description of electron dynamics, coupled to the Ehrenfest scheme for classical molecular dynamics. The ultrafast pulse is explicitly included as a time-dependent external field, while solvents and substrates are modeled implicitly as polarizable continua. Considering ethylene, thiophene, and benzene molecules as building blocks of complex molecular systems, we demonstrate and rationalize the strong interplay between electronic excitations and coupled vibrational modes. The results obtained in such small compounds confirm the prominent role of vibronic coupling in the ultrafast dynamics of molecules.

Invited Talk O 120.7 Fri 12:30 TRE Ma

Resolving Chemical Bond Dynamics at an Electrode Surface — •Tanja Cuk — University of Colorado, Boulder, Boulder USA

Catalytic mechanisms at electrode surfaces guide the development of electrochemically-controlled energy storing reactions and chemical synthesis. The intermediate steps of these mechanisms are challenging to identify in real time, but are critical to understanding the speed, stability, and selectivity of product evolution. In my group, we employ photo-triggered vibrational and electronic spectroscopy to time-resolve the catalytic cycle at a surface, identifying meta-stable intermediates and critical transition states which connect one to another. The talk will focus on the highly selective water oxidation reaction at the semiconductor (SrTiO3)-aqueous interface, triggered by an ultrafast light pulse in an electrochemical cell. Here, I will describe the dynamics from the birth of the initial intermediates that trap charge (Ti-O* and Ti-O*-Ti) through the next event, suggested to be the formation of the first O-O bond of O2 evolution. The dynamics of charge screening at the interface, a hallmark of electrochemically controlled reactions, will be addressed in both aqueous and non-aqueous (battery) electrolytes. While many open questions remain, these experiments provide and benchmark the opportunity to quantify intermediates at an electrode surface and their associated dynamics.

O 121: Solid-Liquid Interface IV: Structure and Spectroscopy

Time: Friday 10:30–13:30 Location: TRE Phy

O 121.1 Fri 10:30 TRE Phy

Implementation of a high-pressure cell in a UHV setup — •Jiri Pavelec, Florian Kraushofer, Francesca Mirabella, Jian Xu, Manuel Ulreich, Michael Schmid, Ulrike Diebold, and Gareth S. Parkinson — Institut of Applied Physics, Vienna University of Technology, Austria

The importance of bridging the pressure gap in studies of model catalysts has been recognized for decades. Here we will discuss a novel design for a high-pressure cell that allows us to study reactions occurring on UHV-prepared metal-oxide single-crystal samples at pressures up to 1 bar and temperatures up to 500 °C. In our setup, only the sample surface and the inner surface of a quartz tube are exposed to the gas at elevated temperature, which minimizes contamination. The maximum operational temperature is currently limited by quartz purity. Case studies of the Fe$_3$O$_4$(001) surface exposed to water vapour [1] and the oxidation of reduced rutile TiO$_2$ will be presented.

[1] Kraushofer, Mirabella, Xu, Pavelec, Balajka, Müllner, Resch, Jakub, Hulva, Meier, Schmid, Diebold, and Parkinson; "Self-limited growth of an oxyhydroxide phase at the Fe3O4(001) surface in liquid and ambient pressure water." Chem. Phys. 151: 154702 (2019)

O 121.2 Fri 10:45 TRE Phy

Wet-chemically prepared porphyrin-layers on rutile TiO$_2$(110) — •Daniel Wechsler[1], Cynthia Carolina Fernández[2], Julia Köbl[1], Hans-Peter Steinrück[1], Federico José Williams[2], and Ole Lytken[1] — [1]Chair of Physical Chemistry II, University Erlangen-Nürnberg, 91058 Erlangen, Egerlandstraße 3, Germany — [2]Department of Inorganic, Analytical and Physical Chemistry, University of Buenos Aires, Buenos Aires C1428EHA, Argentina

Porphyrins are large organic molecules that are interesting for different applications like photovoltaic cells, gas sensors or in catalysis. For many of these applications the interactions between adsorbed molecules and surfaces play a crucial role.

Recent surface science publications focused mainly on systems that were prepared by standard ultra-high vacuum (UHV) procedures, like sputtering, annealing and physical vapor deposition. This results in well-defined and impurity-free samples but neglects effects arising from the interaction with solutions or air occurring during a preparation process outside of UHV.

In this study, we present a way to wet-chemically prepare porphyrin layers on rutile TiO$_2$(110) surfaces in a reproducible way while keeping the amount of impurities at a minimum. X-ray photoelectron spectroscopy measurements show the differences between in-solution and pure UHV prepared samples.

The project is supported by the DFG through FOR 1878 (funCOS).

Invited Talk O 121.3 Fri 11:00 TRE Phy

Photoelectron spectroscopy at liquid/solid interfaces — •Hendrik Bluhm — Fritz Haber Institute of the Max Planck Society, Berlin

Solid/liquid interfaces are ubiquitous in technological applications and the environment and govern numerous important phenomena, including corrosion, electroplating, and weathering of rocks. A detailed understanding of these processes requires the investigation of solid/liquid interfaces with chemical sensitivity and interface specificity under operating conditions. Ambient pressure X-ray photoelectron spectroscopy is an excellent method to probe the heterogeneous chemistry of these interfaces, and provides in addition the opportunity to measure the local potentials simultaneously with the chemical composition through the observation of shifts in the kinetic energy of the photoelectrons, which serve as a non-contact probe. The challenge for photoelectron experiments on solid/liquid interfaces under ambient conditions is not only the elevated pressure at which these experiments have to be carried out, but equally so the preparation of well controlled samples with high cleanliness and reproducibility. This talk shows examples of the application of APXPS to solid/liquid interfaces and discusses some of the remaining challenges that still need to be overcome in these investigations.

O 121.4 Fri 11:30 TRE Phy

Spectroscopic Insights into Liquid Metal Solutions for Catalysis — •Haiko Wittkämper[1], Mathias Grabau[1], Sven Meisel[2], Mingjian Wu[3], Andreas Görling[2], Erdmann Spiker[3], Hans-Peter Steinrück[1], and Christian Papp[1] — [1]Chair of Physical Chemistry 2, FAU Erlangen-Nürnberg — [2]Chair of Theoretical Chemistry, FAU Erlangen-Nürnberg — [3]Chair of Micro- and Nanostructure Research, FAU Erlangen-Nürnberg

Supported catalytically active liquid metal solutions (SCALMS) are deactivation resilient and highly active dehydrogenation catalysts, based on binary transition metal Gallium alloys. The remarkable properties of these catalysts, especially their good resiliency towards deactivation, are attested to the atomic dispersion of the active transition metal in liquid Gallium nano-droplets and the dynamics at the liquid metal/gas interface. The concept was pioneered at FAU and over the recent years we published findings on PdGa, PtGa and most recently RhGa alloys. Herein we present XPS studies on macroscopic alloy droplets and model catalyst particles, including in situ heating and comparative near ambient pressure oxidation studies for Pd-, Pt- and RhGa alloys. In all cases transition metal enrichment at the surface is observed, the development during the oxidation however suggests that despite their similarity the chemical origin of the enrichment effects differ for the transition metals.

O 121.5 Fri 11:45 TRE Phy

Understanding metal dissolution at Mg/H$_2$O interfaces from first-principles modelling — •Sudarsan Surendralal, Mira Todorova, and Jörg Neugebauer — Deparment of Computational Materials Design, Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf-40237, Germany

The fundamental reaction that governs the corrosion of metals in an aqueous environment is the electrochemical dissolution reaction. Using our recently developed ab initio potentiostat scheme [1], we study the atomistic mechanism of metal dissolution at the vicinal Mg(1 2 -3 15)/water interface using density functional theory based molecular dynamics simulations under conditions of anodic polarization. Our results show water dissociation and the subsequent adsorption of OH groups at low coordinated kink sites of the electrode. This adsorption process is found to make these sites prone to dissolution. Analysis of our calculated trajectories confirms that a kink Mg atom dissolves as a divalent cation with a six-fold solvation shell. In addition, the anomalous hydrogen evolution reaction reported for anodically polarized Mg/H$_2$O interfaces is also observed. Based on our observations, we propose a reaction mechanism of Mg dissolution involving water dissociation.

[1] S. Surendralal, M. Todorova, M. W. Finnis, J. Neugebauer, *Phys. Rev. Lett.* **120**, 246801 (2018)

O 121.6 Fri 12:00 TRE Phy

Investigation of ion mobility and material transport on KBr surfaces in air in dependence of the relative humidity. — •Dominik Kirpal, Korbinian Pürckhauer, and Franz J. Giessibl — University of Regensburg

On every surface exposed to humid air a thin film of water molecules forms. The presence of water plays an important role for chemical reactions, material exchange and movement. The effect of condensed water layer, present in ambient conditions plays a significant role especially on surfaces that dissolve easily in water [1]. Surface atoms can easily diffuse into the thin water layer and, when surface conditions are favourable, they can re-attach to the surface. We collected FM-AFM images of the KBr surface in a climate-controlled glove box at various values of relative humidity. By scratching the surface with the AFM tip, we construct energetically unfavourable hills and scratch sites. We observed an exponential decay of the size of the defects and material accumulations, and from this data we determined energy barriers to dissolution and aggregation of approximately 0.9 eV [2].

[1] M. Luna, et al., Journal of Physical Chemistry A, 102.34 (1998) 6793-6800.

[2] D. Kirpal, et al. Beilstein Journal of Nanotechnology, 10.1 (2019): 2084-2093.

O 121.7 Fri 12:15 TRE Phy

Comparative AFM and STM study of the ionic liquid

[C1C1Im][Tf2N] on Au(111) from 110 K to Room Temperature — •Manuel Meusel, Matthias Lexow, Afra Gezmis, Andreas Bayer, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany

Ionic liquids (IL) have raised increased interest in surface science due to their low vapour pressure and the unique possibility to investigate liquid systems using UHV methods. For catalytic concepts involving thin layers of ionic liquids (SCILL and SILP), the understanding of the IL/solid and IL/gas interface is crucial. Therefore, we investigated the adsorption behaviour of [C1C1Im][Tf2N] deposited on Au(111) via AFM and STM from 110 K to room temperature (RT). While it was easier to obtain high sub-molecular resolution images with STM, AFM provided a more stable imaging, especially over the micrometer scale. At 110 K, we observe a closed wetting layer (WL) of anions and cations, showing up two different appearances: a striped and a hexagonal pattern. We assign these two patterns to different molecular orientations resulting in different superstructures. Around 200 K, transitions between both superstructures occur but none of them is dominant after further annealing. Even at RT the molecular ordering of the WL is still present, however the superstructures have vanished.

M.M., M.L. and H.P.S. thank the European Research Council (ERC) for financial support of this research in the context of an Advanced Investigator Grant to H.P.S (No. 693398-ILID).

O 121.8 Fri 12:30 TRE Phy

Potential and distance dependent measurements of tunneling barrier-heights at the interface of gold(111) in ionic liquids — •Marcel Lang and Rolf Schuster — Karlsruher Institut für Technologie, Deutschland

The structure of the solid-liquid interface of ionic liquids on charged surfaces depends on the cell potential. E.g. multi-layered structures are found at polarization negative of the pzc.

To investigate these structures perpendicular to an Au(111) electrode we measured the distance dependence of the tunneling current, from which we calculated the local tunneling barrier-heights in four different ionic liquids ([BMP][TFSI], [BMP][FSI], [EMIM][TFSI], [EMIM][FSI]). The measurements were performed using a STM under inertgas atmosphere operating at room temperature.

The measured tunneling barrier-heights are very low at positive potentials. At positive to moderatly negative potentials we observed an almost linear increase in tunneling barrier-height with increasing distance. At more negative potentials (<- 0.9 V vs Pt) strong variations of the tunneling barrier-heights were observed. These variations of the tunneling barrier-heights can be correlated to the local electron density, indicating the formation of up to 3 layers, consisting of alternating kation and anion enriched layers.

O 121.9 Fri 12:45 TRE Phy

Bulk ion conductivity and near surface composition of Ionic Liquid and Zwiterion Ionic Liquid based electrolyte for lithium battery applications — •Fabian Ullmann, Anna Dimitrova, and Stefan Krischok — Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, Germany

In this contribution we focus on the bulk conductivity and the near surface composition of several tertiary electrolytes, which consist of Ionic Liquid (IL), Zwitterion Ionic Liquid (ZwIL) and a Li salt. Two ILs and ZwIL are chosen: IL: 1-ethyl-3-methylimidazolium bis-(trifluoromethylsulfonyl)imide - [EMIm][Tf2N] and 1-butyl-1-methylpyrrolidinium bis-(trifluoromethylsulfonyl)imide - [Py1,4][Tf2N]; ZwIL: 3-(3-methylimidazolium-1-yl)Propane-1-sulfonate and 3-(3-vinylimidazolium-1-yl)Propane-1-sulfonate. As lithium precursor - bis(trifluoromethylsulfonyl)imide - Li[Tf2N] was used. Different Li[Tf2N]/ZwIL ratios are considered and studied. Electrochemical Impedance Spectroscopy (EIS) enables us to determine the ion conductivity of the electrolyte. The results reveal that the presence of ZwILs enhances the ion conductivity, although they itself are not ion conductive. Further, by using X-Ray Photoelectron Spectroscopy (XPS) we analyze the near surface chemical composition at UHV-conditions. The XPS analysis displays a cation/anion/ZwIL distribution as depended on the concentration of Na[Tf2N] and the type of IL and ZwIL used. The spectroscopic results revealed solute-solvent interactions which modify the ion mobility.

O 121.10 Fri 13:00 TRE Phy

Bulk ion conductivity and near surface composition of Ionic Liquid and Zwitterion Ionic Liquid based electrolyte for sodium battery applications — •Thimo Brendel, Anna Dimitrova, and Stefan Krischok — Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, Germany

With this contribution we discuss the bulk ion conductivity, as well as the near surface chemical composition of ternary electrolytes containing Ionic Liquid (IL), sodium salt and Zwitterion Ionic Liquids (ZwIL). Two ILs and ZwIL are chosen: IL: 1-ethyl-3-methylimidazolium bis-(trifluoromethylsulfonyl)imide - [EMIm][Tf2N] and 1-butyl-1-methylpyrrolidinium bis-(trifluoromethylsulfonyl)imide - [Py1,4][Tf2N]; ZwIL: 3-(3-methylimidazolium-1-yl)Propane-1-sulfonate and 3-(3-vinylimidazolium-1-yl)Propane-1-sulfonate. As sodium precursor - bis(trifluoromethylsulfonyl) imide ([Na][Tf2N] was used. Different Na[Tf2N]/ZwIL ratios are considered and studied. By using Electrochemical Impedance Spectroscopy (EIS) and X-Ray Photoelectron Spectroscopy (XPS) we were able to measure the ion conductivity of the electrolytes in the temperature range 263K-323K and to determine the near surface chemical composition at UHV-conditions. The EIS results reveal that the presence of ZwILs enhances the ion conductivity, although they itself are not ion conductive. This implies to an ion decoupling in the other two electrolyte components. The XPS analysis displays a cation/anion/ZwIL (cation: [Py1,4]+, [EMIm]+, Na+; anion: [Tf2N])- distribution as depended on both: the concentration of Na[Tf2N] and the type of IL and ZwIL used.

O 121.11 Fri 13:15 TRE Phy

Temperature-dependent sticking coefficient measurements of hydrocarbons on ionic liquid surfaces using molecular beam techniques — •Leonhard Winter, Radha G. Bhuin, Matthias Lexow, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Ionic Liquids (ILs) are a class of compounds consisting only of cations and anions, which are usually liquid already below room temperature. Besides numerous other applications, IL thin films are the key components in the catalytic concepts Supported Ionic Liquid Phase (SILP) and Solid Catalyst with Ionic Liquid Layer (SCILL). These catalysts show improved behavior e.g. in hydrogenation and hydroformylation reactions. In these processes, the phase transfer of hydrocarbons through the ionic liquid/gas interface plays a crucial role.

We have built a new ultra-high vacuum apparatus dedicated for the investigations of ILs with molecular beam techniques. It was used to study the interaction of n-butane with alkylimidazolium ionic liquids with varying chain length ($[C_nC_1Im][Tf_2N]$). Based on the temperature-dependent behavior of the initial sticking coefficient at low temperatures, measured by the direct method of King and Wells, we discuss the adsorption dynamics on the different surfaces and their correlation with the molecular structure of the ILs.

L.W., R.G.B, M.L. and H.P.S. thank the European Research Council (ERC) for financial support of this research in the context of an Advanced Investigator Grant to H.P.S (No. 693398-ILID).

O 122: Topology and Symmetry Protected Materials II

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

O 122.1 Fri 10:30 WIL A317

Coupling of topologically protected edge states on the TCI (Pb,Sn)Se(001) — •Johannes Jung, Robin Boshuis, Artem Odobesko, and Matthias Bode — Physikalisches Institut, Lehrstuhl für Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074, Würzburg, Germany

In a recent publication [1] we reported on the existence of one-dimensional (1D) edge states at odd step edges of the (001) surface of the topological crystalline insulator (Pb,Sn)Se, which were found to be extraordinarily robust against high temperatures and magnetic fields. It was also observed, that the edge states vanish if two steps merge into each other. In this contribution we present a systematic STM and STS

study of converging, wedge-shaped step edges. Our results elucidate a distance-dependent coupling between adjacent 1D edge states. Three regimes with qualitatively different electronic structures are found: (i) At step–step distances larger than about 20 nm the tunneling spectrum of either step features a single peak at the Dirac point, which—within our signal-to-noise level—is indistinguishable from individual 1D edge state. In contrast, (ii) wherever the inter-step distance decreases below this value, we observe a splitting into a double peak. (iii) As the distance decreases below a critical limit of about 5 to 10 nm, the double peak vanishes and the 2D surface spectra remains. The results will be discussed in terms of the crystal structure and the symmetry at odd step edges.
[1] P. Sessi *et al.*, Science **354**, 1269 (2016).

O 122.2 Fri 10:45 WIL A317

Topological transport quantization by dissipation in fast Thouless pumps — •Zlata Fedorova, Haixin Qiu, Stefan Linden, and Johann Kroha — Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität Bonn, Nussallee 12, 53115 Bonn, Germany.

Quantized particle pumping in a slowly varying one-dimensional potential has played a prominent role in the development of topology as a concept in condensed matter physics. In the adiabatic regime, the net particle transfer per pumping cycle is an integer given by the Chern number, i.e., a topological invariant, and therefore is robust against topology-preserving perturbations. However, at finite driving frequencies the system becomes topologically trivial due to the coupling between forward- and backward-propagating states. As a result, the particle transport deviates from perfect quantization, which poses a problem for the experimental observation of Thouless pumping. Here, on the example of the driven Rice-Mele model we introduce time-periodic modulation of dissipation as a new concept to overcome this problem. The basic idea is to selectively suppress transport in one direction, while allowing it in another by making use of the distinct spatial and temporal amplitude distributions of the eigenstates moving in the corresponding directions. Restoration of quantized pumping under such periodic losses is confirmed by the Floquet analysis and by the experiments based on plasmonic waveguide arrays.

O 122.3 Fri 11:00 WIL A317

First-principles investigation of strained Weyl semimetals — •Yangjun Lee[1,2,3] and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

A Weyl semimetal is characterized by pairs of Weyl points, which are topologically protected band degeneracies. Weyl semimetals host interesting phenomena such as Fermi arc surface states and chiral anomaly. There have been fascinating theoretical studies on strained Weyl semimetals, e.g., Refs. [1-3]. In this talk, we present the results of our first-principles calculations on the electronic structure of strained Weyl semimetals. From these results, we provide some of the relevant materials parameters related to the electron-phonon coupling in Weyl semimetals.

[1] Cortijo, Alberto, et al, Physical Review B 94.24 (2016): 241405. [2] Arjona, Vicente, and María AH Vozmediano, Physical Review B 97.20 (2018): 201404. [3] Chernodub, M. N., and María AH Vozmediano, arXiv preprint arXiv:1904.09113 (2019).

O 122.4 Fri 11:15 WIL A317

Dichroic spin- and angle-resolved soft X-ray photoemission on a Weyl semimetal TaAs — •Maximilian Ünzelmann[1], Tim Figgemeier[1], Philipp Eck[2], Matthias Kalläne[3], Kai Rossnagel[3,4], Domenico Di Sante[2], Giorgio Sangiovanni[2], Hendrik Bentmann[1], and Friedrich Reinert[1] — [1]Experimentelle Physik 7, Universität Würzburg — [2]Theoretische Physik 1, Universität Würzburg — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — [4]Deutsches Elektronen-Synchrotron DESY

The interplay of inversion symmetry breaking (ISB) and spin-orbit coupling (SOC) lifts the spin degeneracy of electronic states in solids. In Weyl semimetals (WSM) structural ISB leads to spin-splittings in their bulk band structure, a key requirement for the formation of topologically protected Weyl points. Here we use angle-resolved soft x-ray photoemission to study the bulk electronic structure of the paradigmatic WSM TaAs. By means of spin-resolved measurements, we directly demonstrate the expected spin-splitting of the bulk bands. Moreover, circular dichroic measurements are in excellent agreement with the calculated momentum dependent orbital angular momentum (OAM). In contrast to spin angular momentum (SAM), OAM shows a parallel alignment in the spin-split states. This behavior is expected in materials where the characteristic energy scale of the ISB dominates over SOC [1,2].

[1] V. Sunko et al., Nature 549, 492 (2017), [2] J.-H. Park et al., Phys. Rev. B 85, 195401 (2012)

O 122.5 Fri 11:30 WIL A317

Terahertz driven nonequilibrium dynamics of Dirac fermions in Cd$_3$As$_2$ — •Semyon Germanskiy, Chris Reinhoffer, Paul H. M. van Loosdrecht, and Zhe Wang — Institute of Physics II, University of Cologne, 50937 Cologne, Germany

Cd$_3$As$_2$ is a well-established three-dimensional Dirac semimetal material with intriguing non-linear and nonequilibrium dynamical properties. By using intense terahertz pump pulses, we study the driven dynamics of Dirac fermions in Cd$_3$As$_2$ with various probe techniques. Particularly, we observe a very efficient generation of terahertz high-order harmonics, which reflects the unconventional nonequilibrium dynamical properties and is associated with the characteristic linear dispersion relation of the Dirac fermions.

O 122.6 Fri 11:45 WIL A317

Fermi arc transport in nanowires of Dirac and Weyl semimetals — •Pavlo Sukhachov[1], Mykhailo Rakov[2], Olena Teslyk[3], and Eduard Gorbar[3,4] — [1]Nordita, KTH Royal Institute of Technology and Stockholm University, Roslagstullsbacken 23, SE-106 91 Stockholm, Sweden — [2]Institut für Mathematische Physik, Technische Universität Braunschweig, Mendelssohnstraße 3, 38106 Braunschweig, Germany — [3]Faculty of Physics, Kyiv National Taras Shevchenko University, 64/13 Volodymyrska st., 01601 Kyiv, Ukraine — [4]Bogolyubov Institute for Theoretical Physics, 03680 Kyiv, Ukraine

The electron states and transport properties in cylinder nanowires of topological Dirac and Weyl semimetals are investigated. The presence of the Fermi arc surface states makes the electric charge and current density distributions in nanowires strongly nonuniform. By using the Kubo linear response approach, both direct and alternating current conductivities are calculated and it is found that their spatial profiles are nontrivial. By explicitly separating the contributions of the surface and bulk states, it is shown that when the electric chemical potential is small, the conductivity is determined primarily by the Fermi arcs and is much higher at the surface than in the bulk of the wire. Due to the rise of the surface-bulk transition rate, the relative contribution of the surface states to the total conductivity gradually diminishes with the increase of the chemical potential and the frequency. A nontrivial spatial profile of the conductivity in the case of the alternating current response might allow for a novel Fermi arc skin effect, where the localization is significantly enhanced.

O 122.7 Fri 12:00 WIL A317

Probing non-trivial topology at Weyl nodes by dichroic photoemission — •Hendrik Bentmann[1], Maximilian Ünzelmann[1], Tim Figgemeier[1], Philipp Eck[2], Chul Hee Min[3], Jeniffer Neu[4], Theo Siegrist[4], Domenico Di Sante[2], Giorgio Sangiovanni[2], and Friedrich Reinert[1] — [1]Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [2]Theoretische Physik I and and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — [4]National High Magnetic Field Laboratory, Tallahassee, USA

Weyl nodes are topologically protected intersections between non-degenerate bands and constitute the defining feature of Weyl semimetals. At these special points in momentum space the Bloch wave functions show a special behavior: in the bulk the Weyl nodes constitute monopoles of Berry flux and at the surface their projections define the termination points of Fermi-arc surface states. In this contribution we discuss how these effects can be addressed experimentally by use of dichroic angle-resolved photoemission spectroscopy (ARPES). In particular, we have studied the Weyl semimetal TaAs by VUV and soft X-ray ARPES to probe the surface and bulk electronic structure, respectively. Analyzing the linear and circular dichroism in comparison to first-principles calculations we observe direct indications of the topological behavior at the Weyl nodes [1]. [1] C. H. Min, HB, et al., Phys. Rev. Lett. 122, 116402 (2019).

O 122.8 Fri 12:15 WIL A317

Experimental observation and spin texture of a Dirac node arc in tetradymite topological metals — •Ji Dai[1,2], Emmanouil Frantzeskakis[1], Kuan-Wen Chen[3,4], Franck Fortuna[1], Taichi Okuda[5], François Bertran[6], Julien Rault[6], Patrick Le Fèvre[6], Ryan Baumbach[3,4], and Andrés Felipe Santander-Syro[1] — [1]CSNSM, Université Paris-Sud, Orsay, France — [2]Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland — [3]National High Magnetic Field Laboratory, Florida State University, USA — [4]Department of Physics, Florida State University, USA — [5]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hrioshima, Japan — [6]Synchrotron SOLEIL, Gif-sur-Yvette, France

Topological metals of the tetradymite family M_2Te_2X (with M=Ti, Zr or Hf and X=P or As) have been recently proposed to possess multiple Dirac cones, different topological characteristics and a Dirac node arc [1-4]. Here we use spin- and angle-resolved photoemission spectroscopy to directly probe the electronic dispersion and -for the first time- the spin texture of the topological surface states in Hf_2Te_2P and Ti_2Te_2P. Our results confirm a persistent spin polarization of these states along a high symmetry direction of the Brillouin zone, thereby establishing the presence of a Dirac node arc, regardless of the weak (Hf_2Te_2P) or strong (Ti_2Te_2P) character of the topological invariant.

[1] H. Ji, et al., Physical Review B **93**, 045315 (2016).

[2] K.-W. Chen, et al., Physical Review B **97**, 165112 (2018).

[3] M. M. Hosen, et al., Nature Communication **9**, 3002 (2018).

O 122.9 Fri 12:30 WIL A317

Unconventional Surface Conductivity in Correlated Honeycomb Transition Metal Oxide Mott Insulators — •Thomas Dziuba[1], Máté Stark[1], Ina Pietsch[2], Philipp Gegenwart[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Lehrstuhl für Experimentalphysik VI, Zentrum für Elektronische Korrelationen und Experimentalphysik, Universität Augsburg, Germany

The correlated honeycomb transition metal oxides attract large attention for the theoretical prospect of topological non-triviality as well as being a possible realization of the magnetic Kitaev exchange model. The Mott insulating sodium iridate Na_2IrO_3 is prototypical among these materials with the promising prospect to bridge the field of strongly correlated systems with topology [1]. By using home-built STM and STS combined with macroscopic conductivity measurements of freshly cleaved Na_2IrO_3 surfaces in UHV we measure the properties provided by the sample surface. We report on the rather unconventional linear-dispersion in-gap conductivity found by tunneling spectroscopy. The addressability of such states strongly depends on the electronic properties of the probe and local surface structures. We will further discuss the found conductivity of the Na_2IrO_3 surface in the light of macroscopic measurements, complementing previous (bulk) results [2].

References

[1] Phys. Rev. B 91, 041405(R) (2015)

[2] Phys. Rev. B 82, 064412 (2010)

O 122.10 Fri 12:45 WIL A317

MBE Growth of 3D Topological Insulators on Sapphire — •Christoph Ringkamp, Gregor Mussler, and Detlev Grützmacher — PGI-9, Forschungszentrum Jülich & JARA Jülich-Aachen Research Alliance, Germany

Topological insulators (TI) possess topologically protected, conducting surface states, which are predicted to show Majorana signatures in conjunction with superconductors (SC). A prerequisite for this is a high transparency between the TI and the SC, and that is why an in-situ fabrication of the TI/SC heterostructures is crucial. On Si(111) substrates, we have already established the selective area growth and a shadow mask technique to fabricate such heterostructures via molecular-beam epitaxy (MBE) [1]. However, one major problem in transport experiments still poses the impact of the Si substrate, as the Si/TI interface may serve as an additional conducting channel. Hence, we intend to grow the TI/SC heterostructures on sapphire, as it is a purely insulating substrate which may allow to investigate the topological properties of the TI films in transport experiments in more detail.

I will report on the MBE growth of Bi2Te3, Bi2Se3, Sb2Te3 and its alloys on sapphire substrates, and I will show a substantial reduction of crystal defects in the TI films on sapphire compared to Si(111). Furthermore, I will present first results of selective area growth of TIs on sapphire, using a combination of lithographically defined SiO2 and Si3N4 structures as a growth mask.

[1] Schüffelgen et al., Nature Nanotechnology 14, 825 (2019)

O 123: Nanostructured Surfaces and Thin Films III: Dots, Particles, Clusters (joint session O/CPP)

Time: Friday 10:30–13:00 Location: WIL B321

O 123.1 Fri 10:30 WIL B321

Reconfigurable Polaritonics using Phase Change Materials — •Christina M. Spägele[1], Xinghui Yin[1], Michele Tamagnone[1], Kundan Chaudhary[1], Stefano L. Oscurato[1,2], Jiahan Li[3], Christoph Persch[4], Ruoping Li[1], Noah A. Rubin[1], Luis A. Jauregui[5], Kenji Watanabe[6], Takashi Taniguchi[6], Philip Kim[1], Matthias Wuttig[4], James H. Edgar[3], Antonio Ambrosio[1,7], and Federico Capasso[1] — [1]Harvard University, USA — [2]Unina, Italy — [3]KSU, USA — [4]RWTH, Germany — [5]UCLA, USA — [6]NIMS, Japan — [7]CNST-IIT, Italy

Polaritons garnered significant interest due to their ability of confining light to the nanoscale. They arise when light couples strongly to material excitations such as excitons, plasmons or phonons. To date, methods to control these highly confined states of light are not well-suited for free-form manipulation of polaritons. Moreover, they create systems that are unalterable after the initial fabrication process.

Placing the hyperbolic vdW-material hexagonal boron nitride on the phase change material (PCM) Ge3Sb2Te6, we successfully achieved spatial control of the propagation of surface phonon polaritons (SPhP) by structuring the PCM. The exponentially decaying tail of the guided SPhP modes interacts with the PCM, which can be optically switched to a higher refractive index crystalline phase, slowing the SPhP. We demonstrate rewritable waveguides and refractive optical elements such as lenses and prisms for mid-IR polaritons. Moreover, we will discuss reconfigurable metalenses that allow for precise wavefront engineering and diffraction-limited focusing.

O 123.2 Fri 10:45 WIL B321

Synthesis of 3D ZnO nanostructures on different substrates for gas sensor applications — Hanaa Seso, Stefan Ostendorp, •Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, Westfälische-Wilhelms-Universität, Wilhelm-Klemm-Str.10, 48149 Münster, Germany

Three-dimensional (3D) ZnO nanostructures have been synthesized via atomic layer deposition (ALD) on different types of templates to act as a gas sensing active material. The used template structures range from anodic aluminum oxide (AAO) template synthesized by a two-step anodization method, a polymer template prepared by infiltration of a polymer solution into an AAO structure to a porous gold template fabricated by de-alloying of an Au-Ag solid solution. The morphology of the templates and the nanostructured ZnO-based carbon monoxide (CO) sensors were investigated by scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray diffraction (XRD) and transmission electron microscopy (TEM). The gas-sensing performance of sensors based on the different templates was measured successfully in terms of electrical response to detect CO as a hazardous gas. The tremendously increased surface to volume ratio of ZnO on an AAO (alike) template or porous gold template is thereby supposed to provide an enhanced sensing capability compared to 2D thin film or bulk sensor structures.

O 123.3 Fri 11:00 WIL B321

Thinking inside the box: Quantum corrals as artificial atoms and molecules — •Saoirse Freeney, Jaap Harteveld, Sam Borman, and Ingmar Swart — Utrecht University, Utrecht, Netherlands

The electronic behaviour that underlies the field of chemistry is essentially a result of the confining potential of an atom's nucleus on its electrons. Due to their confinement, the allowed energies that electrons can take in an atom are quantised, and their wavefunctions are well-defined . If we were to create our own potential that confines electrons within, we could emulate real atoms and change their properties at will. In fact, a quantum corral is exactly this. To create one, adsorbates on a metal surface are accurately manipulated with an STM tip to predetermined positions. Much like a particle-in-a-box, the surface state electrons are then confined, exhibiting discrete energy levels analogous to an atom. We can liken the measured wavefunctions to those of s, p, d etc orbitals in an atom. Beyond this, we can pair two quantum corrals together and observe that bonding and antibonding orbitals arise. Here, we use CO molecules to scatter the Cu(111) surface state and investigate the relation of size and shape on the energy and wavefunction, and secondly we tailor the strength of coupling in "molecular" quantum corrals. Several artificial lattices have been made before with the CO/Cu(111) platform. The information presented is useful for designing such lattices.

O 123.4 Fri 11:15 WIL B321

Ordered structures with functional units from artificial alumina membranes — •Wenxin Wang — Photonic Materials Group, College of Physics and Optoelectronic Engineering, Harbin Engineering University,15001 Harbin, China

Constructing ordered structures with functional units (OSFU) gives opportunities to improve, modify intrinsic performances of ordered structures, even render novel properties. Here I report an approach to realize OSFU through artificial alumina membranes (AAMs), single and multi-order structure(s) are functionalized with plasmonic and (or) smart polymer unit to check their mesoscopic optical behaviors. For instance, AAMs are directly used as OSFU to achieve structural color imaging with high reflectivity. Second, functionalize units with plasmonic materials to obtain enhanced local field and resonance modes hybridization, in order to manipulate the linear and nonlinear optical performances. Third, functionalize units with polymer to realize reversible structures for dynamic optical modulation. Finally, multi-order OSFU is designed by inducing diverse lattice arrangements for photonic band engineering. The second-order elements are embedded on special points that corresponding high symmetry points in k-space that will arise Dirac cone and flat band.

O 123.5 Fri 11:30 WIL B321

Comsol modeling of the role of nanostructured current collectors in supercapacitor — •Maximilian Kaupenjohann, Long Liu, Huaping Zhao, and Yong Lei — Technische Universität Ilmenau, 98393, Ilmenau, Germany

Current collector is an important component in supercapacitors and its main role is to transport charge carriers from/to electroactive materials during the charge-discharge process. The charge transport efficiency is believed to be dominated by the resistance at the electroactive-material/current-collector interfaces. Owing to the large specific surface area, nanostructured current collectors have been designed, fabricated, and investigated intensively for supercapacitors. Especially for pseudocapacitive materials that have theoretically high specific capacitance but intrinsically low electric conductivity, nanostructured current collectors enable one to achieve a much higher specific capacitance even nearly reach the theoretical value. The improved performance is generally attributed to the improved electrical and ionic transport kinetics endowed by nanostructured current collectors. In this work, the role of nanostructured current collectors in supercapacitor electrode is further identified by using COMSOL Multiphysics simulations in combination with the experiment results.

O 123.6 Fri 11:45 WIL B321

Global Optimization of Copper Clusters on ZnO Surfaces Utilizing a Neural Network Potential — •Martín Leandro Paleico and Jörg Behler — Universität Göttingen, Theoretische Chemie, Tammannstr. 6, 37077 Göttingen, Germany

The catalyst used in the industrial synthesis of methanol is composed of large copper and zinc oxide nanoparticles. Studying the structure of this system requires a simulation method capable of handling thousands of atoms with ab initio accuracy, but with computational efficiency comparable to classical empirical potentials. To meet these requirements, a Neural Network Potential (NNP) has been trained to reproduce the potential energy surface of the system based on DFT reference calculations.

We have utilized this potential to carry out the tens of thousands of energy and force evaluations required to perform global optimization searches employing genetic algorithms. With this, we are able to optimize pure copper and binary copper-zinc clusters with up to 30 atoms on two different zinc oxide surfaces. This allows us to investigate structural and energetical trends in cluster growth and cluster-substrate interactions, as well as to identify possible active sites and their distribution in the clusters.

O 123.7 Fri 12:00 WIL B321

Deposition and annealing of Fe$_x$Ni$_{1-x}$ nanoparticles on a W(110) surface — •Mahboobeh Ravankhah, Dennis Jagenburg, and Mathias Getzlaff — Institute of Applied Physics, University Düsseldorf

3d bimetallic nanoparticles have received lots of attention because of their technological application. In comparison to pure Fe and Ni, alloys of Fe$_x$Ni$_{1-x}$ have much more complex structural phases under different conditions. Different FeNi alloys are used: Fe$_{0.50}$Ni$_{0.50}$, Fe$_{0.25}$Ni$_{0.75}$ and Fe$_{0.75}$Ni$_{0.25}$. All nanoparticles are prepared by a magnetron sputtering source under UHV condition on a W(110) surface, therefore contaminations are avoided. The deposited nanoparticles are subsequently annealed between 500-800K. Particle's size, shape and structure will be investigated by Transmission Electron Microscopy (TEM) and Scanning Tunneling Microscopy (STM). We report on the influence of different parameters like size of nanoparticles, stoichiometry and annealing temperature on the melting behavior.

O 123.8 Fri 12:15 WIL B321

Cu2+ Detection by Carbon Quantum Dots Derived from Water Hyacinth (Eichhornia crassipes) — •Eduardo Magdaluyo Jr[1], Gerald Mari Quiachon[2], and Persia Ada de Yro[2] — [1]Department of Mining, Metallurgical and Materials Engineering, University of the Philippines, 1101 Diliman, Quezon City, Philippines — [2]Materials Science Division, Industrial Technology Development Institute, Department of Science and Technology, Bicutan, Taguig, Metro Manila, Philippines

Preparation of carbon quantum dots (CQDs) was derived from water hyacinth (Eichhornia crassipes) leaves as a carbon source using facile approach of hydrothermal treatment in acidic medium. The as-synthesized CQDs exhibited coagulation in aqueous solution and a strong blue fluorescence under UV light at 365 nm. Infrared spectra analysis confirmed the presence of functional groups such as hydroxyl (OH), carboxyl (COO) and carbonyl (CO) on the surface of the CQDs. The functional groups were analyzed using zeta potential and was found to induce surface charges which allow the attraction of copper ions and bind with the CQDs. These surface charges were utilized in the application of the CQDs as a biosensor for the detection of Cu2+ ions based on ion-induced fluorescence quenching of CQDs. The photoluminescence spectra confirmed this process and it was found to have excellent affinity toward Cu2+ as the PL of CQD with copper solution was quenched relative to pure CQD solution. The highest quantum yield of the CQD sample being measured against deionized water was found to be at 6.48.

O 123.9 Fri 12:30 WIL B321

Electronic and optical properties of quantum-confined nanoparticles — •Marius Buerkle and Vladimir Svrcek — National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

We discuss the electronic and optical properties of semiconducting nanoparticles in the quantum-confinement regime. Here we focuse on how do quasi-band-like features emerge from finite electronic states with increasing particle size. This is discussed for Si, SiC, and Sn nanoparticles. Particularly interesting is the transition from an indirect to direct bandgap semiconductor for ultra-small Sn nanoparticles.

O 123.10 Fri 12:45 WIL B321

Developing a GAP machine-learned potential for iridium dioxide nanoparticles — •Jakob Timmermann, Christoph Scheurer, and Karsten Reuter — Technische Universität München

Iridium dioxide is currently the preferred material for highly active, yet chemically stable nanoparticle catalysts enabling the electrochemical oxygen evolution reaction (OER) in proton exchange membrane electrolyzers. Full ab initio molecular dynamics (MD) simulations of the reactive processes at the electrified nanoparticle surface would be highly desirable for mechanistic catalyst improvement, but are computationally not tractable for a foreseeable time. To overcome the limitations regarding system size and propagation time, MDs based on machine-learned interatomic potentials are an appealing alternative.

Here, we present a corresponding Gaussian Approximation Potential (GAP) for IrO_2 combining two-body and smooth overlap of atomic positions (SOAP) descriptors to capture the atomic environment. The potential is trained with density-functional theory (DFT) data comprising IrO_2 bulk, various surface slabs, Wulff shape nanoparticles, as well as semi-amorphous structures iteratively obtained from short MD trajectories based on the developing GAP. The final GAP is found to faithfully provide a wide range of static geometric and energetic key parameters. MD simulations based on this GAP now provide first insight into stability and special OER active sites offered by nanoparticles of varying size and shape.

O 124: Development of Novel Methods II

Time: Friday 10:30–13:30 Location: WIL C107

O 124.1 Fri 10:30 WIL C107

Michelson Interferometry with Spiral Phase Plates — •Michael Reichenspurner[1], Nicola Kerschbaumer[1], Michael Fedoruk[2], Theobald Lohmüller[1], and Jochen Feldmann[1] — [1]Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität, Königinstr. 10, 80539 Munich, Germany — [2]Vortex Photonics, Lindwurmstr. 115, 80337 Munich, Germany

Interferometry for highly accurate distance or surface profile measurements is widely applied in various fields of research and engineering. The basic principle of most interferometric approaches is that two propagating transverse beams are superimposed to generate a Newton*s rings interference pattern. Here, we demonstrate a different idea, using an optical vortex instead of a transverse beam for distance measurements in a Michelson configuration. By using a spiral phase plate, we generate a donut-shaped laser beam with helical propagation. The interference of two such helical beams, when they have opposite rotations, results in a characteristic flower shaped intensity distribution. Any phase difference introduced between these beams, either by a length difference or a change in refractive index in one of the beam paths, leads to a specific rotation of the flower pattern, which is even observable by the naked eye.

O 124.2 Fri 10:45 WIL C107

Cryogenic Single Nanoparticle Action Spectroscopy (cryo-SNAS) - A New Tool for Surface Science of Single Nanoparticles — •Tim Esser[1], Benjamin Hoffmann[2], and Knut Asmis[2] — [1]University of Oxford, Oxford, UK — [2]Universität Leipzig, Leipzig

Nanoparticles (NPs) with diameters from 10 to 100 nm have unique size and shape dependent properties due to their large surface-to-volume ratio and quantum effects. They are relevant in atmospheric and astro chemistry and applied in catalysis, energy storage, opto-electronics and bio-medicine. Their fundamental properties can be obscured in experiments that rely on averaging and interaction with surfaces or solutions. Action spectroscopy is a sensitive alternative to direct absorption spectroscopy for gas phase clusters and macroscopic surfaces, but was not previously applied to NPs due to limited sensitivity and resolution of most mass spectrometers above 1 MDa. Here we present a nanoparticle mass spectrometer which enables cryogenic single nanoparticle action spectroscopy (cryo-SNAS) for the first time. NPs from an electrospray ion source are trapped in a temperature controllable (8 to 350 K) split-ring electrode ion-trap. The mass-to-charge ratio and absolute mass of a single NP is determined non-destructively by optical means. Mass variations can then be monitored as a function of the trap temperature, pressure, laser power and wavelength.

First cryo-SNAS spectra of dye labeled SiO_2 NPs are shown followed by a discussion of future applications.

O 124.3 Fri 11:00 WIL C107

Observation of bulk electronic states with HAXPES on the heavy fermion system YbRh2Si2 — •Steinn Ymir Agustsson[1], Sergey Chernov[1], Sergey Babenkov[1], Olena Fedchenko[1], Dmitry Vasilyev[1], Katerina Medjanik[1], Christoph Schlueter[2], Andrei Gloskovskii[2], Yury Matveyev[2], Kristin Kliemt[3], Cornelius Krellner[3], Gerd Schoenhense[1], Jure Demsar[1], and Hans-Joachim Elmers[1] — [1]JGU Mainz — [2]DESY Hamburg — [3]Goethe Universität Frankfurt

The study of elastic strain induced effects on strongly correlated systems requires in situ mechanical deformations, which is best achieved with bulk single crystal samples. Observation of the electronic band structures using low energy photoemission techniques, however, requires additional surface cleaning methods, such as cleaving, which result challenging in combination with applying mechanical deformation. We demonstrate the use of hard x-ray photoemission (HAXPES) as an effective probe for observing bulk electronic band structures, overcoming the surface quality bottleneck, on the prototypical heavy fermion (HF) system YbRh2Si2. We successfully observed bulk states at the Fermi surface, probed with 5keV photons in a time-of-flight momentum microscope spectrometer at different temperatures. Our results agree with previous low energy photoemission experiments as well as with ab-initio calculations, and highlight the changes in the hybridized valence band and Yb 4f band dispersions between 25K and 300K.

O 124.4 Fri 11:15 WIL C107

In-plane and out-of-plane nanomechanical characterization of HOPG at the atomic scale — •Anna Lisa Eichhorn and Christian Dietz — TU Darmstadt

Multifrequency atomic force microscopy enables high resolution imaging of flat surfaces such as HOPG down to the atomic scale. The technique is based on the simultaneous excitation and detection of two or more cantilever eigenmodes. Depending on the type of the oscillation modes (flexural, torsional or lateral), out-of-plane elastic and dissipative sample properties or the in-plane shear behavior can be analyzed. Here, a bimodal approach was developed where the second flexural eigenmode amplitude was used for the topographical feedback. Additionally, either the first torsional or the first lateral eigenmode was excited at a constant amplitude while the frequency shift was recorded. Using the described setup atomic resolution was achieved in both imaging channels at ambient conditions, yet in the flexural topography images only every second carbon atom could be resolved, resulting in a triangular appearance. This effect is a result of the Bernal stacking of graphite monolayers, leading to two distinguishable carbon atom sites. Mapping the torsional/lateral frequency shift, however, provided a more comprehensive image, resolving the complete hexagonal arrangement of the carbon atoms. We aim to study the change in nanomechanical properties originating from single defects artificially generated within the structure by oxygen plasma treatment.

O 124.5 Fri 11:30 WIL C107

Electrospray Ion Beam Deposition as Universal Preparation Method for Electron Microscopy Imaging of Molecules on Ultrathin Supports — •Stephan Rauschenbach — Department of Chemistry, University of Oxford Mansfield Road, Oxford, UK

Recent developments in electron microscopy (EM) instrumentation, such as aberration corrected lenses and high speed, single electron detectors have enabled the observation of individual atoms and molecules at sub-angstrom resolution. This finds applications in structural biology through cryo-EM, however the imaging of many species is hindered by absence of a general sample preparation method.

Here we present soft-landing electrospray ion beam deposition (ES-IBD)as universal preparation method for single molecule imaging on ultra-thin substrates (graphene/carbon membranes) EM. We show applications ranging from native folded proteins to small, few-atom cluster species. The experiment enables structure determination based on direct imaging or averaging in the case of radiation sensitive molecules. In addition, the control of the ion beam offered in ES-IBD allows for chemical isolation of a target species and for the controlled activation in surface collision.

O 124.6 Fri 11:45 WIL C107

Developing descriptors for the prediction of adsorption energies on metal oxides — •Wenbin Xu, Mie Andersen, and Karsten Reuter — Chair for Theoretical Chemistry and Catalysis Research Center, Technical University of Munich, Garching, Germany

Linear scaling relations of adsorption energy arise at transition metal (TM) catalysts as a consequence of the adsorbate valency, together with the properties of the d electrons of the surface. Already, this linearity is only approximate, with outlier adsorption energies easily deviating from the trend by up to 1 eV. At other materials classes, deviations can be even more significant [1], calling for improved approaches that yield reliable adsorption energies at still comparably low computational cost.

To this end, we have recently demonstrated the usefulness of a compressed sensing approach for TM and TM alloy catalysts [2]. The corresponding SISSO (sure independence screening and sparsifying operator) approach [3] allows the prediction of adsorption energies from descriptors that are expressed as nonlinear functions of intrinsic properties of the clean catalyst surface (so-called primary features), e.g. coordination numbers, d-band moments, and work function. Here, we extend this approach to TM oxide catalysts and oxygen evolution catalysis. Next to establishing a systematic first-principles database for the SISSO training, a key aspect of our work is to identify primary features for this class of materials. [1] X. Hong, et al., ACS Catal., 6, 4428 (2016). [2] M. Andersen, et al., ACS Catal., 9, 2752 (2019). [3] R. Ouyang, et al., Phys. Rev. Mater., 2, 083802 (2018).

O 124.7 Fri 12:00 WIL C107

Towards an efficient sarin detector: a combined theory-experiment approach — •Hazem Aldahhak[1], Paulina Powroźnik[2], Piotr Pander[3], Fernando B. Dias[3], Wolf Gero Schmidt[1], Uwe Gerstmann[1], and Maciej Krzywiecki[2] — [1]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany — [2]Institute of Physics, Center for Science and Education, Silesian University of Technology, Gliwice, Poland — [3]Department of Physics, Durham University, South Road, Durham, DH1 3LE, United Kingdom

Detecting hazardous agents is vital for efficiently preventing their effects. A prominent example in this respect is sarin gas, one of the most toxic nerve agents. Therefore, sensing devices are required to are able to detect sarin rapidly and in extremely concentration.

Here, density-functional theory (DFT) is used to analyze the interaction of sarin with single metal-centered phthalocyanines (MPc) as well as MPc layer structures, and to identify a benign model system. The calculations show almost coincident behaviors of sarin and dimethyl methylophosphonate (DMMP) on different MPcs. Among NiPc, CuPc, CoPc and ZnPc we find the interaction of both sarin and DMMP to be strongest with ZnPc, both in terms of interaction energy and adsorption induced work function change. Zinc phthalocyanine is thus proposed as a promising sensor for sarin detection. Using X-ray photoelectron spectroscopy (XPS), the theoretically predicted charge transfer to ZnPc is confirmed for the model system DMMP and identified as a key component in the sensing mechanism.

O 124.8 Fri 12:15 WIL C107

Self-interaction correction applied to molecules in solution — •Jakob Kraus[1], Sebastian Schwalbe[1], Kai Trepte[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Germany — [2]Central Michigan University, USA

The Fermi-Löwdin orbital self-interaction correction (FLO-SIC [1]) combats the self-interaction error [2] found in common exchange-correlation functionals of density functional theory (DFT), which is otherwise known as numerically efficient and reasonably accurate. While DFT calculations assume $T = 0$ K and the gas phase, many chemical reactions happen near room temperature and in an aqueous solution, frequently leading to shifts in energies. Thus, SIC and other approaches might profit from including thermochemical corrections and solvation effects. Here, electrostatic solvation was studied by combining the conductor-like screening model (COSMO [3]) with DFT, SIC-DFT, and wavefunction methods (HF, CCSD(T)). Using the PySCF [4], PyFLOSIC [5], and ERKALE [6] codes, ionization potentials and standard enthalpies of formation were evaluated in the gas phase and in an aqueous solution.

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O 124.9 Fri 12:30 WIL C107

Reliable electrostatic energies in MPE implicit solvation — •Jakob Filser, Konstantin Jakob, Markus Sinstein, Karsten Reuter, and Harald Oberhofer — Technical University of Munich

Implicit solvation models like the multipole expansion (MPE) model [1] are widely used in first-principles calculations to incorporate solvent effects without the necessity of sampling solvent degrees of freedom. MPE divides the free energy of solvation into the electrostatic interaction between the solute and a dielectric medium, and a remaining, 'nonelectrostatic' term, fitted to experimental reference data. The medium is defined to fill all space outside a 'cavity' around the solute.

In the present work, we solve two shortcomings of the state-of-the-art treatment of electrostatic interactions in MPE: First, for larger and more complex solutes the multipole basis for the potential becomes insufficient to solve the electrostatic problem. Currently, this is partially compensated for in the nonelectrostatic energy contribution. However, an accurate solution which does not rely on such error cancellation is obviously more desirable. We achieve this by dividing space into approximately spherical domains inside each of which a multipole basis is sufficient to express arbitrary harmonic potentials.

Second, the shape of the cavity crucially influences the electrostatic interaction, but there is no unique and straightforward definition of the cavity. This can lead to a systematic error in the electrostatic interaction. As a remedy, we choose a cavity definition which – at least on average – neither over- nor underestimates this term.

[1] M. Sinstein et al., J. Chem. Theo. Comput. 13, 5582, 2018.

O 124.10 Fri 12:45 WIL C107

Boosting size convergence for slab supercell calculations of materials exhibiting spontaneous polarization — •Su-Hyun Yoo[1], Mira Todorova[1], Chris Van de Walle[2], and Jörg Neugebauer[1] — [1]Department of Computational Materials Design, Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Computational Materials Group, Materials Dept., UCSB, USA

The most common approach to describe surfaces in density-functional theory is the repeated slab geometry. A common strategy to avoid artificial charge transfer from one side of the slab to the other is to passivate the backside of the slab. Using the example of ZnO(0001) surfaces we find that conventionally used passivation schemes (e.g. pseudo H or surface reconstructions) break down for materials exhibiting internal polarization. We have therefore developed a generalized passivation method that accounts for the effect of spontaneous polarization and correctly describes the electric field limit for pyroelectric materials. It is robust and ensures quick convergence of total energies and electronic structure with respect to slab thickness as will be demonstrated using the example of wurtzite ZnO.

O 124.11 Fri 13:00 WIL C107

Theoretical study of Ln atoms in complexes and surfaces: valence electrons effect — •Stanislav Avdosheno and Alexey Popov — Leibniz Institute for Solid State and Materials Research (IFW), D-01069 Dresden, Germany

Detailed electronic structure of single atomic magnets is the most crucial bit in the further understanding and design of a new generation of monatomic functional elements on surfaces and in another structural setting. Recently, the inspirational single atomic experiment with Ho on MgO surfaces brought into a new light a possibility to control and manipulate the quantum states of an atom.[1] However, these convincing experiments are puzzling by the insufficient theoretical description. In this contribution, we looked at the exact ab initio model for the Ho atom at the MgO surface under the various levels of complexity in an attempt to resolve an experimental dilemma in the reported data. The research is based on the idea of the imminent need to implement the local d- and p-shell electrons of Ho atom into the active space for proper system consideration. By doing so, we have obtained the solution which complements experimental observations without any additional assumptions.[2]

References

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O 124.12 Fri 13:15 WIL C107

Spin-dependent electron reflection from Au(111) and single-layer MoS_2/Au(111): A comparative study — •Christoph Angrick[1], Andre Reimann[1], Nicole Mutzke[1], Moritz Ewert[2,3],

Lars Buss[2,3], Jens Falta[3], Jan Ingo Flege[2,3], and Markus Donath[1] — [1]University of Münster, Germany — [2]Brandenburg University of Technology Cottbus-Senftenberg, Germany — [3]University of Bremen, Germany

In the field of spin-integrated photoemission experiments, major parts of the occupied electronic band structure are obtained in a short time by parallel detection of electrons with different energies and/or angles. Spin-polarizing electron mirrors (spin mirrors) are added to the experimental setups to obtain spin resolution [1,2]. The concept of these spin mirrors is based on the reflection of very-low-energy electrons from targets influenced by spin-orbit or exchange interaction.

In this work, Au(111) and single-layer MoS_2/Au(111) are put to a test as scattering targets. Both are influenced by spin-orbit interaction and therefore, are possible candidates for the use as a spin mirror. Maps of the reflectivity, Sherman function and figure of merit are derived from spin-dependent very-low-energy electron reflection measurements for a wide range of incident electron polar and azimuthal angles and energies [3]. The targets are compared with respect to preparation procedure, target stability and efficiency.

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O 125: Overview Talk: Roland Wiesendanger (joint session O/CPP/DS)

Time: Friday 14:00–14:45 Location: HSZ 02

Topical Talk O 125.1 Fri 14:00 HSZ 02

Surface Science Aspects of Topological States of Matter — •Roland Wiesendanger — Universität Hamburg

Topological states of matter have raised great excitement in solid state physics in the past years, e.g. in the fields of topological insulators, topological spin textures (magnetic skyrmions), and topological superconductors hosting Majorana states. Surface and interface science plays a crucial role for all these fields, as has been demonstrated, e.g., by the discovery of ultimately small-scale skyrmions stabilized by interfacial Dzyaloshinskii-Moriya interactions [1,2] or the direct real-space observation of the emergence of Majorana states in atomic-scale magnet-superconductor hybrid systems [3,4]. In particular, the preparation of extremely clean surfaces of elemental s-wave superconductors, such as Re, Ta, La, and Nb has boosted recent studies of topological superconductivity in bottom-up constructed 1D and 2D hybrid systems, allowing for the atomic-scale design of Majorana states and a one-to-one comparison between results of theoretical toy models and experimental observations. Bringing together surface science concepts and advanced techniques for the fabrication of atomically well defined magnet-superconductor hybrid systems is a key ingredient for this exciting new research area which ultimately will allow for the realization of topological quantum computation schemes. [1] N. Romming et al., Science 341, 6146 (2013). [2] S. Heinze et al., Nature Physics 7, 713 (2011). [3] H. Kim et al., Science Advances 4, eaar5251 (2018). [4] A. Palacio-Morales et al., Science Advances 5, eaav6600 (2019).