Thin Films Division
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Overview of Invited Talks and Sessions

(Lecture rooms CHE 89 and CHE 91; Posters P2-EG and P1C)

Gaede Prize Talk

O 43.1	Tue	15:30–16:00	WIL C307	**STM-induced light emission: from molecular LED to sub-nanometric optical microscopy.** — •Guillaume Schull

Invited Talks

DS 2.1	Mon	9:30–10:00	CHE 89	**Inhomogeneities in chalcopyrites and kesterites** — •Claudia S. Schnohr
DS 2.2	Mon	10:00–10:30	CHE 89	**Impact of growth condition on defect generation in Cu(In,Ga)Se2** — •Takeaki Sakurai, Muhammad Islam, Akira Uedono, Shogo Ishizuka, Hajime Shibata, Shigeru Niki, Katsuhiro Akimoto
DS 2.4	Mon	11:00–11:30	CHE 89	**Inhomogeneities in chalcopyrites for solar cells** — •Daniel Abou-Ras
DS 2.5	Mon	11:30–12:00	CHE 89	**Understanding the defects in Cu(In,Ga)Se2 solar cell: a correlative microscopy approach** — •Oana Cojocaru-Mirédin, Torsten Schwarz, Roland Mainz, Daniel Abou-Ras
DS 12.1	Mon	15:00–15:30	CHE 89	**Defects in Chalcopyrites** — •Susanne Siebentritt
DS 20.1	Tue	9:30–10:00	CHE 89	**Driving nanophotonics to the atomic scale** — •Javier Aizpurua
DS 20.2	Tue	10:00–10:30	CHE 89	**Transverse and Longitudinal Resonances in Plasmonic Gold Tapers** — Surong Guo, Nahid Talebi, Wilfried Sigle, Ralf Vogelgesang, Gunther Richter, Martin Esmann, Simon F. Becker, Christoph Lienau, •Peter A. van Aken
DS 20.3	Tue	10:30–11:00	CHE 89	**Nanoimaging and control of polaritons in 2D materials** — •Rainer Hillenbrand
DS 20.4	Tue	11:15–11:45	CHE 89	**Switchable infrared nanophotonic elements enabled by phase-change materials** — •Thomas Taubner
DS 20.5	Tue	11:45–12:15	CHE 89	**Nonlocal response in plasmonic nanoparticles: How much quantum?** — •N. Asger Mortensen
DS 20.6	Tue	12:15–12:45	CHE 89	**Short-range plasmonics** — •Harald Giessen
DS 28.1	Wed	9:30–10:00	CHE 89	**Self-consistent hybrid functional calculations: Electronic and optical properties of oxide semiconductors** — •Daniel Fritsch, Benjamin Morgan, Aron Walsh
DS 28.6	Wed	11:15–11:45	CHE 89	**Exceptional Points in Oxide Bulk and Metamaterials** — •Marius Grundmann
DS 28.8	Wed	12:00–12:30	CHE 89	**Kinetics and thermodynamcis of binary and ternary oxides during molecular beam epitaxy** — •Patrick Vogt, Oliver Bierwagen
DS 32.1	Wed	14:45–15:15	CHE 89	**Defect induced magnetic or optical properties in gallium-based oxides** — •Laurent Binet, Didier Gourier
DS 32.3	Wed	15:30–16:00	CHE 89	**Vacancy defects and electrical compensation in gallium oxide** — •Filip Tuomisto
DS 32.5	Wed	16:30–17:00	CHE 89	**Integration of Oxide Semiconductors with Traditional Semiconductors - A New Twist** — •Scott Chambers

DS 38.1	Thu	9:30–10:00	CHE 89	**Memristive devices for neuromorphic systems** — •Martin Ziegler
DS 38.2	Thu	10:00–10:30	CHE 89	**Learning in Silico: neuromorphic models of long-term plasticity** — •Elisabetta Chicca
DS 38.6	Thu	11:30–12:00	CHE 89	**Design and CMOS Co-Integration of ReRAM Devices and Crossbar Arrays for Neuromorphic Applications** — •Yusuf Leblebici
DS 38.7	Thu	12:00–12:30	CHE 89	**Neuromorphic Memristive Systems** — •Bernabe Linares-Barranco
DS 40.1	Thu	15:00–15:30	CHE 89	**Brain-inspired neurocomputing with memristive synapses** — •Daniele Ielmini
DS 40.2	Thu	15:30–16:00	CHE 89	**Exploring evolutionary biology and neuromorphic computing with quantum materials** — •Shriram Ramanathan

Invited talks of the joint symposium SYCE

See SYCE for the full program of the symposium.

SYCE 1.1	Mon	15:00–15:30	HSZ 02	**Ferroelectric domain walls: from conductors to insulators and back again** — •Petro Maksymovych
SYCE 1.2	Mon	15:30–16:00	HSZ 02	**Zoology of skyrmions and the role of magnetic anisotropy in the stability of skyrmions** — •Istvan Kezsmarki, Sandor Bordacs, Jonathan White, Vladimir Tsurkan, Alois Loidl, Peter Milde, Hiroyuki Nakamura, Andrey Leonov
SYCE 1.3	Mon	16:00–16:30	HSZ 02	**Magnetic imaging of topological phenomena in ferroic materials** — •Weida Wu
SYCE 1.4	Mon	17:00–17:30	HSZ 02	**Topological skyrmion textures in chiral magnets** — •Markus Garst
SYCE 1.5	Mon	17:30–18:00	HSZ 02	**Learning through ferroelectric domain dynamics in solidstate synapses** — Sören Boyn, Gwendal Lecerf, Stéphane Fusil, Sylvain Saïghi, Agnès Barthélémy, Julie Grollier, Vincent Garcia, •Manuel Bibes

Invited talks of the joint symposium SYNS

See SYNS for the full program of the symposium.

SYNS 1.1	Wed	15:00–15:30	HSZ 02	**The Limits to Lithography: How Electron-Beams Interact with Materials at the Smallest Length Scales** — •Karl K. Berggren
SYNS 1.2	Wed	15:30–16:00	HSZ 02	**High precision fabrication for light management at nanoscale** — •Saulius Juodkazis, Armandas Balcytis
SYNS 1.3	Wed	16:00–16:30	HSZ 02	**Directed self-assembly of performance materials** — •Paul Nealey
SYNS 1.4	Wed	16:45–17:15	HSZ 02	**Nanometer accurate topography patterning using thermal Scanning Probe Lithography** — •Armin W. Knoll
SYNS 1.5	Wed	17:15–17:45	HSZ 02	**High resolution 3D nanoimprint lithography** — •Hartmut Hillmer

Invited talks of the joint symposium SYQO

See SYQO for the full program of the symposium.

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

Invited talks of the joint symposium SYLM

See SYLM for the full program of the symposium.

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

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

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

Sessions

DS 1.1–1.13	Mon	9:30–13:00	HSZ 204	**Transport: Topological Insulators (jointly with DS, MA, HL, O)**
DS 2.1–2.6	Mon	9:30–12:15	CHE 89	**Focused Session: Inhomogeneous Materials for Solar Cells I**
DS 3.1–3.13	Mon	9:30–13:00	CHE 91	**Thin Film Characterisation: Structure Analysis and Composition I**
DS 4.1–4.9	Mon	9:30–12:45	POT 81	**Focus Session: Two-dimensional materials I (jointly with HL/TT)**
DS 5.1–5.9	Mon	10:15–13:00	ZEU 222	**Fundamentals of Perovskite Photovoltaics I (jointly with CPP)**
DS 6.1–6.10	Mon	10:30–13:00	REC/PHY C213	**2D Materials Beyond Graphene I (jointly with O)**
DS 7.1–7.3	Mon	12:30–13:15	CHE 89	**Atomic Layer Deposition**
DS 8.1–8.10	Mon	14:45–18:15	POT 81	**Focus Session: Two-dimensional materials II (jointly with HL/TT)**
DS 9.1–9.12	Mon	15:00–18:15	HSZ 204	**Transport: Graphene and Carbon Nanostructures (jointly with HL/MA/TT)**
DS 10.1–10.11	Mon	15:00–18:00	HSZ 304	**Transport: Topological Phases (jointly with DS/MA/TT)**
DS 11.1–11.9	Mon	15:00–18:15	ZEU 222	**Fundamentals of Perovskite Photovoltaics II (jointly with CPP/DS/HL)**
DS 12.1–12.3	Mon	15:00–16:15	CHE 89	**Focused Session: Inhomogeneous Materials for Solar Cells II**
DS 13.1–13.7	Mon	15:00–16:45	CHE 91	**Phase Change/Resistive Switching**
DS 14.1–14.10	Mon	16:00–18:30	REC/PHY C213	**2D Materials Beyond Graphene II (jointly with CPP)**
DS 15.1–15.3	Mon	16:30–17:15	CHE 89	**Focussed Session: Frontiers in Exploring and Applying Plasmonic Systems I** **(Joint Session of CPP, DS, HL, MM, and O, organized by DS)**
DS 16.1–16.6	Mon	17:00–18:30	CHE 91	**Layer Properties: Electrical, Optical, and Mechanical Properties I**
DS 17.1–17.5	Mon	17:45–19:00	CHE 89	**Thermoelectric Materials**
DS 18.1–18.8	Tue	9:30–11:45	HSZ 201	**Transport: Topological Semimetals 1 (jointly with MA/TT)**

DS 19.1–19.10	Tue	9:30–12:30	ZEU 222	**Fundamentals of Perovskite Photovoltaics III (jointly with CPP/HL)**
DS 20.1–20.6	Tue	9:30–12:45	CHE 89	**Focussed Session: Frontiers in Exploring and Applying Plasmonic Systems II** **(Joint Session of CPP, DS, HL, MM, and O, organized by DS)**
DS 21.1–21.13	Tue	9:30–13:00	CHE 91	**Thin Film Characterisation: Structure Analysis and Composition II**
DS 22.1–22.12	Tue	9:30–13:15	POT 51	**Two-dimensional materials III (jointly with HL/TT)**
DS 23.1–23.13	Tue	9:30–13:15	POT 251	**Organic Semiconductors (jointly with CPP/HL)**
DS 24.1–24.7	Tue	14:00–16:00	ZEU 222	**Fundamentals of Perovskite Photovoltaics IV (jointly with CPP/HL)**
DS 25.1–25.1	Tue	15:30–16:00	WIL C307	**Gaede Prize Talk (jointly with O)**
DS 26.1–26.5	Tue	18:30–20:30	P1C	**Metallic Nanowires on Semiconductor Surfaces (jointly with O)**
DS 27.1–27.20	Tue	18:30–20:30	P2-EG	**2D Materials beyond Graphene (jointly with O)**
DS 28.1–28.10	Wed	9:30–13:00	CHE 89	**Focussed Session: Oxide Semiconductors for Novel Devices I**
DS 29.1–29.14	Wed	9:30–13:15	CHE 91	**Organic Thin Films I**
DS 30.1–30.13	Wed	9:30–13:15	POT 51	**Two-dimensional materials IV (jointly with HL/TT)**
DS 31.1–31.10	Wed	10:30–13:00	WIL A317	**2D Materials Beyond Graphene III (jointly with O)**
DS 32.1–32.8	Wed	14:45–17:45	CHE 89	**Focussed Session: Oxide Semiconductors for Novel Devices II**
DS 33.1–33.10	Wed	15:00–17:45	HSZ 204	**Transport: Topological Semimetals 2 (jointly with MA/TT)**
DS 34.1–34.8	Wed	15:00–17:00	CHE 91	**Organic Thin Films II**
DS 35.1–35.10	Wed	15:00–17:45	WIL A317	**2D Materials Beyond Graphene IV (jointly with O)**
DS 36.1–36.54	Wed	17:00–19:00	P2-EG	**Postersession I**
DS 37.1–37.8	Thu	9:30–13:00	HSZ 03	**Focus Session on 2D Materials: Ballistic Quantum Transport in Graphene (jointly with HL, MA, TT)**
DS 38.1–38.10	Thu	9:30–13:15	CHE 89	**Focussed Session: Memristive Devices for Neuronal Systems I**
DS 39.1–39.14	Thu	9:30–13:15	CHE 91	**Thin Film Applications**
DS 40.1–40.5	Thu	15:00–16:45	CHE 89	**Focussed Session: Memristive Devices for Neuronal Systems II**
DS 41.1–41.7	Thu	15:00–16:45	CHE 91	**Layer Properties: Electrical, Optical, and Mechanical Properties II**
DS 42.1–42.11	Thu	15:00–17:45	WIL C107	**Metallic Nanowires on Semiconductor Surfaces (jointly with O)**
DS 43.1–43.2	Thu	17:00–17:30	CHE 91	**Quantum Optics at the Nanoscale: From Fundamental Physics to Quantum Technologies** **(Joint Session HL, DS, O, and TT, organized by DS)**
DS 44.1–44.54	Thu	17:00–19:00	P1C	**Postersession II**
DS 45.1–45.8	Fri	9:30–11:30	HSZ 03	**Transport: Spintronics, Spincalorics and Magnetotransport (jointly with HL, MA)**
DS 46.1–46.6	Fri	9:30–11:00	CHE 89	**Ion and Electron Beam Induced Processes**
DS 47.1–47.8	Fri	9:30–11:45	CHE 91	**Organic-Inorganic Hybride Interfaces**
DS 48.1–48.10	Fri	9:30–12:45	POT 51	**Oxide Semiconductors (jointly with HL)**
DS 49.1–49.5	Fri	10:30–13:00	HSZ 02	**Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond (SYES)**
DS 50.1–50.4	Fri	11:15–12:15	CHE 89	**Optics and Light-Matter Interaction with Excitons in 2D Materials** **(Joint Session HL, DS, O, and TT, organized by DS)**

Annual Meeting of the Thin Films Division

Wednesday 19:00–20:00 CHE 89

- Annual Report

DS 1: Transport: Topological Insulators (jointly with DS, MA, HL, O)

Time: Monday 9:30–13:00 Location: HSZ 204

DS 1.1 Mon 9:30 HSZ 204

Magnetic excitations in the symmetry protected, topological Haldane phase of $\mathrm{SrNi_2V_2O_8}$ — Vladimir Gnezdilov[1,2], Vladimir Kurnosov[2], •Peter Lemmens[1], A. K. Bera[3], A. T. M. N. Islam[3], and Bella Lake[3] — [1]TU-BS, Braunschweig — [2]ILTP Kharkov — [3]HZB Berlin

We report results of a single-crystal Raman scattering study of the coupled spin-1 Haldane chain compound $\mathrm{SrNi_2V_2O_8}$. In addition to the one-and two-magnon excitations, broad gapless and temperature dependent continua are detected with light polarization parallel to the basal plane. This feature is discussed in terms of spinon-like excitations related to a symmetry protected topological state, of which the Haldane phase in 1D is a preeminent example.

Work supported by RTG-DFG 1952/1, Metrology for Complex Nanosystems and the Laboratory for Emerging Nanometrology, TU Braunschweig.

DS 1.2 Mon 9:45 HSZ 204

Low-temperature magnetotransport in Mn-doped $\mathrm{Bi_2Se_3}$ topological insulators — V. Tkáč[1], V. Komanicky[2], R. Tarasenko[1], M. Vališka[1], V. Holý[1], G. Springholz[3], V. Sechovský[1], and •J. Honolka[4] — [1]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, CZ — [2]Institute of Physics, P. J. Šafárik University, SK — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University, AT — [4]Institute of Physics, Academy of Sciences of the Czech Republic, CZ

Magnetic impurities can break the time-reversal symmetry of 3D topological insulators (TI), thereby opening an energy gap Δ at the Dirac point of a topological surface state with large consequences for transport properties in the thin film limit. In magnetotransport a transition from weak antilocalisation to weak localisation is expected, strongly dependent on contributions from possible coexisting 2D quantum well and bulk states. We present a low-T magnetotransport study ($T = 0.3$ K - 300 K, $B_{\max} = 14$ T) of MBE-grown $\mathrm{Bi_2Se_3}$ films of 20 nm - 500 nm thickness with varying Mn concentrations up to 8% and Curie temperatures $T_C = 5 - 7$ K [1,2]. The results are interpreted following mainly theory by Lu et al. [3] as a competition of quantum corrections to the conductivity σ (phase coherence length $l_\phi \propto T^{-1/2} \sim 50 - 150$nm for pure $\mathrm{Bi_2Se_3}$) and 2D e-e interaction corrections both in the ferro- and paramagnetic phase.

[1] M. Valiska et al., Appl. Phys. Lett. 108, 262402 (2016).
[2] R. Tarasenko et al., Physica B 481, 262 (2016).
[3] H.-Z. Lu et al., Phys. Rev. Lett. 112, 146601 (2014).

DS 1.3 Mon 10:00 HSZ 204

Proximity-induced superconductivity and quantum interference in topological crystalline insulator SnTe devices — •Robin Klett[1], Joachim Schönle[2], Denis Dyck[1], Karsten Rott[1], Shekhar Chandra[3], Claudia Felser[3], Wolfgang Wernsdorfer[2], and Günter Reiss[1] — [1]CSMD, Bielefeld University, Germany — [2]CNRS, Institut Neél, France — [3]MPI for Chemical Physics of Solids, Germany

Topological states of matter host a variety of new physics that is promising for future technology. Among these phenomena, the emergence of metallic symmetry-protected topological surface states (TSS) are of major interest. The coupling of topological matter to a nearby superconductor is forsaken to host unconventional proximity-induced superconductivity. We demonstrate the fabrication of superconducting Quantum interference devices (SQUIDs) out of SnTe/Nb hybrid structures. Our findings show strong proximity-induced superconductivity in the surface of SnTe. Transport contributions of Majorana Bound States are predicted to enter with a shift in periodicity to DC SQUID experiments. The Analysis of the SQUID response suggest the absence of periodicity shifts, but show additional features expected for TSS carried supercurrents, such as unconventional Fraunhofer shapes.

DS 1.4 Mon 10:15 HSZ 204

Emergence of topological and topological crystalline phases in $\mathrm{TlBiS_2}$ and $\mathrm{TlSbS_2}$ — •Udo Schwingenschlögl, Qingyun Zhang, and Yingchun Cheng — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

Using first-principles calculations, we investigate the band structure evolution and topological phase transitions in $\mathrm{TlBiS_2}$ and $\mathrm{TlSbS_2}$ under hydrostatic pressure as well as uniaxial and biaxial strain. The phase transitions are identified by parity analysis and by calculating the surface states. Zero, one, and four Dirac cones are found for the (111) surfaces of both $\mathrm{TlBiS_2}$ and $\mathrm{TlSbS_2}$ when the pressure grows, which confirms trivial-nontrivial-trivial phase transitions. The Dirac cones at the $\bar{\mathrm{M}}$ points are anisotropic with large out-of-plane component. $\mathrm{TlBiS_2}$ shows normal, topological, and topological crystalline insulator phases under hydrostatic pressure, thus being the first compound to exhibit a phase transition from a topological to a topological crystalline insulator. [1] Scientific Reports **5**, 8379 (2015)

DS 1.5 Mon 10:30 HSZ 204

Perfect filter for triplet superconductivity on the surface of a 3DTI — •Daniel Breunig[1], Pablo Burset[1], François Crépin[2], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, Wuerzburg University, 97074 Wuerzburg, Germany — [2]Laboratoire de Physique Théorique de la Matière Condensée, UPMC, Sorbonne Universités, 75252 Paris, France

We study a NSN junction on the surface of a 3D topological insulator (TI), where N is a normal region and S is a s-wave proximity-induced superconducting region. Spin-orbit coupling in the TI breaks spin rotational symmetry and induces unconventional triplet superconductivity.

From the anomalous Green function, we identify the singlet and triplet pairing amplitudes and perform a symmetry classification on these quantities. Pauli exclusion principle demands the antisymmetry of the Green function under simultaneous exchange of its space, time and spin variables. The pairing amplitudes can thus be classified as ESE, OSO, ETO or OTE. Here, the first (last) letter specifies the time/frequency (parity) symmetry (Even or Odd) and the second one describes the spin (Singlet or Triplet). A special feature of our system is the emergence of the exotic odd-frequency pairing.

Interestingly, we find that for a bipolar junction, where the chemical potentials in the N leads only differ in their signs, the non-local singlet pairing amplitude is completely suppressed and only triplet pairing occurs. As a result, the non-local conductance across the junction can be dominated by purely spin triplet crossed Andreev reflections, while electron cotunneling is absent.

DS 1.6 Mon 10:45 HSZ 204

Ferromagnetic transition and fluctuation-induced Dzyaloshinskii-Morya interaction at the surface of three-dimensional topological insulators — •Flavio Nogueira[1], Ferhat Katmis[2], and Ilya Eremin[2] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum — [2]Deparment of Physics and Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology

A ferromagnetic insulator (FMI) proximate to the surface of a three-dimensional topological insulator (TI) generate a gap in the spectrum of surface Dirac fermions, provided an out-of-plane exchange exists. We study the ferromagnetic transition in TI-FMI structures and show that fluctuations from Dirac fermions induce a Dzyaloshinskii-Morya (DM) interaction in the effective free energy of the FMI. This DM interaction arises only if the chemical potential is nonzero. Thus, if the proximity effect gaps the Dirac fermions, this means that the Fermi level must be outside the gap in order for a DM term to be induced. We also show that the Curie temperature of the ferromagnetic state at the interface between the TI and FMI is necessarily higher than the bulk Curie temperature of the FMI. This result is corroborated by recent experiments in $\mathrm{Bi_2Se_3}$-EuS bilayer structures. These results imply an interface critical behavior very different from the bulk FMI.

DS 1.7 Mon 11:00 HSZ 204

A time-reversal symmetric topological magnetoelectric effect in 3D topological insulators — •Heinrich-Gregor Zirnstein and Bernd Rosenow — Institut für Theoretische Physik, Universität Leipzig, Germany

One of the hallmarks of time-reversal symmetric (TRS) topological insulators in 3D is the topological magnetoelectric effect (TME). So far, a time-reversal breaking variant of this effect has been discussed, in the sense that the induced electric charge changes sign when the direction of an externally applied magnetic field is reversed. Theoretically, this effect is described by the so-called axion term. Here, we discuss a time-reversal symmetric TME, where the electric charge depends only on the magnitude of the magnetic field but is independent of its sign. We obtain this non-perturbative result by a combination of analytic and numerical arguments, and suggest a mesoscopic setup to demonstrate it experimentally.

In particular, we show that threading a thin magnetic flux tube of one flux quantum through the material and applying a uniform electric field will induce a half-integer charge $\Delta Q = e/2\,\mathrm{sgn}\,\mathbf{E}_z$ on the surface of the topological insulator. The sign of the induced charge is independent of the direction of the magnetic field.

15 min. break.

DS 1.8 Mon 11:30 HSZ 204

Single-electron injection in the edge states of a 2D topological insulator — •Giacomo Dolcetto and Thomas Schmidt — Physics and Materials Science Research Unit, University of Luxembourg

The realization of single-electron sources in integer quantum Hall systems has paved the way for exploring electronic quantum optics experiments in solid-state devices. Recently, two-dimensional topological insulators have also been considered as an interesting playground for implementing electron quantum optics. Here, two electron waveguides emerge at the edge, one for spin-up and one for spin-down electrons. Scattering between the two channels is strongly suppressed and phase-coherent ballistic transport is predicted. In this talk I will characterize the injection of single Kramers pairs from a mesoscopic capacitor: a periodic voltage drive results in the emission of periodic trains of electron and hole Kramers pairs. Due to spin-momentum locking and to the geometry of the device, the injected state is in general a superposition of many different orthogonal states, thus representing an interesting playground not only to study the transport properties, but also to investigate and to measure the entanglement production.

DS 1.9 Mon 11:45 HSZ 204

Odd-frequency superconductivity at the Helical Edge of a 2D Topological Insulator — •Felix Keidel[1], Pablo Burset[1], François Crépin[2], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, Würzburg University, 97074 Würzburg, Germany — [2]Laboratoire de Physique Théorique de la Matière Condensée, UPMC, Sorbonne Universités, 75252 Paris, France

By virtue of the basic laws of quantum mechanics, the Pauli principle demands the Cooper pairs in superconductors to be odd under exchange of the two constituent electrons. Consequently, even-parity singlets are formed in conventional s-wave superconductivity. Exotic unconventional pairing symmetries emerge once the classification is extended to frequency, additionally to orbital and spin degrees of freedom.

In our work, we study a helical edge of a two-dimensional topological insulator in proximity to an s-wave superconductor and ferromagnetic insulators. While helicity and the magnetic field induce triplet correlations in addition to the inherited singlet pairing, both even- and odd-parity contributions arise since translational invariance and inversion symmetry are broken. In such a hybrid junction, odd-frequency amplitudes thus occur naturally as all combinations of spin and parity symmetry appear. On the basis of a Green's function analysis, we find signatures of these unconventional pairing amplitudes in the local density of states and in the non-local conductance. Strikingly, our method allows to track the emergence of unconventional superconductivity and make a connection to transport and pairing properties of the system.

DS 1.10 Mon 12:00 HSZ 204

Parity anomaly driven topological transitions in magnetic field — •Jan Böttcher, Christian Tutschku, and Ewelina M. Hankiewicz — Institut für Theoretische Physik und Astronomie, Uni Würzburg, 97074 Würzburg, Germany

Recent developments in solid state physics give a prospect to observe the parity anomaly in (2+1)D massive Dirac systems. We show, that the charge neutrality condition for a quantum anomalous Hall (QAH) state in orbital magnetic fields gets modified by an additional term originating from an intrinsic Chern-Simons term in the one loop Lagrangian. This can be utilized to experimentally differentiate the QAH from the quantum Hall (QH) state at charge neutrality [1]. As a result, an experimental signature of the QAH phase in magnetic fields is a long $\sigma_{xy} = e^2/h$ ($\sigma_{xy} = -e^2/h$) plateau in $\mathrm{Cr}_x(\mathrm{Bi}_{1-y}\mathrm{Sb}_y)_{2-x}\mathrm{Te}_3$ (HgMnTe quantum wells). Furthermore, we predict a new transition between the quantum spin Hall (QSH) and the QAH state in magnetic fields without magnetic impurities but driven by effective g-factors and particle-hole asymmetry.

[1] J. Böttcher, C. Tutschku, E. M. Hankiewicz, arXiv:1607.07768v1

DS 1.11 Mon 12:15 HSZ 204

Tunable edge states and their robustness towards disorder — •Maik Malki and Götz S. Uhrig — Lehrstuhl für Theoretische Physik 1, TU Dortmund, Germany

The interest in the properties of edge states in Chern insulators and in $\mathbb{Z}_2$ topological insulator has increased rapidly in recent years. We present calculations on how to influence the transport properties of chiral and helical edge states by modifications of the edges in the Haldane and in the Kane-Mele model. The Fermi velocity of the chiral edge states becomes direction-dependent as does the spin-dependent Fermi velocity of the helical edge states. Moreover, it is possible to tune the Fermi velocity by orders of magnitude. Additionally, we explicitly investigate the robustness of edge states against local disorder. The edge states can be reconstructed in the Brillouin zone in presence of disorder. The influence of the width and of the length of the system is studied as well as the dependence on the strength of the disorder.

DS 1.12 Mon 12:30 HSZ 204

Instability of interaction-driven topological insulators against disorder — Jing Wang[1,2], Carmine Ortix[1,3], Jeroen van den Brink[1], and •Dmitri Efremov[1] — [1]IFW Dresden, Germany — [2]University of Science and Technology of China, Hefei, China — [3]Utrecht University, Netherlands

We analyze the effect of disorder on the weak-coupling instabilities of quadratic band crossing point (QBCP) in two-dimensional Fermi systems, which, in the clean limit, display interaction-driven topological insulating phases. In the frame of the weak-coupling renormalization group procedure, which treats fermionic interactions and disorder on the same footing, we test all possible instabilities and identify the corresponding ordered phases in the presence of disorder for both single-valley and two-valley QBCP systems. We find that disorder generally has a strong influence on the stability of the interaction-driven topological insulating phases – it strongly suppresses the critical temperature at which the topologically non-trivial order sets in – and can even trigger a phase transition to different, topologically trivial, ordered phases.

DS 1.13 Mon 12:45 HSZ 204

Effect of disordered geometry on transport properties of three dimensional topological insulator nanowires — •Emmanouil Xypakis[1], Jun Won Rhim[1], Roni Ilan[2], and Jens H. Bardarson[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Department of Physics, University of California, Berkeley, California

Three dimensional topological insulator nanowires are materials which, while insulating in the bulk, have a metallic boundary described by a two dimensional Dirac Hamiltonian with antiperiodic boundary conditions. Transport properties of this system have been extensively studied in the limit where the surface manifold is conformally at (e.g., a cylinder) in the presence of a random disordered scalar potential. In this talk I will discuss how this picture is altered when a more realistic surface manifold is chosen, such as a cylinder with a randomly fluctuating radius.

DS 2: Focused Session: Inhomogeneous Materials for Solar Cells I

Although multinary compound semiconductors exhibit a variety of inhomogeneities - such as strong local concentration fluctuations, built-in vertical concentration gradients, rough interfaces, and a high density of grain boundaries - they are among the leading solar cell technologies. In this focused session, the impact of inhomogeneities on the carrier transport in solar cells shall be addressed with emphasis on material growth, characterization, and modeling. Therefore, state-of-the-art research and challenges will be highlighted for a broad range of related materials such as chalcopyrites, kesterites, perovskites, and group III-nitrides.

Organizers: Roland Scheer (MLU Halle Wittenberg), Frank Bertram (OvGU Magdeburg), and Jürgen Christen (OvGU Magdeburg)

Time: Monday 9:30–12:15 Location: CHE 89

Topical Talk DS 2.1 Mon 9:30 CHE 89

Inhomogeneities in chalcopyrites and kesterites — •Claudia S. Schnohr — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Thin film solar cells based on $Cu(In,Ga)(Se,S)_2$ have reached a record efficiency of 22.6 %, thus closing the gap to silicon-based technology. $Cu_2ZnSn(Se,S)_4$ has also attracted great attention as non-toxic, earth-abundant alternative and a record efficiency of 12.6 % has already been demonstrated. Both material systems typically feature inhomogeneities such as grain boundaries, interfaces, and compositional variations, that may deteriorate or improve the device performance. We therefore applied high-resolution X-ray fluorescence analysis using a synchrotron nanobeam to study the elemental composition of chalcopyrite- and kesterite-type thin films on a micrometer and submicrometer scale. To that end, thin cross section lamellas were prepared with a focused ion beam system. For $Cu(In,Ga)(Se,S)_2$, the depth-dependent Ga gradient shows a strong dependence on the growth conditions in a sequential two-stage process. Furthermore, we find subtle lateral variations in the material composition and a significant In enrichment for some of the grain boundaries. For highly non-stoichiometric $Cu_2ZnSn(Se,S)_4$, different binary secondary phases coexist within a distance of only a few micrometers and the local compositions of the kesterite-type domains differ tremendously from the integral layer composition. Detailed knowledge of these compositional variations, which directly affect the electronic properties of the material, will thus help to exploit the full potential of chalcopyrite- and kesterite-based thin film solar cells.

Topical Talk DS 2.2 Mon 10:00 CHE 89

Impact of growth condition on defect generation in Cu(In,Ga)Se2 — •Takeaki Sakurai[1], Muhammad Islam[1], Akira Uedono[1], Shogo Ishizuka[2], Hajime Shibata[2], Shigeru Niki[2], and Katsuhiro Akimoto[1] — [1]University of Tsukuba, Tsukuba, Japan — [2]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

Characterization of defects in Cu(In,Ga)Se2 (CIGS)-based solar cells is an important research subject for understanding its carrier recombination processes. In this decade, the optical and electrical response of the defect states have been intensely studied using various analytical methods. Nevertheless, the origin and distribution of the defects in CIGS have not been fully understood yet due to its complex device structures and multinary compositions. During the growth of CIGS, in particular, segregation of the secondary phase, selenization, and alkali metal diffusion occur, and the difficulty in the control of the growth process mainly results in fluctuation of their optoelectronic properties. Therefore, a systematic study on the relation between the thin film growth and the generation of defects is necessary. In this study, we have investigated the impact of growth condition (Se flux and Ga concentration) on defect generation in CIGS by using various characterization techniques. We want to point out that the defect level centered around 0.8 eV from the valence level may act as a recombination center at room temparature. We will discuss whether this defect level acts as a recombination ceneter by using two-wavelength excited photoluminescence method.

DS 2.3 Mon 10:30 CHE 89

On the impact of material inhomogeneities on the time-resolved luminescence decay — •Matthias Maiberg, Torsten Hölscher, and Roland Scheer — Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle, Germany

Time-resolved luminescence is the method of choice for determination of material parameters, e.g. the minority carrier lifetime in a semiconductor. However, due to the size of the excited area the obtained data are mostly mean values averaged over a typical region of $10^4\,cm^{-2}$. In our work, we study the impact of lifetime fluctuations, band gap inhomogeneities, and potential fluctuations on the time-resolved luminescence decay by means of three-dimensional simulation. It turns out that inhomogeneous charge carrier lifetimes will increase the luminescence decay time, if the ratio of the structure size and the average diffusion length is larger than 1. For ratios smaller than 1, however, inhomogeneous charge carrier lifetimes will lead to reduced luminescence decay times. In contrast to the strong impact of lifetime inhomogeneities, band gap fluctuations are shown to have a negligible effect on the luminescence decay. In the end, it is demonstrated that the effect of potential fluctuations, which numerous of the thin-film semiconductors are prone to, is rather similar to that of space charges in a semiconductor junction. In particular the decay time will always be smaller than the recombination lifetime due to occuring drift effects. For this reason, potential fluctuations may not explain the often observed long decay times in compensated semiconductors such as $Cu(In,Ga)Se_2$ or $Cu_2ZnSnSe_4$.

15 min. break.

Topical Talk DS 2.4 Mon 11:00 CHE 89

Inhomogeneities in chalcopyrites for solar cells — •Daniel Abou-Ras — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Thin-film solar cells with polycrystalline Cu(In,Ga)(S,Se)2 absorber layers have exhibited record conversion efficiencies of up to 22.6%. Although parallel to the substrate, the concentrations of the matrix elements in these Cu(In,Ga)(S,Se)2 thin films do not vary substantially, obvious inhomogeneities are the [In]/[Ga] and also (in case S is present) [S]/[Se] gradients perpendicular to the substrate. Moreover, also indications for various net doping concentrations in neighboring grains have been reported, which may be explained by locally varying point-defect concentrations. On the (sub)nanometer scale, compositional variations at different line and planar defects in Cu(In,Ga)(S,Se)2 thin films have been detected. The present contribution will give an overview of all these imhomogeneities existing on different length scales, but all affecting the potential landscape of chalcopyrite-type Cu(In,Ga)(S,Se)2 absorber layers.

Topical Talk DS 2.5 Mon 11:30 CHE 89

Understanding the defects in Cu(In,Ga)Se2 solar cell: a correlative microscopy approach — •Oana Cojocaru-Mirédin[1], Torsten Schwarz[2], Roland Mainz[3], and Daniel Abou-Ras[3] — [1]University of RWTH Aachen, I. Institut of Physics, Sommerfeldstraße 14, 52056 Aachen, Germany — [2]Max-Planck Institut für Eisenforschng, Max-Planck Straße 1, 40237 Düsseldorf, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109 Berlin, Germany

In Cu(In,Ga)Se2 solar cells, interfaces between individual layers in a thin-film stack, such as p-n heterojunctions, or structural defects such as grain boundaries or stacking faults, often influence substantially the performance of the device [1]. To further develop these solar devices, one needs to understand the relationship between structural and chemical properties for specific interfaces and defects. Diffraction techniques in transmission electron microscopy or scanning electron microscopy are excellent tools for structural investigations, i.e., the crystallographic structure of stacking faults and grain boundary. The present work shows an advanced, correlative study combining atom-probe tomography and various electron microscopy techniques on defects in Cu(In,Ga)Se2 absorber. Indeed, different approaches for determining structural and chemical property relationships will be presented. The experimental results to be presented will also be compared directly with the existing theoretical models on defects and phase formation in photovoltaic materials.

[1] M. Müller et al., Journal of Applied Physics 115 (2014) 023514.

DS 2.6 Mon 12:00 CHE 89

Controllable crystallization of chalcogenide thin films for photovoltaic and electrical applications — •Ilia Korolkov, Michel Cathelinaud, Xian-Hua Zhang, and Jean-Luc Adam — Verres et céramique, ISCR, Université de Rennes 1, Rennes, France

Chalcogenide materials (i.e. materials containing sulfur (S), selenium (Se) and/or tellurium (Te)) are of great importance in the context of solar energy harvesting because of their suitable electronic properties such as extended absorption spectrum, direct band gap and high absorption coefficient.

In this work we present the investigation on chalcogenide thin films of 40Sb2Se3-40GeSe2-20CuI composition, which upon the crystallization showed the formation of the conductive percolation network formed by Sb2Se3 rods covered with Cu2GeSe3 microcrystals. We optimized targets composition varying the amount of iodine and copper iodide. Various deposit and heating treatment regimes were applied as well. We revealed an important role of the iodine which dopes Sb2Se3, increasing drastically its conductivity and serving as an electron donor. We established that pre-deposit of a very thin film of CuI (about 3nm) prior to a major thin film deposit influences positively on crystallization and conductive channels formation during the heating treatment. A simple photovoltaic cell of [ITO|ZnO (or Sb2Se3 : I)|40Sb2Se3-40GeSe2-20CuI|Au] configuration shows the short circuit current up to 10mA/cm2 and open circuit voltage up to 0,2V.

DS 3: Thin Film Characterisation: Structure Analysis and Composition I

Time: Monday 9:30–13:00 Location: CHE 91

DS 3.1 Mon 9:30 CHE 91

Ti valence mapping in LAO/STO with resonant soft X-ray reflectometry — •Martin Zwiebler[1], Emiliano Di Gennaro[2], Jorge Enrique Hamann-Borrero[1], Fabio Miletto Granozio[2], Enrico Schierle[3], Eugen Weschke[3], Bernd Büchner[3], George Sawatzky[4], Robert Green[4], and Jochen Geck[5] — [1]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]CNR-SPIN and Dipartimento di Finica, Complesso Universitario di Monte S. Angelo, Via Cintia, 80126 Naples, Italy — [3]Helmholtz-Zentrum Berlin, BESSY, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [4]University of British Columbia 6224 Agricultural Road Vancouver, B.C. V6T 1Z1 Canada — [5]Institut fuer Strukturphysik Technische Universität Dresden, 01062 Dresden, Germany

The two dimensional electron gas (2DEG) at the LaAlO3/SrTiO3 heterointerface exhibits intriguing features, which are currently not well understood. When at least four UCs of LAO are deposited on a STO substrate, mobile electrons accumulate at interfacial Ti sites. In order to establish the underlying physics, it is essential to know the charge density distribution of the 2DEG around the interface. Exactly this point, however, remained highly controversial so far. In order to clarify this issue, we performed X-ray reflectivity measurements at the Ti $L_{2,3}$ edge to determine the Ti stoichiometry and the depth-dependent electron content at the interface with resolution at the atomic scale. We demonstrate that the electron distribution is strongly T-dependent. From the polarization dependence of the reflectivity we gain new results on the anisotropy of orbital energies and electron density.

DS 3.2 Mon 9:45 CHE 91

XPD experiments and simulation of GaAs(001)-c(8x2) — •Karim Shamout[1,2], Philipp Espeter[1,2], Peter Roese[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik I - Technische Universität Dortmund, Otto-Hahn-Str. 4a, D-44221 Dortmund — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund

The III-V compound semiconductor gallium arsenide is an applicable substrate for spin-tronic multilayer systems due to its electronical and magnetic properties. GaAs(001) is found in various reconstructions determined by the Ga-As ratio in the top atom surface layer. In this work, we analyse of the GaAs surface reconstructions, and here especially the GaAs(001)-c(8x2) structure where huge uncertainties arise. Photoelectron diffraction (XPD) provides detailed information of the surface and interface of the sample. Thereby Ga or As dimers located 5 Å beneath the surface can be resolved. In literature, 8 different possible structures of the GaAs-c(8x2) surface have been shown. These structures differ by the number of Ga dimers, the sub-dimers or the arrangement of Ga-As rings. Here we present the experimental data of the GaAs-c(8x2) surface measured with XPD at the U55 beamline 11 at DELTA. For each possible structure an XPD pattern has been simulated and compared to the experimental data. As a result, the structure suggested by Kumpf et al. fits best to the data. Further, the precise location of the Ga-dimers is found. Moreover, we analyse the interface of Co/GaAs(001)-c(8x2) and investigate on the stability of the GaAs reconstruction beneath Co.

DS 3.3 Mon 10:00 CHE 91

ARXPS study of the growth behaviour of ultrathin ionic liquid layers on metal surfaces — •Matthias Lexow, Benjamin May, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Ionic liquids (IL) are ionic compounds with a relatively low melting point, often even below room temperature. In addition to numerous applications as a solvent or electrolyte, the extremely low vapour pressure of ILs also led to the development of completely new concepts for catalytically active systems. Thin layers of ILs on solid materials are applied e.g. in SCILL (Solid Catalyst with Ionic Liquid Layer) catalysis.

In this context, the structure and composition of the IL/solid interface is studied by our group with angle-resolved X-ray photoelectron spectroscopy (ARXPS). Recently it was shown that by deposition of sub-monolayer amounts of Pd on single-crystalline Au(111) the growth mode of ILs can be switched from three-dimensional to two-dimensional growth, i.e. from non-wetting to wetting behaviour.

Aiming to understand the behaviour of applied catalyst systems containing Ag and Pd, the ARXPS studies are extended to the Ag(111) surface. The results offer possible explanations for the beneficial influence of the IL layer on heterogeneous metal alloy catalysts.

M.L., B.M 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.!

DS 3.4 Mon 10:15 CHE 91

Multiparamter Characterization of Subnanometre Cr/Sc Multilayers Based on Complementart Measurements — •Anton Haase[1], Saša Bajt[2], Philipp Hönicke[1], Victor Soltwisch[1], and Frank Scholze[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany — [2]Photon Science, DESY, Notkestr, 85, 22607 Hamburg, Germany

Cr/Sc multilayer systems can be used as near-normal incidence mirrors for the water window spectral range. It is shown that a detailed characterization of these multilayer systems with 400 bilayers of Cr and Sc, each with individual layer thicknesses below < 1 nm, is attainable by the combination of several analytical techniques. We used EUV and X-ray reflectance measurements, resonant EUV reflectance across the Sc L edge, as well as X-ray standing wave fluorescence measurements. The parameters of our multilayer model were determined based on a particle swarm optimizer and validated using a Markov-chain Monte Carlo maximum likelihood approach. For the determination of the interface roughness, diffuse scattering measurements were conducted.

DS 3.5 Mon 10:30 CHE 91

3D-Analysis of fine-grained metallic thin films. — •Ahu Öncü[1], Thomas Hempel[1], Bodo Kalkofen[2], Thorsten Halle[3], and Dana Zöllner[1] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg — [2]Institute of Micro and Sensor Systems, Otto-von-Guericke-University Magdeburg — [3]Institute of Materials and Joining Technology, Otto-von-Guericke-University Magdeburg

Fine-grained thin films play an important role in many technical applications. It is also known that grain microstructures of polycrystalline metals and alloys have an immense impact on materials properties. That is why it is important to understand the processes of grain growth not just as surface effects, but also as mechanisms in the entire layer like in bulk materials.

Commonly, thin layers are measured in 2D and compared with 2D simulations and analytic theories. However, two-demensional analytic size distributions or topological correlations between grains rarely capture the experimental features. One reason of this disagreement can be found in the simple fact that the experimental samples are of 3D nature. In the present work, we analyze the grain microstructures of thin aluminum films experimentally and compare the results to 3D computer simulations.

DS 3.6 Mon 10:45 CHE 91

Synchrotron radiation damage on Copper Naphthalocyanine layers — •Peter Roese[1,2], Philipp Espeter[1,2], Karim Shamout[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik I - Technische Universität Dortmund, Otto-Hahn-Str. 4a, D-44221 Dortmund — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund

The organic semiconductor naphthalocyanine includes a delocalized π-electronic system. The fascinating properties of naphthalocyanine are based on the delocalized π-electronic system. For applications the molecule is being studied as a perspective candidate for organic solar cells, organic LED's and molecular switches. Furthermore, using naphthalocyanines as a photosensibilisator in cancer treatment utilizes the strong absorption properties in the visible spectrum. Here, we present the investigation of synchrotron radiation damage on copper- and free-base naphthalocyanine layers (CoNc, H2Nc) on an Ag(110) surface using x-ray photoelectron spectroscopy (XPS) at the U55 beamline 11 at DELTA. In this study we report on synchrotron radiation damage induced changes at the nitrogen bonds while no changes at the C 1s signals occur. Furthermore, the reduction of the photon density by moving the experimental chamber out of focus reduced radiation damage significantly. Now, it was possible to perform photoelectron diffraction (XPD) measurements with these systems.

DS 3.7 Mon 11:00 CHE 91

Real time investigation of optical properties and morphology during the co-sputter deposition of Au/Ag nanoparticles — •Deniza Chekrygina[1], Matthias Schwartzkopf[2], André Rothkirch[2], Ivan Baev[1], Pallavi Pandit[2], Marc Gensch[1], Calvin Brett[1,2], Wiebke Ohm[2], Bjoern Beyersdorff[2], Jan Rubeck[2], Stephan Roth[2,3], Wilfried Wurth[1], and Michael Martins[1] — [1]UHH, Luruper Chaussee 149, D-22761 Hamburg — [2]DESY, Notkestr. 85, D-22607 Hamburg — [3]KTH, Teknikringen 56-58, SE-100 44 Stockholm

Binary alloys and multicomponent metallic thin films containing one or more noble metals are of great interest now due to their possible applications as catalysts, sensors and photonic devices. We concentrated in our work on investigation of the binary alloy system of Au/Ag, which is considered to be very promising in the field of nonlinear optical materials [1]. In this work, we present the results of in situ Grazing Incidence Small-Angle X-ray scattering (GISAXS) and UV/Vis spectroscopy for the simultaneous radio-frequence (r.f) co-sputtering process from two metallic targets with different ratio and geometry of deposition. Post-sputtering growth characterization for the set of samples was made using Atomic Force Microscopy (AFM), GISAXS, Grazing Incidence Wide-Angle X-ray scattering (GIWAXS) and X-ray emission spectroscopy (XES). We will present comparison of the physical and structural properties depending on the ratio of the metal in bialloys and the geometry of the deposition. [1] Faupel et al., Adv. Eng. Mater. 12, 1177 (2010).

15 min. break.

DS 3.8 Mon 11:30 CHE 91

Reactive ion beam sputter deposition of TiO2: Influence of deposition parameters on thin film properties — •Thomas Lautenschläger, Daniel Spemann, Annemarie Finzel, Erik Thelander, Micheal Mensing, Frank Frost, and Carsten Bundesmann — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, 04318 Leipzig, Germany

In physical vapor deposition (PVD), the properties of film forming particles strongly influence the growth process. Ion beam sputter deposition (IBSD) is a versatile PVD technique, as it offers several possibilities to alter the properties of the film forming particles. Reactive IBSD was used to deposit TiO2 thin films. The influence of sputtering geometry, ion energy, and ion species on thin film characteristics was investigated. The growth rate shows an over-cosine angular distribution, tilted in forward direction, and was found to increase with increasing ion energy and incidence angle. This behavior is in good agreement with the well-known dependence of the sputtering yield. The deposited films were amorphous, stoichiometric, and contained a considerable amount of primary particles. The concentration of inert gas was found to depend mainly on sputtering geometry and ion species. Surface roughness was well below 1 nm and depends mainly on sputtering geometry. Similarly, the refractive index changes systematically with the scattering geometry. These changes are strongly correlated with systematic variations in the mass density. The observations are assigned to variations of the angular and energy distribution of the sputtered target particles and the backscattered primary particles.

DS 3.9 Mon 11:45 CHE 91

Properties of SiO2 films grown by ion beam sputter deposition — •Maria Mateev, Thomas Lautenschläger, Daniel Spemann, Annemarie Finzel, Michael Mensing, Frank Frost, and Carsten Bundesmann — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, 04318 Leipzig, GER

Ion beam sputter deposition (IBSD) is an established physical vapor deposition technique that provides several possibilities to study the influence of certain process parameters on the film properties. Sputtering of a Si target in a reactive oxygen atmosphere using Ar and Xe as primary ions was used to grow SiO_2 films on silicon substrates. The sputtering geometry, ion energy and ion species were varied systematically and their influence on the sputtering yield and film properties was investigated. Thickness, index of refraction, composition, mass density, and surface roughness were determined with the help of ellipsometry, Rutherford backscattering spectrometry, X-ray reflectometry and atomic force microscopy, respectively. The SiO_2 growth rate increases with increasing ion energy and incidence angle between ion beam and target normal. Furthermore, thickness, index of refraction, stoichiometry, mass density and surface roughness show a strong correlation with the sputtering geometry. The ion species also has an impact on the film properties, the influence of the ion energy is rather small. A considerable amount of primary inert gas particles is found in the deposited films.

DS 3.10 Mon 12:00 CHE 91

Magneto-optical polarization spectroscopy on graphene-metal interfaces in the soft-x-ray regime — •Christine Jansing[1], Hans-Christoph Mertins[1], Markus Gilbert[1], Maxim Krivenkov[2], Andrei Varykhalov[2], Oliver Rader[2], Andreas Gaupp[2], Andrey Sokolov[2], Hud Wahab[3], Heiko Timmers[3], Dominik Legut[4], and Peter M. Oppeneer[5] — [1]Münster University of Applied Sciences, Stegerwaldstr. 39, D-48565 Steinfurt — [2]HZB, Albert Einstein Str. 15, D-12489 Berlin — [3]Uni. of New South Wales, Canberra, ACT 2600, Australia — [4]IT4Innovations Center, VSB-Technical University of Ostrava, CZ-708 33 Ostrava, Czech Republic — [5]Dept. of Physics and Astronomy, Uppsala University, Sweden

We present magneto-optical polarization and x-ray natural linear dichroism measurements [1] at the C 1s edge of graphene on metallic substrates. Graphene-metal interfaces show a strong hybridization between graphene π-states and 3d-states of the metallic substrate. Intercalation of gold in the graphene/Ni system leads to a change in the orientation and strength of this bonding which is deduced quantitatively. Additionally we observe a shift of the conduction bands (CB) at the Dirac point while the CB at the M-point is not affected. Furthermore the XMCD as well as T-MOKE of graphene/Ni is presented, which allows for the determination of the spin split density of states of the CB and the determination of the magnetic moment of magnetized graphene showing that magnetism in graphene is carried by the π-orbitals. [1] C. Jansing, H.-Ch. Mertins et al., Phys. Rev. B 94, 045422 (2016)

DS 3.11 Mon 12:15 CHE 91

Insights into epitaxial growth of thin film samples of the ferromagnetic shape memory alloy Fe_7Pd_3 — •Alina J. Bischoff[1], Kenneth Hua[1], and Stefan G. Mayr[1,2] — [1]Leibniz-Institut für Oberflächenmodifizierung, Leipzig — [2]Abteilung Oberflächenphysik, Fakultät für Physik und Geowissenschaften, Universität Leipzig

Single crystalline-like thin film Fe_7Pd_3 samples allow to study the physics of this promising ferromagnetic shape memory alloy. We demonstrate how to prepare such samples using electron beam evaporation and investigate the impact of variable deposition parameters such as growth temperature and deposition interruptions. We are able to epitaxially grow 500 nm thin Fe_7Pd_3 samples in austenitic and martensitic phases and the latter with visible surface twinning structures. Ideal growth conditions are given around 700 °C because deposition at temperatures below 690 °C results in demixing of samples while film quality is reduced at higher temperatures due to lattice misfit effects. Our investigations enabled us to identify a deposition procedure, which is realizable without much effort, to grow samples of increased and satisfyingly good quality so that subsequent processing of samples is rendered unnecessary.

DS 3.12 Mon 12:30 CHE 91

Interphase Formation and Band Bending in Organic and Inorganic Semiconductor Films Examined with Hard X-ray Photoelectron Spectroscopy — •Martin Schmid, Benedikt P. Klein, Claudio K. Krug, Stefan R. Kachel, Malte Sachs, Min Chen, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg

Hard X-ray photoelectron spectroscopy (HAXPES) allows to extend the information depth of photoelectron spectroscopy up to several tens of nanometers into a bulk material. This is achieved by using high energy photons ($h\nu = 2 - 10$ keV) to generate photoelectrons with high kinetic energies and accordingly larger mean free paths within solid materials. In a HAXPES experiment one integrates the signal contributions from many layers within the material, however the extraction of quantitative local information with regard to individual layers from the integral signal is in general not trivial. We will demonstrate how genetic optimization routines can be used to accomplish this task with two examples. In a first example we use this approach to characterize the reaction zone between 2H-tetraphenylporphyrin (2HTPP) films and metallic cobalt and iron layers. We find that the width of the reaction zone crucially depends on the sample temperature during preparation. In a second example we examine the depth dependent, local electrostatic potential (band bending) at a GaP/Si(001) heterojunction. Funding by DFG through SFB 1083 and by Verband der Chemischen Industrie e.V. is gratefully acknowledged.

DS 3.13 Mon 12:45 CHE 91

The effect of substrate miscut in epitaxial PMN-PT thin films — •Paul Chekhonin[1,3], Michael Mietschke[1,2], Darius Pohl[1], Frank Schmidt[1,2], Sebastian Fähler[1], Werner Skrotzki[3], Kornelius Nielsch[1,2], and Ruben Hühne[1] — [1]Institute for Metallic Materials, IFW Dresden — [2]Institut für Werkstoffwissenschaft, Technische Universität Dresden — [3]Institut für Strukturphysik, Technische Universität Dresden

The perovskite (1-x)Pb(Mg1/3Nb2/3)O3-xPbTiO3 (or (1-x)PMN-xPT) exhibits excellent ferroelectric and electrocaloric properties. The use of epitaxial films of PMN-PT facilitates the analysis of predetermined crystal orientations and the application of strain. Therefore, PMN-PT thin films were grown on SrTiO3 (STO) substrates using pulsed laser deposition. In comparison to standard (001) oriented substrates, such with a certain miscut allow the growth in a much broader parameter range. To advance the understanding of the substrate miscut, the microstructure of 0.68PMN-0.32PT thin films grown on La0.7Sr0.3CoO3 buffered STO substrates, with and without miscut, is compared in detail applying X-ray diffraction and high resolution transmission electron microscopy. The PMN-PT layers in both cases exhibit strain relaxation. While in the film without miscut perfect misfit dislocations are observed, in the film with miscut partial dislocations and stacking faults dominate the microstructure. These results may be useful to comprehend the stabilisation of the perovskite PMN-PT phase on miscut substrates.

DS 4: Focus Session: Two-dimensional materials I (jointly with HL/TT)

Time: Monday 9:30–12:45 Location: POT 81

Invited Talk DS 4.1 Mon 9:30 POT 81

Van der Waals heterostructures: tunnelling and interaction with light — •Artem Mishchenko — School of Physics and Astronomy, The University of Manchester, Manchester, UK

When graphene or other conducting 2D crystals are separated by an atomically thin insulating 2D crystal (e.g. hexagonal boron nitride), quantum mechanical tunnelling leads to the appreciable interlayer current between the two 2D conductors due to the overlap of their wave functions. These tunnel devices reveal exciting physics and great potential for applications: resonant tunnelling, negative differential conductance, light emission and detection, to name a few. Here, I will update on a current status and perspectives of tunnelling devices and quantum wells based on 2D materials assembled into van der Waals heterostructures. Particularly, I will present the results on tunnelling in mono- and bilayer graphene, tunnelling in 2D crystal-based quantum wells, and tunnelling in superconducting 2D materials. I will overview such effects as momentum and chirality conservation, phonon- and impurity-assisted tunnelling. Furthermore, interaction with light (i.e. photovoltaics, solar cells, light emission, lasing and plasmonics) within these heterostructures will be discussed. Finally, possible practical applications will be outlined.

DS 4.2 Mon 10:00 POT 81

Quantum emission from low dimensional materials — •Nathan Chejanovsky[1,2], Youngwook Kim[2], Andrea Zappe[1], Rainer Stöhr[1], Felipe Favaro de Oliveira[1], Durga Dasari[1,2], Amit Finkler[1], Jurgen H. Smet[2], and Jörg Wrachtrup[1,2] — [1]3rd Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Quantum emitters (QEs) in semi-conductors are at the forefront of optical research. 3D solid state systems [1] and quantum dots [2] are known sources of QEs. Nevertheless, quantum dots have constraints on temperature operation, broad linewidths and emission intermittency rendering these systems problematic. 3D systems suffer from light scattering and are difficult to process into tailored nano-structures.

Low dimensional wide band-gap materials (e.g. Van der Waals crystals) open possibilities for circumventing these obstacles, accessing intra-band gap states using sub-band gap excitation. Fulfilling this criteria, hexagonal boron nitride (h-BN), hosts room temperature QEs. [3] I summarize developments in this field and present results from our recent publication: [3] connecting structural features and QE location, generation of QEs using chemical etching/ion irradiation and analyzing their spectral features and photodynamics.

[1] Jelezko, F. et al. phys. stat. sol. (a) 2006, 203(13), 3207-3225
[2] Lodahl, P. et al. Reviews of Modern Physics 2015, 87 (2), 347-400
[3] Chejanovsky, N. et al. Nano letters 2016, 16, 7037-7045

DS 4.3 Mon 10:15 POT 81

Layered semiconductors coupled to an optical microcavity — •Michael Förg[1], Hisato Yamaguchi[2], David Hunger[3,4], and Alexander Högele[1] — [1]Fakultät für Physik and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Germany — [2]Materials Physics and Applications Division, Los Alamos National Laboratory, USA — [3]Ludwig-Maximilians-Universität München, Schellingstr. 4, München, Germany — [4]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, Garching, Germany

Two-dimensional atomic crystals of transition metal dichalcogenides exhibit remarkable optoelectronic properties in the limit of direct bandgap monolayers [1]. Bilayer heterostructures, on the other hand, feature long-lived indirect excitons potentially viable for studies of condensation phenomena [2]. In the scope of this work we investigate excitons in CVD grown layered semiconductors coupled to an optical microcavity. In our experiments we use a tunable open-access cavity with one curved fiber-based mirror and one planar mirror which supports laterally extended semiconductor flakes. This configuration allows us to combine controlled inter-mirror spacing with lateral scanning capabilities. While the former parameter is used to explore the light-matter coupling as a function of the cavity length, the latter enables two-dimensional cavity imaging of extended monolayer flakes to probe variations in the local crystal quality and the dielectric environment.

[1] Xu et al., Nat. Phys. 10, 343 (2014)
[2] Rivera et al., Nat. commun. 6 (2015)

DS 4.4 Mon 10:30 POT 81

Understanding single-photon emission from defects in hexagonal boron nitride

— •Sten Haastrup and Kristian S. Thygesen — Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark

Point defects in sheets of hexagonal boron nitride have recently been studied as potential single-photon emitters: Experimental studies have shown that the emission from point defect color centers has extremely narrow bandwidth and mainly takes place in the zero phonon line. From an engineering perspective, a high-quality source of single photons would be extremely useful for many applications including quantum computing and quantum communications. Currently, it is not clear which defect systems in boron nitride have the right properties for use as single-photon emitters; different experimental studies have observed emission at very different energies, indicating that multiple different defect states can produce single photons. This is the starting point for our investigation into which properties of defects are important for single-photon emission, and which properties of boron nitride make it suitable as host. We have used density functional theory to explore the potential energy surfaces of the ground- and lowest excited states around different point defects in hBN. Our calculations shed light on the observed narrow band nature of the emission lines and indicate potential routes for tuning emission energy, line width and lifetime.

DS 4.5 Mon 10:45 POT 81

On the Dynamics of Excitons in Perovskite Nanoplatelets

— •Alexander F. Richter[1,2], Verena A. Hintermayr[1,2], Florian Ehrat[1,2], Bernhard Bohn[1,2], Thomas Simon[1,2], Lakshminarayana Polavarapu[1,2], Alexander S. Urban[1,2], and Jochen Feldmann[1,2] — [1]Chair of Photonics and Optoelectronics, Department of Physics and Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität München (LMU), Amalienstraße 54, 80799 Munich, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 Munich, Germany

Organic-inorganic halide perovskites have received great attention in the past few years due to their remarkably high solar energy conversion efficiency. Their functionality is even more widespread showing vast improvements in light-emitting applications, especially in the form of nanocrystals. We have successfully synthesized two-dimensional perovskite nanoplatelets with a controllable thickness down to a single unit cell. This leads to exciton binding energies in the hundred meV range. Here, we present experimental results on the dynamics of excitons in such nanoplatelets. Time-resolved photoluminescence reveals an increased exciton recombination rate with decreasing crystal thickness. In addition, we derive exciton-phonon scattering rates from a linewidth analysis of linear optical spectra. These results are compared to exciton dephasing rates obtained by transient four-wave-mixing experiments.

Coffee break

Invited Talk DS 4.6 Mon 11:30 POT 81

Excitons in ultra-thin perovskites & van der Waals crystals

— •Alexey Chernikov — Department of Physics, University of Regensburg, Germany

Excitons, as first introduced by J. Frenkel in 1931, are fundamental quasiparticles in semiconductors, composed from an excited electron and the remaining hole with an effective positive charge bound together by the Coulomb interaction. The excitons strongly influence the materials‘ response to external fields and perturbations, and are of particular importance for a variety of applications, including solar cells, light emitters, lasers, modulators, and detectors. In addition, they play a major role in more advanced concepts, such as entangled photons from biexciton sources, excitonic qubits, carrier multiplication, and Bose-Einstein condensation.

In this talk, I will focus on the properties of excitonic particles in nanostructured two-dimensional materials: single layers of semiconducting organic-inorganic perovskites and van der Waals crystals as thin as a single unit cell. I will discuss the nature of an unusually strong and unconventional Coulomb interaction shared by these systems and demonstrate how it results in exciton binding energies as large as 0.5 eV with highly efficient light-matter interaction, largely determining the optical response of these ultra-thin layers. Finally, I will outline how the excitons can be externally tuned either by electrical and optical injection of charge carriers or through the dielectric engineering of the environment in heterostructures.

DS 4.7 Mon 12:00 POT 81

Carrier dynamics in MoS2

— •Michael Lorke, A. Steinhoff, M. Florian, C. Gies, M. Roesner, T. Wehling, and F. Jahnke — Institute for Theoretical Physics, University of Bremen, Germany

In the context of the current interest in transition-metal dichalcogenides, we study the optical generation and relaxation of excited carriers and their influence on optical properties. In these two-dimensional atomically thin semiconductors, the Coulomb interaction is known to be much stronger than in quantum wells of conventional semiconductors like GaAs, as witnessed by the up to 50 times larger exciton binding energy. The question arises, whether this translates into equivalently faster carrier-carrier Coulomb scattering of excited carriers. We answer this question by combining ab-initio band-structures and single-particle wave functions with kinetic equations for the Coulomb-induced carrier scattering in the full Brillouin zone, We find an ultrafast redistrubution of carriers into different valleys of the band structure on a 100fs timescale. The other main source of carrier relaxation is the interaction of the excited carriers with phonons. To analyze carrier-phonon scattering and dephasing, we solve kinetic equations, based on ab-initio carrier-phonon interaction matrix elements, both for carriers and phonons, including heating effects due to the excitation of non-equilibrium phonons. We find that within 100fs the electrons have relaxed into the valleys of the bandstructure, demostrating fast carrier dynamics, which is accompanied by the generation of non-equilibrium phonons. This process is followed by carrier cooling on a timescale of about 1ps, which is consistent with recent experimental findings.

DS 4.8 Mon 12:15 POT 81

Optical Properties of WSe_2 monolayers on metal films

— •Laxmi Narayan Tripathi, Oliver Iff, Simon Betzold, Sven Hoefling, and Christian Schneider — Technische Physik and Wilhelm-Conrad-Roentgen Research Center for Complex Material Systems, Universitaet Wuerzburg, Wuerzburg, Am Hubland, D-97074 Germany

Single photon generation is essential for quantum communications. For efficient quantum communication devices, a core requirement are single photon sources which are stable, bright, and which can be replicated. Recently, quantum light emission from inorganic two dimensional layers of transition metal dichalcogenides (TMDC), such as WSe_2, has been demonstrated.

In this contribution, we present our spectroscopy results from a metal-TMDC hybrid device. We performed low temperature (5K) photoluminescence measurement on a WSe_2 monolayer transferred mechanically on metal surface and obtained stable and sharp emission features as compared to bare TMDC monolayer on dielectric substrate. The nanoscale metal surface sample were prepared in the group of Prof Dai-Sik Kim, Seoul National University, South Korea. We envisage that the results will find application in quantum photonics.

DS 4.9 Mon 12:30 POT 81

Tamm-Plasmon Exciton-Polaritons with a WS2 monolayers at room temperature

— •Sebastian Stoll[1], Nils Lundt[1], Christian Schneider[1], and Sven Höfling[1,2] — [1]Technische Physik and Wilhlem-Conrad-Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Am Hubland, Germany — [2]SUPA, School of Physics and Astronomy, University of St. Andrews KY 16 9SS, UK

We demonstrate the formation of room temperature Tamm-plasmon Exciton-polaritons with a WS2 monolayer. Due to their high oscillator strength and stable excitonic complexes at 300 K, transition metal dichalcogenide monolayers have awaken strong interest in the field of light-matter interaction at high temperatures. Recently, WS2 was brought into the strong coupling regime by embedding it into both an open-cavity [1] and a Fabry-Perot-cavity consisting of two silver mirrors [2]. In this experiment, the use of a Tamm structure provides us with a narrower cavity linewidth and thus with a higher cavity Q-factor. The exciton-polariton dispersion was measured by momentum-resolved PL spectroscopy. The acquired dispersion shows the expected avoided crossing behaviour of the two polariton branches and yields a Rabi splitting of around 27 meV. References: [1] L.C. Flatten et al., Scientific Reports 6, 33134 (2016) [2] S. Wang et al., Nano Letters 16, 7 (2016)

DS 5: Fundamentals of Perovskite Photovoltaics I (jointly with CPP)

Time: Monday 10:15–13:00 Location: ZEU 222

Invited Talk DS 5.1 Mon 10:15 ZEU 222

The Versatility of Mesoscopic Solar Cells — •Anders Hagfeldt — Laboratory of Photomolecular Science, Swiss Federal Institute of Technology Lausanne (EPFL), CH-1015, Lausanne, Switzerland

In our work on solid-state dye-sensitized solar cells (ssDSSC) we have recently [1] shown that copper phenanthroline complexes can act as an efficient hole transporting material, achieving power conversion efficiencies of more than 11%.

In our work on perovskite solar cells (PSC) we have achieved efficiencies above 20% with a mixed composition of iodide/bromide and methyl ammonium/formamidinium. With the use of SnO2 compact underlayers as electron acceptor contacts we have constructed planar perovskite solar cells with a hysteresis free efficiency above 20% [2]. We have taken the cation mixing of the perovskite film further by including Cs+ and Rb+. Larger grains grown in a monolithic manner are observed and for example reproducibility and device stability are improved [3]. At the meeting we will discuss our champion data; up to 22% efficiency with an external electroluminescence of 4%, and an outstanding open-circuit voltage of 1.24 V at a band gap of 1.63 eV. Furthermore, we will report a breakthrough in stability at 85 oC for 500 h under full solar illumination.

References [1]*Freitag et al., Energy & Envir. Sci., DOI: 10.1039/C5EE1204J [2]*Correa et al., Energy & Envir. Sci., DOI:10.1039/C5EE02608C [3]*M. Saliba et al., Science 10.1126/science.aah5557 (2016)

DS 5.2 Mon 10:45 ZEU 222

Impact of Preparation Conditions on Properties of Perovskite Thin Films — •Alexander Hinderhofer[1], M. Ibrahim Dar[2], Jan Hagenlocher[1], Neha Arora[2], Michael Grätzel[2], and Frank Schreiber[1] — [1]Institute of Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]Laboratory of Photonics and Interfaces, EPFL, CH-1015 Lausanne, Switzerland

The performance of light emitting and light harnessing perovskite thin film devices depend strongly on their structural features. The so-called two-step conversion for preparing perovskite thin films, involves the deposition of lead halide precursor onto a substrate and the subsequent transformation of the resulting films into the perovskite phase by spin coating (drop casting) or dipping into an isopropanol solution containing a defined amount of methylammonium halide (CH_3NH_3X) (X=I,Br). It is well-known that the morphology and structural properties of perovskite depend strongly on the exact preparation conditions.

We applied grazing incidence wide angle x-ray scattering (GIWAXS) to determine the domain size and preferred orientation in several perovskite thin films. We will discuss the impact of different solvents and preparation methods (spin coating, dip coating) on the structure and morphology of the different perovskite films and we comment on the device performance. Finally, we will comment on the time scale of the crystallization process in $CH_3NH_3PbI_3$ perovskite thin films, which is accessible by in situ real time x-ray scattering.

DS 5.3 Mon 11:00 ZEU 222

Analysis of electronic trap states in methylammonium lead halide perovskite solar cells via thermally stimulated current — •Philipp Rieder[1], David Kiermasch[1], Mathias Fischer[1], Kristofer Tvingstedt[1], Andreas Baumann[1,2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research ZAE, 97074 Würzburg

While power conversion efficiencies already exceeding 22% have been achieved for organo lead halide perovskite solar cells, a complete understanding of its fundamental working principles is still missing, but nonetheless essential to further improve this type of thin film photovoltaic. To address the impact of electronic trap states on device performance, we probed solution processed methylammonium lead halide perovskite solar cells via thermally stimulated current (TSC) analysis. Thereby, after cooling the sample down to 10 K, possible trap states are filled optically and gradually released again by heating the sample back up to 300 K. This causes a weak current to flow, which allows to draw conclusions about the trap state density as well its energetic depth. We probed perovskite solar cells in normal as well as inverted device configuration to identify the influence of different transport layers on the energetic trap landscape and observe a substantial addition in the case of the commonly used TiO_2. Additionally, we studied the effect of incorporating bromine as well as chlorine to partly replace the iodine on the electrically active trap state distribution of the photoactive semiconductor.

DS 5.4 Mon 11:15 ZEU 222

Strong impact of processing parameters on morphology and crystal orientation of hybrid perovskite thin films for photovoltaic application — •Johannes Schlipf[1], Lukas Oesinghaus[1], Yinghong Hu[2], Nadja Giesbrecht[2], Sigrid Bernstorff[3], Thomas Bein[2], Pablo Docampo[4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]Department of Chemistry and CENS, LMU München, 80539 München — [3]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, 34149 Trieste, Italy — [4]Newcastle University, School of Electrical and Electronic Engineering, Newcastle upon Tyne NE1 7RU, UK

After five years of rapid research, power conversion efficiencies of hybrid perovskite solar cells (PSC) around 20% have become feasible for solution-processed multicrystalline thin films. However, photovoltaic performance, reproducibility and stability of PSC devices depend on crystal size and orientation which in turn are affected by processing parameters during synthesis. We investigate hybrid perovskite thin films with small and wide angle X-ray scattering (GISAXS, GIWAXS) and thereby identify key crystallization mechanisms that strongly influence film morphology and crystal orientation [1,2]. This not only shows the importance of rigorous control of processing parameters, but also renders film morphologies tunable which allows for a rational development of new synthesis methods for high efficiency PSC. [1] J. Schlipf et al., J. Phys. Chem. Lett. 2015, 6, 1265. [2] L. Oesinghaus et al., Adv. Mater. Interfaces 2016, 1600403.

15 min break

DS 5.5 Mon 11:45 ZEU 222

Local Time-Dependent Charging in a Perovskite Solar Cell — Victor W. Bergmann[1], Ilka M. Hermes[1], Dan Li[1], Alexander Klasen[1], Simon Bretschneider[1], Eiichi Nakamura[2], Rüdiger Berger[1], and •Stefan A.L. Weber[1,3] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]The University of Tokyo, Tokyo 113-0033, Japan — [3]Johannes Gutenberg University Mainz, 55128 Mainz, Germany

Efficient charge extraction within solar cells explicitly depends on the optimization of the internal interfaces. Potential barriers, unbalanced charge extraction or interfacial trap states can prevent cells from reaching high power conversion efficiencies. Furthermore, in perovskite solar cells, slow processes happening on timescales of seconds cause hysteresis. Here, we report on local and time-dependent potential measurements with Kelvin probe force microscopy (KPFM) on cross sections [1] of planar methylammonium lead iodide (MAPI) perovskite solar cells. The KPFM revealed distinct differences in the charging dynamics at interfaces of the MAPI to adjacent layers [2]. Illumination experiments showed that more than one process is involved in hysteresis. By locally resolving these processes we found distinct differences in the charging dynamics in different regions of the device. Our results support the scenario of mobile ions and interfacial trap states for explaining the hysteresis in our device. [1] Nat. Commun. 2014, 5. [2] ACS Appl. Mater. Interfaces, 2016, 8 (30), 19402.

DS 5.6 Mon 12:00 ZEU 222

Effect of Thermal and Structural disorder on Electronic Structure in Methylammonium Lead Halide Perovskites — •Cheng Li[1], Shivam Singh[2], Fabian Panzer[3], K L. Narasimhan[2], Yu Zhong[1], Anna Gräser[1], Tanaji Gujar[1], Mukundan Thelakkat[1], Anna Köhler[3], Dinesh Kabra[2], and Sven Huettner[1] — [1]Macromolecular Chemistry I, Universität Bayreuth, Universitätstr. 30, 95447 Bayreuth, Germany — [2]Indian Institute of Technology Bombay, Powai, 400076 Mumbai, Indian — [3]Experimentalphysik II, Universität Bayreuth, Universitätstr. 30, 95447 Bayreuth, Germany

In this work, to understand the structure of perovskite materials, we investigate the temperature dependence of optical properties of perovskite from room temperature (300K) to 6K. Unlike typical inorganic semiconductor, in both tetragonal (T>163K) and orthorhombic (T<163K) phases of MAPbI3, the band gap decreases with decrease in temperature. We indicate that this temperature dependence of the band gap is governed by the lattice expansion term instead of the electron-phonon interaction. The exciton linewidth is homogeneously broadened in both phases. The absorption, at the low energy edge of the exciton absorption, increases exponentially with energy, i.e reminiscent of Urbach tail absorption. The Urbach energy which is used to characterize order of structure, is modelled using thermal and static disorder for both phases separately.This work provides important insights to the electronic and structural properties of MAPbI3 based perovskites, and this method is transferable to many related perovskites.

DS 5.7 Mon 12:15 ZEU 222

Impact of bromine doping on recombination kinetics in perovskite solar cells — •David Kiermasch[1], Phillip Rieder[1], Kristofer Tvingstedt[1], Andreas Baumann[2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern) Bayern, 97074 Würzburg

Organo metal halide perovskite solar cells exhibit exceptionally good power conversion efficiency values exceeding already 20%. To allow further improvements it is important to understand the limiting processes e.g. charge carrier recombination in this new photovoltaic technology. Most of the recombination studies presented so far have been focused on perovskite films or crystals but only a few have studied the charge carrier dynamics in solar cell devices. We report on charge carrier lifetime values in bromine containing planar perovskite solar cells with varying the bromine content. The lifetime and corresponding charge carrier density has been derived from transient photovoltage (TPV) and charge carrier extraction (CE) experiments. We found increased lifetime values in solar cells with bromine ($\mathrm{MAPb(I_{3-x}Br_x)_3}$) compared to pure methylammonium lead iodine ($\mathrm{MAPbI_3}$). Furthermore, the CE signals from the bromine containing solar cells can be divided in two different extraction parts on different time scales leading to anomalously high extracted charge values. We discuss the experimental findings in regard of possible different contributions to the CE signal.

DS 5.8 Mon 12:30 ZEU 222

Reduced Recombination for High-Open-Circuit Voltages in CH3NH3PbI3 Solar Cells — •Christian M. Wolff[1], Fengshuo Zu[2], Andreas Paulke[1], Lorena Perdigon Toro[1], Norbert Koch[2], and Dieter Neher[1] — [1]Universität Potsdam, Institut für Physik und Astronomie — [2]Humboldt-Universität zu Berlin, Institut für Physik

Perovskite solar cells with all-organic transport layers have shown efficiencies rivalling their counterparts that employ inorganic transport layers while avoiding high temperature processing. We investigate how the choice of the fullerene derivative employed in the electron-transporting layer of inverted perovskite cells affects the open circuit voltage. Non-radiative recombination mediated by the electron-transporting layer is the determining factor for the open-circuit voltages in our cells. By inserting an ultra thin layer of an insulating polymer between the active CH3NH3PbI3 perovskite and the fullerene layer, external radiative efficiencies of up to 0.3%, open-circuit voltages (Voc) as high as 1.16V and with efficiencies up to 19.4% were realised. Our results show that reduction of non-radiative recombination due to charge-blocking at the perovskite/organic interface is more important than proper alignment in the search for ideal selective contacts for high Voc.

DS 5.9 Mon 12:45 ZEU 222

On the chemical origins of crystalline preferred orientations in hybrid organometallic lead halide perovskite thin films — •Shambhavi Pratap, Johannes Schlipf, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Solar cells based on organometallic lead halide perovskites have established themselves as a promising alternative to commercial thin film solar cells. The crystallographic versatility of the material allows the possibility of extensive chemical tuning, which manifests in the material as a spectra of properties that may be obtained. This entices research on hybrid perovskite structures combining different organic and inorganic groups into a crystalline framework. Preferential orientations of the crystalline hybrid perovskites (1) are reported and correlated to their morphological and chemical characteristics by grazing incidence wide angle x-ray scattering (GIWAXS). Remarkably, perovskite thin films prepared by the same methodologies displayed varying behaviors of preferred orientations, as their chemical composition was varied. Moreover, the route and rate of crystallization (2) is known to radically influence crystalline preferred orientations as well, giving rise to information regarding kinetic and thermodynamic orientations. These results, for the first time propose the possibility of controlling crystallinity of spin-coated thin films by tuning the ingredients of and the treatment of the solution used for spin coating.

(1) Oesinghaus et al., Adv. Mater. Interfaces 2016, 3, 1600403

(2) Giesbrech et al., ACS Energy Lett. 2016, 1, 150-154

DS 6: 2D Materials Beyond Graphene I (jointly with O)

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

DS 6.1 Mon 10:30 REC/PHY C213

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

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

We present a 2D $\mathrm{SiO_2}$ bilayer film, prepared on a Ru(0001) substrate via CVD. The atomic structure has been investigated using scanning probe microscopy.[1] Extended honeycomb structures and glass-like network structures were identified, while DFT calculations and STS measurements indicate a band gap larger than 6.5 eV.[2,3]

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

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

DS 6.2 Mon 10:45 REC/PHY C213

Photocarrier dynamics and interaction effects of interlayer excitons in $\mathrm{WSe_2/MoSe_2}$ heterostructures — •Philipp Nagler, Gerd Plechinger, Alexey Chernikov, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Regensburg, Germany

Atomically thin transition metal dichalcogenides (TMDCs) such as $\mathrm{WSe_2}$ or $\mathrm{MoSe_2}$ have lately emerged as a promising platform to study the physics of excitons in strongly confined systems. Thereby, the use of transfer techniques allows for the fabrication of van der Waals heterostructures by deterministic stacking of individual monolayers. It is expected that type-II band alignment of the individual monolayers results in the formation of spatially indirect excitons. Here, we present a detailed study of the optical properties of interlayer excitons in a $WSe_2/MoSe_2$ heterostructure using static and time-resolved photoluminescence measurements. At low temperatures, we observe the emergence of an energetically separated (1.4 eV) and spectrally sharp (FWHM < 20meV) feature, which we attribute to the emission of interlayer excitons. Power-dependent measurements show a considerable blue shift of the interlayer exciton peak position due to dipolar exciton-exciton interaction effects. Finally, we employ a streak camera system in order to reveal the photocarrier dynamics of interlayer excitons for varying temperatures. The lifetime at low temperatures amounts to several nanoseconds, which is a consequence of the reduced oscillator strength of the interlayer exciton.

DS 6.3 Mon 11:00 REC/PHY C213

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

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

DS 6.4 Mon 11:15 REC/PHY C213

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

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

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

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

DS 6.5 Mon 11:30 REC/PHY C213

Realization of stanene on the surface of Au(111) — •Mahalingam Maniraj[1], Benjamin Stadtmüller[1], Wujun Shi[2], Dominik Jungkenn[1], Sebastian Emmerich[1], Johannes Stöckl[1], Lu Lyu[1], Jobynson Kollamana[1], Zheng Wei[1], Anatol Jurenkow[1], Sebastian Jakobs[1], Yongli Gao[3], Mirko Cinchetti[4], Binghai Yan[2], Stefan Mathias[5], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Department of Physics and Astronomy, University of Rochester, Rochester, NY 14627 — [4]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany — [5]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

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

DS 6.6 Mon 11:45 REC/PHY C213

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

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

DS 6.7 Mon 12:00 REC/PHY C213

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

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

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

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

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

DS 6.8 Mon 12:15 REC/PHY C213

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

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

DS 6.9 Mon 12:30 REC/PHY C213

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

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

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

DS 6.10 Mon 12:45 REC/PHY C213

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

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

[1] Akcöltekin S. et al. *Applied Physics Letters*, 98 (2011) 103103
[2] Ochedowski O. et al. *NimB*, 340 (2014) 39.
[3] Ochedowski O. et al. *Nanotechnology*, 26 (2015) 465302

DS 7: Atomic Layer Deposition

Time: Monday 12:30–13:15 Location: CHE 89

DS 7.1 Mon 12:30 CHE 89

Atomic layer deposition (ALD) for the fabrication of HfO_2- and TiO_2- based resistive switching memories — •Alexander Hardtdegen, Hehe Zhang, and Susanne Hoffmann-Eifert — Peter Grünberg Institute and JARA-Fit, Forschungszentrum Jülich, 52425 Jülich, Germany

One common growth method for ultrathin metal oxide layers used in resistive switching devices is atomic layer deposition. Often used materials for these devices are e.g. HfO_2 and TiO_2, which are generally deposited in the amorphous phase. Nevertheless resistive switching behaves differently even in cells out of the apparently same material, as the switching properties are very sensitive to the amount of oxygen in the functional layers.

In this study, plasma-enhanced ALD HfO_2 is combined with three qualitative different (sub-)stoichiometric TiO_2-layers, comparing either layers which were deposited with liquid injection and bubbler supplied TDMAT or thermal processes with processes based on oxygen plasma as co-reactant. The bilayers were integrated into metal-insulator-metal structures and electrically characterized. The switching behavior gives information about the oxygen amount within the different TiO_2-layers.

DS 7.2 Mon 12:45 CHE 89

Al_2O_3 ALD on pristine graphene — •Marcel Junige[1], Julia Kitzmann[2], Marion Geidel[1], Grzegorz Lupina[2], Matthias Albert[1], Christian Wenger[2], and Johann W. Bartha[1] — [1]Technische Universität Dresden — [2]IHP GmbH, Frankfurt (Oder)

Coating monolayer graphene (here: CVD-G) with ultra-thin ($<10\,\mathrm{nm}$), continuous (pinhole-free), smooth, and electrically well-insulating films is prerequisite for graphene-based applications in electronics, sensors, etc., but has yet been very challenging due to graphene's lack of dangling bonds. Thus, the nucleation of a dielectric's Atomic Layer Deposition (ALD) on CVD-G has commonly been inhibited and the corresponding Volmer-Weber island growth mode has produced sporadic, rough, and electrically leaky deposits, preferentially decorating defects.

Apart from a previous improvement[1] by pre-treating CVD-G with NF_3, we studied here a lower Al_2O_3 ALD set-point temperature of 200 °C compared to 400 °C on pristine CVD-G. The reduced deposition temperature indeed supported a faster and more dense Al_2O_3 ALD nucleation upon the plane CVD-G surface. The ALD growth initiation, the CVD-G integrity, and the coating morphology were investigated by a unique metrology combination of *in-situ* real-time Spectroscopic Ellipsometry, *in-vacuo* X-Ray Photoelectron Spectroscopy, and Atomic Force Microscopy, respectively.

[1] Junige, M. *et al.* in *Proc. of SPIE Vol. 9519*, p. 951915 – DOI:10.1117/12.2181242.

DS 7.3 Mon 13:00 CHE 89

A hybrid molecular beam epitaxy based growth method for large-area synthesis of stacked hexagonal boron nitride/graphene heterostructures — •Siamak Nakhaie[1], Joseph M. Wofford[1], Thilo Krause[1], Xianjie Liu[2], Manfred Ramsteiner[1], Michael Hanke[1], Henning Riechert[1], and J. Marcelo J. Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]Department of Physics, Chemistry and Biology, Linköping University, SE-58183 Linköping, Sweden

Devices based on the graphene/hexagonal boron nitride (h-BN) materials system offer a host of potential advantages, including high speed, extremely low power consumption, and various novel functionalities. As a result, the large-area synthesis of this material has been extensively researched over the past few years using various crystal growth techniques. In this contribution, we introduce a method for the production of h-BN/graphene heterostructures which allows both materials to form on the surface of the Ni substrate. We exploit the finite solubility of C in Ni by first saturating the metal film, then depositing a few-layer thick h-BN film from elemental B and N on the exposed Ni surface, and finally ramping the sample temperature down to controllably precipitate the C and form graphene at the interface between the h-BN and Ni. The resulting heterostructures are studied using various characterization techniques, such as UV and visible Raman spectroscopy, x-ray photoelectron spectroscopy and synchrotron-based grazing incidence spectroscopy to learn about their structural properties and quality.

DS 8: Focus Session: Two-dimensional materials II (jointly with HL/TT)

Time: Monday 14:45–18:15 Location: POT 81

Invited Talk DS 8.1 Mon 14:45 POT 81

2D / 3D Heterostructures for Optoelectronis — •Max Lemme — University of Siegen, Germany

Broad spectral optical detection is of high interest for imaging, sensing, communication and spectroscopy. Two-dimensional (2D) materials are very promising for such applications due to their high optical absorption, potential wide detection range and material flexibility.

In this talk, graphene / silicon Schottky diodes made of chemical vapor deposited (CVD) graphene on n-type Si substrates will be discussed. Broad spectral response of 60 - 407 mA/W is measured from ultraviolet to near infrared light. In contrast to graphene, bulk molybdenum disulfide (MoS_2) is an n-type semiconducting 2D material with an indirect band gap of 1.3 eV. MoS_2/Si hybrid diodes made with multilayer, CVD grown MoS_2 yield a maximum spectral response of 8.6 mA/W.

Hybrid integration of large area CVD graphene as transparent conductive electrodes with amorphous silicon (a-Si) will be discussed for applications as multispectral photodetectors. A strong enhancement of the detectors' spectral response is observed in the ultraviolet region compared to reference devices with conventional aluminum doped zinc oxide electrodes. The maximum responsivity of these multispectral PDs can be tuned in their wavelength from 320 nm to 510 nm by external biasing, which allows single pixel detection of UV to visible light. The material combination of graphene and a-Si enables flexible diodes on polyimide substrates. Bilayer graphene boosts the maximum photoresponsivity of these flexible diodes up to 239 mA/W.

DS 8.2 Mon 15:15 POT 81

Optical properties of atomically thin MoS2 exposed to helium ions — •Anna Nolinder[1], Julian Klein[1,2], Agnieszka Kuc[4], Marcus Altzschner[1], Jakob Wierzbowski[1], Florian Sigger[1], Franz Kreupl[3], Thomas Heine[4], Jonathan Finley[1,2], Ursula Wurstbauer[1,2], Alexander Holleitner[1,2], and Michael Kaniber[1] — [1]Walter Schottky Institut und Physik Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 München, Germany — [3]Department of Hybrid Electronic Systems, Technische Universität München, Arcisstr. 21, 80333 Munich, Germany — [4]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstr. 2, 04103 Leipzig, Germany

We present a spectroscopic study on atomically thin MoS2 exposed to helium ions. Distinct changes of the first-order Raman bands, additional defect luminescence and strong modification of the intrinsic valley spin relaxation properties are observed, shedding light on the effect of disorder on the optical properties and valley spin relaxation mechanisms. Moreover, our observations are in good qualitative agreement with Density Functional Theory calculations.

DS 8.3 Mon 15:30 POT 81

Coulomb Engineering of Excitonic Transitions in Transition Metal Dichalcogenides for New Non-Classical Light Sources — •Sven Borghardt[1], Jhih-Sian Tu[1], Tim Flatten[2], Frank Matthes[2], Daniel Bürgler[2], Detlev Grützmacher[1], and Beata Kardynal[1] — [1]Peter Grünberg Institute 9 (PGI-9), Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Peter Grünberg Institute 6 (PGI-6), Forschungszentrum Jülich, D-52425 Jülich, Germany

The spatial confinement of excitons is a key prerequisite for the creation of non-classical light sources. Since the dielectric environment of transition metal dichalcogenide monolayers (TMD-MLs) changes the screening of electrostatic fields and, thus, the interaction of charge carriers within the MLs, both the single particle band gap and the binding energy of exciton complexes in TMD-MLs can be tuned by modifying the dielectric properties of the environment.

In our experiments, we prepare TMD-MLs in different environments and apply optical spectroscopy methods in order to quantify the effects of the dielectric environment on the transition energies of exciton complexes. Furthermore, we correlate the results with single particle band gaps estimated from excited exciton states and single particle band gaps measured in scanning tunnelling spectroscopy experiments. This correlation gives access to the binding energy of exciton complexes.

In addition to TMD-MLs in laterally homogeneous environments, we examine lateral heterostructures of TMD-MLs in environments with laterally changing dielectric properties, paving the way towards controllable confinement of excitons within TMD-MLs.

DS 8.4 Mon 15:45 POT 81

Exciton-trion competition and single photon emission in III-V- monolayer hybrid architectures — •Oliver Iff[1], Yu-Ming He[1], Nils Lundt[1], Sebastian Stoll[1], Vasilij Baumann[1], Sven Hoefling[1,2], and Christian Schneider[1] — [1]Technische Physik and Wilhelm Conrad Roentgen Research Center for Complex Material Systems, Physikalisches Institut, Universitaet Wuerzburg, Am Hubland, D-97074 Wuerzburg, Germany — [2]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

Atomic monolayers represent a novel class of materials to study localized and free excitons in two dimensions and to engineer optoelectronic devices based on their significant optical features. Here, we investigate the role of epitaxially grown III-V substrates on the photoluminescense response from exfoliated MoSe2 and WSe2 monolayers in comparison to regular SiO2 substrates. In the case of MoSe2, we observe a significant qualitative modification of the emission spectrum, which is widely dominated by the trion resonance on InGaP substrates. Even more remarkably, in sheets of WSe2, we notice emission lines from localized excitons with linewidths down to 70 μeV, only limited by our system resolution. Furthermore, these spectral signatures are identified as single photon or even photon pair emitters without any sign of spectral jitter or blinking. Overall, the results outline the enormous potential of hybrid III-V- monolayer architectures in obtaining high quality emission signals from atomic monolayers, enhancing their optical properties.

DS 8.5 Mon 16:00 POT 81

The Influence of the Substrate Material on the Optical Properties of Tungsten-Diselendide Monolayers — Sina Lippert[1], •Lorenz Schneider[1], Dylan Renaud[1], Kyung Nam Kang[2], Obafunso Ajayi[3], Marc Halbich[1], Oday Abdulmunem[1], Xing Lin[1], Jan Kuhnert[1], Khaleel Hassoon[1], Saideh Edalati-Boostan[1], Young Duck Kim[3], Wolfram Heimbrodt[1], Eui-Hyeok Yang[2], James Hone[3], and Arash Rahimi-Iman[1] — [1]Faculty of Physics, Philipps-Universität, Marburg 35032, Germany — [2]Department of Mechanical Engineering, Stevens Institue of Technology, Hoboken, New Jersey, 07030, USA — [3]Department of Mechanical Engineering, Columbia University, New York, New York, 10027, USA

In recent years 2D materials based on transition metal dichalogenides (TMDs) have come up as an interesting material system mainly due to their remarkable properties in the monolayer regime after the successful exploration of graphene. While the main optical properties of these materials have been studied and understood well, the influence of the substrate material on the energy levels and the recombination dynamics are not yet sufficiently discussed. Here, we present a systematic comparison of the optical properties of monolayered WSe$_2$ on different substrates including SiO$_2$, sapphire, Si$_3$N$_4$-hBN and MgF$_2$. In addition to the exfoliated monolayers, a CVD grown monolayer on sapphire is included. While similarities have been found for the Raman signal and PL of these samples, small differences regarding excitonic features, emission characteristics and decay dynamics have been observed in dependence on the substrate.

Coffee Break

Invited Talk DS 8.6 Mon 16:45 POT 81

Excitons in colloidal 2D-CdSe nanocrystals — •Ulrike Woggon — Institut für Optik und Atomare Physik, TU Berlin, Str. des 17. Juni 135, 10623 Berlin, Germany

Two-dimensional II-VI semiconductor nanoplatelets (NPLs) gained increasing interest because of their unique electronic and optical properties, such as the Giant Oscillator Strength, strong electroabsorption response, low exciton-phonon interaction and high impact of dielectric confinement on exciton binding energies [1]. CdSe platelets are of special importance since they combine large particle volumes with ultrastrong confinement. We present a comprehensive study of the influence of dimensionality, size and shape on excitons in CdSe NPLs. They are an attractive system allowing to control not only the exciton energy states by thickness (z-direction) but also with lateral size variation the LO-phonon coupling (x,y-direction) [2]. The larger the particles' aspect ratio, the greater is the confinement related electronic contribution to the increased two-photon absorption and CdSe NPLs are ideally suited for two-photon imaging and non-linear opto-electronics [3-5]. [1] A.W. Achtstein et al., Nano Letters 12, 3151 (2012); [2] A.W. Achtstein et al., Phys. Rev. Lett. 116, 116802 (2016); [3] A.W. Achtstein et al., J. Phys. Chem. C 119, 20156 (2015); [4] R. Scott et al., Nano Lett. 15, 4985 (2015); [5] A.W. Achtstein et al., ACS Nano 8, 7678 (2014)

DS 8.7 Mon 17:15 POT 81

Controlled MoS2 deposition by metal-organic vapour phase epitaxy — Matthias Marx[1], Dominik Andrzejewski[2], Annika Grundmann[1], You-Ron Lin[1,3], Gerd Bacher[2], Holger Kalisch[1], Andrei Vescan[1], and •Michael Heuken[1,3] — [1]GaN Device Technology, RWTH Aachen University — [2]WET, University Duisburg-Essen — [3]AIXTRON SE

Recently, layered transition metal dichalcogenides (TMDC) have attracted a lot of attention. Their thermodynamically stable 2D form and their unique electrical and optical properties are very promising for integration in future electronic devices. For systematic scientific studies and in particular for implementation in commercial devices, it will be necessary to achieve a reproducible, homogeneous and scalable deposition on wafer scale. A promising option to achieve this goal is to use metal-organic vapour phase epitaxy (MOVPE) processes employing MO precursors for the TMDC constituents. All deposition experiments reported here are carried out in an AIXTRON horizontal hot-wall reactor. Molybdenum hexacarbonyl (MCO) and Di-tert-butyl sulfide (DTBS) are used as Mo and S sources, respectively. The samples are characterized via Raman spectroscopy, photoluminescence (PL) spectroscopy, atomic force microscopy (AFM) and scanning electron microscopy (SEM) to investigate their optical and structural properties. To reduce and control the nucleation density and to promote a layer-by-layer growth mode, the growth parameters such as DTBS and MCO precursor flows are optimized and temperature treatment was adjusted.

DS 8.8 Mon 17:30 POT 81

Ion implantation of 2D transition metal dichalcogenides monolayers — •Jihih-Sian Tu[1], Sven Borghardt[1], Hans Hofsass[2], Ursel Bangert[3], Quentin Ramasse[4], Detlev Grützmacher[1], and Beata Kardynał[1] — [1]PGI 9, Forschungszentrum Jülich, Jülich, Germany — [2]II. Physikalisches Institut, Georg-August-University Göttingen, Göttingen, Germany — [3]Department of Physics, Univsity of Limerick, Limerick, Ireland — [4]SuperSTEM Laboratory, Daresbury, UK

Monolayer transition metal dichalcogenides (TMDs) have gained interest as material for optoelectronics. In order to realise the technological potential of the TMDs semiconductors, it is desirable to be able to form heterostructures and introduce dopants in the monolayers. In this study, we examine the possibility to do so using ion implantation. We show that chalcogen atoms of the monolayer MoS2 can be substituted using very low energy ion beams (<50 eV) as verified using Raman spectroscopy and scanning transmission electron microscopy. Implantation levels of a few percent are realised with no structural damage visible in Raman spectra. Significant changes of the photoluminescence compared with pristine MoS2 monolayers are observed at cryogenic temperature. The technique under development is to be applied for forming lateral heterostructures of 2D TMDs.

DS 8.9 Mon 17:45 POT 81

synthesis of bismuth/reduced graphene oxide composites and their electrochemical properties for Na-ion batteries — •Benrong Hai[1,2], Yang Xu[1], Min Zhou[1], Liying Liang[1], and Yong Lei[1] — [1]TU-ilmenau, Ilmenau, Germany — [2]Northeastern University, Shenyang, P. R. China

Recently, Na-ion batteries have been considered as a desirable alternative to Li-ion batteries, because of the greater abundance and lower cost of sodium-containing precursors. Even though Na-ion batteries have attracted great attention, more research is needed to enhance their performance. Reduced graphene oxide sheets have extraordinary electronic transport properties, large surface area and mechanical flexibility. Therefore, reduced graphene oxide sheets have been considered as a matrix material to improve electrochemical performance of metal nanoparticles. Here, we demonstrate a facile strategy to prepare bismuth/reduced graphene oxide composites. Such composites exhibit high specific capacity and enhanced cycling performance as anode. Compared to pure bismuth nanoparticles, the enhancement of sodium storage could be attributed to the introduction of reduced graphene oxide sheets that not only buffer the large volume changes during the reaction of sodium and bismuth, but also provide a highly conductive network for rapid electron transport in electrochemical reaction.

DS 8.10 Mon 18:00 POT 81

Optical properties of boron vacancies and boron vacancy complexes in hexagonal boron nitride — •Mažena Mackoit and Audrius Alkauskas — Center for Physical Sciences and Technology, Vilnius, Lithuania

In this work we perform density functional theory calculations of boron vacancies and boron vacancy complexes with oxygen in hexagonal boron nitride. It is shown that interaction with oxygen significantly lowers the formation energy of boron vacancies. Therefore, when oxygen is present, complexes are more likely to occur that bare vacancies. We find that electronic defect states can be of both σ and π type. This gives rise to various possible configurations of ground and excited states. In particular, it is suggested that intra-defect luminescence can be polarized both in- and out-of-plane. We also provide estimates of intra-defect excitation energies and associated Franck-Condon shifts, making the connection with recent experimental observations of single photon emitters in this material.

DS 9: Transport: Graphene and Carbon Nanostructures (jointly with HL/MA/TT)

Time: Monday 15:00–18:15 Location: HSZ 204

DS 9.1 Mon 15:00 HSZ 204

Creating and steering highly directional electron beams in graphene — Ming-Hao Liu[1,2], •Cosimo Gorini[1], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, Regensburg, Germany — [2]Department of Physics, National Cheng Kung University, Tainan, Taiwan

We put forward a concept to create highly collimated, non-dispersive electron beams in pseudo-relativistic Dirac materials such as graphene or topological insulator surfaces [1]. Combining negative refraction and Klein collimation at a parabolic *pn* junction, the proposed lens generates beams, as narrow as a few Fermi wave lengths, that stay focused over scales of several microns and can be steered by a magnetic field without losing collimation. We demonstrate the lens capabilities by applying it to two paradigmatic settings of graphene electron optics: We propose a setup for observing high-resolution angle-dependent Klein tunneling, and, exploiting the intimate quantum-to-classical correspondence of these focused electron waves, we consider high-fidelity transverse magnetic focusing accompanied by simulations for current mapping through scanning gate microscopy. Our proposal opens up new perspectives for next-generation graphene electron optics experiments.

[1] M.-H. Liu, C. Gorini, K. Richter, arXiv:1608.01730.

DS 9.2 Mon 15:15 HSZ 204

Graphene *p*-*n* junction in a magnetic field as a valley switch — •Tibor Sekera, Rakesh P. Tiwari, and Christoph Bruder — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Low-energy excitations in graphene exhibit relativistic properties due to the linear dispersion relation close to the Dirac points in the first Brillouin zone. Two of the cones located at opposite corners of the first Brillouin zone can be chosen as inequivalent, representing a new *valley* degree of freedom, in addition to the charge and spin of an electron. Using the valley degree of freedom to encode information aroused significant interest, both theoretically and experimentally, and gave rise to the field of *valleytronics*.

We study a graphene *p*-*n* junction in an out-of-plane magnetic field as a platform to generate and controllably manipulate the valley polarization of electrons. We show that by tuning the external potential giving rise to the *p-n* junction we can switch the current from one valley polarization to the other. We also consider the effect of different types of edge terminations and present a setup, where we can partition an incoming valley-unpolarized current into two branches of valley-polarized currents. The branching ratio can be chosen by changing the location of the *p-n* junction.

DS 9.3 Mon 15:30 HSZ 204

Probing electronic wave functions in a nanotube quantum dot via conductance in a magnetic field — Magdalena Marganska[1], Alois Dirnaichner[1,2], Daniel R. Schmid[2], Peter L. Stiller[2], Christoph Strunk[2], Milena Grifoni[1], and •Andreas K. Hüttel[2] — [1]Institute for Theoretical Physics, Universität Regensburg, Regensburg, Germany — [2]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

The tunneling of electrons through a contact between two systems depends on the overlap of their electronic wave functions. In quantum dots the overlap is often tuned via the height of tunneling barriers. Conversely, in carbon nanotubes the unique combination of cylindrical topology and honeycomb atomic lattice allows for a manipulation of the longitudinal component of the electronic wave function via a parallel magnetic field. The amplitude of the wave function at the point of contact with the leads is directly reflected in the coupling strength. Experimentally, we detect the changes in the electronic wave function through the evolution of conductance resonances corresponding to single particle quantum states with magnetic field. The magnitude of the magnetic field in our experiment, up to 17 T, allows us to confirm our prediction of the very different behaviour of the two valley states. The K' valley states experience a strengthening of the tunnel coupling at low magnetic field, followed by subsequent decoupling. In contrast, the K valley states decouple from the leads monotonically, and coupling becomes unmeasurably small already for moderate magnetic fields.

DS 9.4 Mon 15:45 HSZ 204

Electron-electron interaction correction to tunneling in graphene-graphene nanojunctions — •Matthias Popp, Ferdinand Kisslinger, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg (FAU), Erlangen, Germany.

In weakly disordered conductors, electron-electron interaction is expected to provide a zero-bias anomaly in tunneling characteristics [1]. This purely electronic effect is seemingly suppressed in scanning tunneling spectroscopy experiments on graphene due to momentum mismatch, which requires phonon assisted tunneling. [2,3]. In order to overcome this limitation, we fabricate in-plane graphene-graphene nanojunctions by an electro burning process using epitaxial graphene on SiC as starting material. In some junctions with an overall conductance of about e^2/h we indeed observed a zero-bias anomaly at low temperatures which follows the logarithmic scaling characteristics predicted by *Altshuler* and *Aronov*. These experiments offer the opportunity to study the nonlocal aspects of electron tunneling via manipulation of the environment.

[1] Altshuler, B. L. and Aronov, A. G., *Electron-Electron Interaction in Disordered Conductors*, 1985
[2] Brar, V. W. et al., Applied Physics Letters, 2007, 91, 122102
[3] Zhang, Y. et al., Nature Physics, 2008, 4, 627-630

DS 9.5 Mon 16:00 HSZ 204

Electroluminescence of Graphene Nanojunctions — •Christian Ott, Konrad Ullmann, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstr. 7/A3, D-91058 Erlangen, Germany

We report on electroluminescence (EL) detected at graphene nanojunctions, the latter being formed by electroburning of epitaxial graphene ribbons on silicon carbide [1]. The EL shows a broad spectrum with emphasis on the near infrared regime. Its intensity scales with applied current and is temperature independent down to liquid helium temperatures. Surprisingly, we find a weak voltage dependence. The spectrum is similar to blackbody radiation with apparent temperatures well above the damage threshold of graphene and the silicon carbide substrate. A similar phenomenon has already been observed in single atom point contacts [2] and island metal films [3]. There a model was proposed based on hot electron luminescence which goes along with a large mismatch between electron gas temperature and lattice temperature due to a reduced electron-phonon interaction in nanoscopic structures. A critical discussion of the underlying mechanism is provided.

[1] Ullmann et al, Nano Letters 15, 5 (2015)
[2] Downes et al., Applied Physics Letters 81, 7 (2002)
[3] Fedorovich et al., Physics Reports 328 (2000)

DS 9.6 Mon 16:15 HSZ 204

Reversible Photochemical Control of Doping Levels in Supported Graphene — •Marie-Luise Braatz[1,2], Nils Richter[1,2], Hai I. Wang[1], Axel Binder[3], Mischa Bonn[4], and Mathias Kläui[1,2] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz (MAINZ), 55128 Mainz, Germany — [3]BASF SE, 67056 Ludwigshafen, Germany — [4]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

The type and density of carriers in graphene are important parameters to control its properties. Based on Terahertz (THz)-spectroscopy and electrical characterization of Nitrogen-doped graphene, we show that the doping level can be optically tuned between the p-type and intrinsic n-type regime [1]. This is achieved photochemically by controlling the dynamical equilibrium between the oxygen adsorption and desorption process via UV laser pulse irradiation treatment [2]. This approach is reversible, easy to use and contact free. This simple method can be used to write doping structures with spatial control by a focused laser beam, not requiring sophisticated nanostructuring to generate doping for instance by gate electrodes that need to be defined at the time of device fabrication.

[1] H. I. Wang, M.-L. Braatz et al., submitted (2016)
[2] S. M. Hornett et al., Phys Rev B 90 (2014)

15 min. break.

DS 9.7 Mon 16:45 HSZ 204

Time evolution of Floquet states in graphene — •Matteo Puviani[1], Francesco Lenzini[1], and Franca Manghi[1,2] — [1]Dipartimento FIM, Università di Modena e Reggio Emilia — [2]CNR - Institute of NanoSciences - S3, Modena

When a time-periodic field is applied to electrons in a lattice the Bloch theorem can be applied twice, both in space and in time, to describe the photon-dressed quasiparticles which are formed. This is the essence of Floquet theory, which has recently attracted a large renewed interest for its ability to describe topological phases in driven quantum systems. The discovery that circularly polarized light may induce nontrivial topological behavior in materials which would be standard in static condition has opened the way to the realization of the so-called Floquet Topological Insulators. In these systems, the topological phases may be engineered and manipulated by tunable controls such as polarization, periodicity and amplitude of the external perturbation.

In the presence of a continuous time-periodic driving, electrons are in a non-equilibrium steady state characterized by a time-periodic dependence of the wave function, and therefore of the expectation values of any observable. In this talk we will consider the prototypical case of graphene that, under the influence of circularly polarized light, exhibits in its Floquet band structure the distinctive features of a topological insulator, namely a gap in 2D and linear dispersive edge states in 1D (graphene nanoribbon). In particular, we will discuss how these characteristics affect the time behavior of some relevant observables such as energy, charge and current density.

DS 9.8 Mon 17:00 HSZ 204

Quantum chaos and out-of-time order correlation functions in graphene — •Markus Klug, Mathias Scheurer, and Jörg Schmalian — Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Deutschland

Out-of-time order correlation functions of type $C = \langle A(t)B(0)A(t)B(0)\rangle_\beta$ are believed to be a reasonable measure of quantum chaos which manifests in an exponential growth of C with a certain Lyapunov exponent determined by the microscopic model under considerations. Recently, it was conjectured hat this Lyapunov exponent is be bounded by $\lambda \leq 2\pi k_B T/\hbar$ [1].

In this work we investigate the out-of-time order correlation functions in graphene subject to the long range Coulomb interaction. To this end we develop a formalism to capture the relevant effects which determines the dominant time dependence of C. We demonstrate that the critical Dirac fluid graphene is a good candidate for saturating the

bound mentioned above.
[1] J. Maldacena, S.H. Shenker and D. J. Stanford, High Energ. Phys. (2016) 2016: 106.

DS 9.9 Mon 17:15 HSZ 204

Interaction induced Dirac fermions from quadratic band touching in bilayer graphene — •Thomas C. Lang[1], Sumiran Pujari[2], Ganpathy Murthy[2], and Ribhu K. Kaul[2] — [1]Institute for Theoretical Physics, University of Innsbruck, Austria — [2]Department of Physics & Astronomy, University of Kentucky, Lexington, KY

We revisit the effect of local interactions on the quadratic band touching (QBT) of Bernal stacked bilayer graphene models using renormalization group (RG) arguments and quantum Monte Carlo simulations of the Hubbard model. We present an RG argument which predicts, contrary to previous studies, that weak interactions do not flow to strong coupling even if the free dispersion has a QBT. Instead they generate a linear term in the dispersion, which causes the interactions to flow back to weak coupling. Consistent with this RG scenario, in unbiased quantum Monte Carlo simulations of the Hubbard model we find compelling evidence that antiferromagnetism turns on at a finite U/t, despite the $U = 0$ hopping problem having a QBT. The onset of antiferromagnetism takes place at a continuous transition which is consistent with $z = 1$ as expected for Gross-Neveu criticality. We conclude that generically in models of bilayer graphene, even if the free dispersion has a QBT, small local interactions generate a Dirac phase with no symmetry breaking and there is a finite-coupling phase transition out of this phase to a symmetry-broken state.

DS 9.10 Mon 17:30 HSZ 204

Dynamical charge and pseudospin currents in graphene and possible Cooper pair formation — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

With the quantum kinetic equations for systems with SU(2) structure, regularization-free density and pseudospin currents are calculated in graphene realized as the infinite mass-limit of electrons with quadratic dispersion and a proper spin-orbit coupling. The intraband and interband conductivities are discussed with respect to magnetic fields and magnetic domain puddles. The optical conductivity agrees well with the experimental values using screened impurity scattering and an effective Zeeman field. The universal value of Hall conductivity is shown to be modified due to this Zeeman field. The pseudospin current reveals an anomaly since a quasiparticle part appears though it vanishes for particle currents. The density and pseudospin response functions to an external electric field are calculated and the dielectric function is discussed with respect to collective excitations. A frequency and wave-vector range is identified where the dielectric function changes sign and the repulsive Coulomb potential becomes effectively attractive allowing for Cooper pairing.

[1] Phys. Rev. **B 94** (2016) 165415

DS 9.11 Mon 17:45 HSZ 204

Interplay between the long-range Coulomb interaction and edge-state magnetism in zigzag graphene nanoribbons — •Marcin Raczkowski and Fakher Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Quasi-one-dimensional graphene nanoribbons terminated by zigzag edges host partially flat bands at the Fermi energy. Theoretical studies of the Hubbard model with the effective on-site interaction only predict spontaneously induced spin polarizations at the zigzag edges and the associated finite dispersion of the low-energy band. Here, we revisit the stability and dynamical signatures of spin-polarized edge states by performing projective quantum Monte Carlo simulations of a more realistic model with long-range Coulomb interactions. On the one hand, increasing the relative strength of nonlocal interactions with respect to the on-site repulsion reduces noticeably the spin correlation length along the zigzag edge; nevertheless the tendency towards the extended spin polarization along the edges remains dominant over the competing short-range charge correlations. On the other hand, growing charge fluctuations are responsible for the emergence of incoherent low-energy excitations in the dynamical charge structure factor. In addition, we resolve a systematic shift of the dominant low-energy peak in single-particle spectral function on the edge towards higher frequencies that we attribute to quasiparticle scattering from charge excitations.

DS 9.12 Mon 18:00 HSZ 204

Quantum phase transition in effective spin ladders derived from graphene nanoribbons — •Cornelie Koop and Stefan Wessel — Institut für Theoretische Festkörperphysik, RWTH Aachen University

Zigzag edges of graphene nanoribbons host localized edge states, which show a ferromagnetic coupling along each edge and an antiferromagnetic one to the opposite edge. Using an effective model that treats the edge-bulk interaction as a perturbation to the edge-edge interaction, we can drastically reduce the numerical effort needed for this system, and we eventually find a rather general spin ladder model.

We examine this model at low, but finite temperatures by means of Monte-Carlo techniques using the stochastic series expansion method. Susceptibilities and correlation functions can be investigated. We find a quantum-phase transition (QPT), as a function of the antiferromagnetic inter-leg coupling strength, between a weak-coupling phase with long-range ferromagnetic order along each leg, which does not have a spin excitation gap, and a disordered, gapped singlet-phase. The location and estimates for the critical exponents are assessed by numerical methods and compared to known results from renormalization group calculations.

DS 10: Transport: Topological Phases (jointly with DS/MA/TT)

Time: Monday 15:00–18:00 Location: HSZ 304

DS 10.1 Mon 15:00 HSZ 304

Dynamical Buildup of a Quantized Hall Response from Non-Topological States — Ying Hu[1], Peter Zoller[1,2], and •Jan Carl Budich[3] — [1]Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, 6020 Innsbruck, Austria — [2]Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria — [3]Department of Physics, University of Gothenburg, SE 412 96 Gothenburg, Sweden

We consider a two-dimensional system initialized in a topologically trivial state before its Hamiltonian is ramped through a phase transition into a Chern insulator regime. This scenario is motivated by current experiments with ultracold atomic gases aimed at realizing time-dependent dynamics in topological insulators. Our main findings are twofold. First, considering coherent dynamics, the non-equilibrium Hall response is found to approach a topologically quantized time averaged value in the limit of slow but non-adiabatic parameter ramps, even though the Chern number of the state remains trivial. Second, adding dephasing, the destruction of quantum coherence is found to stabilize this Hall response, while the Chern number generically becomes undefined. We provide a geometric picture of this phenomenology in terms of the time-dependent Berry curvature.

DS 10.2 Mon 15:15 HSZ 304

Sign reversal of the quantized topological Hall effect in skyrmion crystals — •Börge Göbel[1], Alexander Mook[1], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — [2]Institut für Physik, Martin-Luther-Universität, D-06120 Halle

The topological Hall effect (THE) of electrons [1] is the hallmark of a skyrmion crystal phase [2]. It can be understood either by coupling of the electrons' spin to the local magnetic texture (Zeeman interaction) or by coupling of the electrons' charge to the emergent field generated by the texture (Peierls substitution).

Here, we study the THE on a triangular lattice, addressing band structure, Hall conductivity, and topological surface states. In this system, the THE is quantized and the transverse conductivity changes sign if the Fermi energy crosses a van Hove singularity. By mapping the THE to a quantum Hall effect (QHE) on a lattice [3], we assign this prominent feature to the cyclotron mass of electron orbits, that is, when constant-energy cuts of the band structure change from electron to hole pockets. Based on this picture, we derive an approximate rule which allows to determine the energy dependence of the topological Hall conductivity in *any* two-dimensional lattice.

[1] K. Hamamoto et al., Phys. Rev. B **92**, 115417 (2015)
[2] S. Mühlbauer et al., Science **323**, 915 (2009)
[3] Y. Hatsugai et al., Phys. Rev. B **74**, 205414 (2006)

DS 10.3 Mon 15:30 HSZ 304

Edge states and topology in finite-length single-wall carbon nanotubes — •Wataru Izumida[1,2], Rin Okuyama[3], Ai Yamakage[4,5], Mikio Eto[3], and Riichiro Saito[1] — [1]Department of Physics, Tohoku University, Sendai 980-8578, Japan — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [3]Faculty of Science and Technology, Keio University, Yokohama 223-8522, Japan — [4]Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan — [5]Institute for Advanced Research, Nagoya University, Nagoya 464-8601, Japan

Edge states in finite-length single-wall carbon nanotubes, which appear in the energy gap of the bulk states, are studied from the topological viewpoint [1,2]. An effective one-dimensional (1D) lattice model is introduced to analyze the quantum system with boundary. By analyzing the 1D lattice model, a bulk-edge correspondence, relationship between the number of edge states in the energy gap and the topological winding number defined in the corresponding bulk system, is given [1]. Manipulation of the edge states by magnetic field [3,4] is suggested in terms of the topological phase transition [2].

[1] W. Izumida, R. Okuyama, A. Yamakage, R. Saito, Phys. Rev. B 93, 195442 (2016).
[2] R. Okuyama, W. Izumida, M. Eto, arXiv:1610.05034.
[3] K. Sasaki, S. Murakami, R. Saito, Y. Kawazoe, Phys. Rev. B 71, 195401 (2005).
[4] M. Marganska, M. del Valle, S. H. Jhang, C. Strunk, M. Grifoni, Phys. Rev. B 83, 193407 (2011).

DS 10.4 Mon 15:45 HSZ 304

Topological invariants in carbon nanotubes with superconducting pairing — •Lars Milz[1], Magdalena Marganska[1], Wataru Izumida[1,2], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93 047 Regensburg, Germany — [2]Department of Physics, Tohoku University, Sendai 980-8578, Japan

The symmetries present in a gapped Hamiltonian system determine the types of topological invariants which can be defined for that system. Our case of interest here is a carbon nanotube, which in its normal state is known to possess a non-trivial integer topological invariant, the winding number. Its value determines the number of edge states. When a superconducting pairing is imposed on the nanotube, the symmetry class of the system changes and it is possible to define also a Z2 Pfaffian topological invariant, exploiting the particle-hole rather than the chiral symmetry. We explore the relationship between the two invariants and their influence on the energy spectrum and eigenstates, in particular the edge modes, of a finite carbon nanotube.

DS 10.5 Mon 16:00 HSZ 304

Renormalization group approach to topological phase transitions — •Wei Chen[1], Manfred Sigrist[1], and Andreas Schnyder[2] — [1]ETH Zurich, Zurich, Switzerland — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Have you thought about this: every time you tie your shoelaces, you are using a scaling procedure (the tying) to make the topology (the knot) more obvious? Akin to knot-tying, a renormalization group approach is proposed to judge topological phase transitions for systems that belong to any dimension and symmetry class, and whether the topological phase transition is driven by noninteracting parameters (hopping, chemical potential, etc) as in the usual topological insulators, or interacting parameters (Hubbard interaction, etc) as in fractional Chern insulators. The meaning of scale invariance at the critical point and the fixed point is shown to be related to the notion of correlation length, which was previously thought to be nonexistent for topological insulators.

[1] W. Chen, J. Phys. Condens. Matter 28, 055601 (2016)
[2] W. Chen, M. Sigrist, and A. P. Schnyder, J. Phys. Condens. Matter 28, 365501 (2016)

DS 10.6 Mon 16:15 HSZ 304

Fermionic topological quantum states as tensor networks — •Carolin Wille, Oliver Buerschaper, and Jens Eisert — Institut für theoretische Physik, Freie Universität Berlin

Tensor network states, and in particular projected entangled pair states, play an important role in the description of strongly correlated quantum lattice systems. They do not only serve as variational states in numerical simulation methods, but also provide a framework for classifying phases of quantum matter and capture notions of topological order in a stringent and rigorous language. The rapid development in this field for spin models and bosonic systems has not yet been mirrored by an analogous development for fermionic models. In this work, we introduce a tensor network formalism capable of capturing notions of topological order for quantum systems with fermionic components. At the heart of the formalism are axioms of fermionic matrix product operator injectivity, stable under concatenation. Building upon that, we formulate a Grassmann number tensor network ansatz for the ground state of fermionic twisted quantum double models. A specific focus is put on the paradigmatic example of the fermionic toric code. This work shows that the program of describing topologically ordered systems using tensor networks carries over to fermionic models.

15 min. break.

DS 10.7 Mon 16:45 HSZ 304

Finite-size scaling around a topological phase transition — •Tobias Gulden[1,2], Yuting Wang[2], and Alex Kamenev[2] — [1]Technion - Israel Institute of Technology — [2]University of Minnesota

The critical point of a phase transition is described by a conformal field theory, where perturbations away from criticality are known to give rise to universal scaling functions. We consider perturbations around a critical point which separates two distinct topological phases. For both energy and entropy we find the existence of scaling functions which depend on the sign of the perturbation, i.e. they discriminate between topological phases. Renyi entropy of the Kitaev model contains two distinct scaling functions which separate a well-known universal part and the topological contribution, while energy has one asymmetric scaling function. The latter is universal for all five Altland-Zirnbauer symmetry classes with non-trivial topology in one spatial dimension.

DS 10.8 Mon 17:00 HSZ 304

Fractionalization of charge and energy after electron injection in 1D helical systems — •Alessio Calzona[1,2,3], Matteo Acciai[1], Matteo Carrega[4], Fabio Cavaliere[1,3], and Maura Sassetti[1,3] — [1]University of Genova, Italy — [2]University of Luxembourg, Luxembourg — [3]SPIN-CNR, Genova, Italy — [4]NEST, Pisa, Italy

The possibility to inject a single electron into ballistic 1D conductors is at the basis of the new and fast developing field of electron quantum optics. In this respect, helical edge states of topological insulators can be used as electronic waveguides and would be an ideal playground [1,2].

Here we thus study and characterize the tunneling of a single electron from a mesoscopic capacitor into a couple of interacting helical edge channels [3]. The injection process leads to the creation of a pair of fractional excitations travelling in opposite directions. Their charge and energy profiles are analyzed. We also show that the energy partitioning between the two fractional excitations depends both on the interaction strength and on the injection parameters. Interestingly, this allows for a situation in which energy and charge mainly flow in opposite directions. In addition, such peculiar behavior of energy partitioning suggests that it can be also used as a tool to probe features of out-of-equilibrium systems [4].

[1] G. Fève et al., Science 316, 1169 (2007)
[2] D. Ferraro et al., PRB 89, 075407 (2014)
[3] A. Calzona et al., PRB 94, 035404 (2016)
[4] A. Calzona et al., arXiv:1610.04492

DS 10.9 Mon 17:15 HSZ 304

Solitons in one-dimensional lattices with a flat band — •Dario Bercioux[1,2], Omjyotu Dutta[1], and Enrique Rico[2,3] — [1]Donostia International Physics Center (DIPC), E-20018 San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation for Science, Maria Diaz de Haro 3, 48013 Bilbao, Spain — [3]Department of Physical Chemistry, University of the Basque Country UPV/EHU, Apartado 644, E-48080 Bilbao, Spain

We investigate the spectral properties of a quasi-one-dimensional lattices in two possible dimerization configurations [1]. Both configurations are characterized by the same lattice topology and the same spectra containing a flat band at zero energy. We find that, one of the dimerized configuration has similar symmetry to an one-dimensional chain proposed by Su-Schrieffer-Heeger [2] for studying solitons in conjugated polymers. Whereas, the other dimerized configuration only shows non-trivial topological properties in the presence of chiral-symmetry breaking adiabatic pumping.

[1] D. Bercioux, O. Dutta & E. Rico, arXiv:1609.06292.

[2] W. P. Su, J. R. Schrieffer, & A. J. Heeger Phys. Rev. Lett. **42**, 1698 (1979).

DS 10.10 Mon 17:30 HSZ 304

Local nature of Quantized Hall Effect — •Afif Siddiki — Mimar Sinan Fine Arts University, Physics Department, Sisli-Istanbul, Turkey 34380

Here, we investigate the electrostatic properties of two dimensional electron system (2DES) in the integer quantum Hall regime. As it is well known, the Landau quantization emerges from strong perpendicular magnetic fields. The (Landau) energy levels are broadened due to impurities, which we embedded their effects in density of states (DOS). As a simple model, DOS have two different forms: the Gaussian and semi-elliptic descriptions, i.e. the self consistent Born approximation (SCBA). Having in hand DOS, we obtain both the longitudinal and Hall (transversal) conductivities (σ_L, σ_H) utilizing Thomas-Fermi-Poisson approximation to calculate the charge density profile and Drude model to obtain transport coefficients. Since, the definition of capacitance is closely related with compressibility, (local) screening properties of 2DES is extremely important. Here we numerically simulate a translational invariant Hall bar subject to high magnetic fields which is perpendicular to the plane of the 2DES using realistic parameters extracted from the related experiments. Using the above mentioned approaches the local capacitances are calculated, numerically. Our findings are in perfect agreement with the related experiment which is based on a dynamic scanning capacitance microscopy technique.

DS 10.11 Mon 17:45 HSZ 304

Properties of non-abelian hierarchy states in the fractional quantum Hall effect — •Yoran Tournois and Maria Hermanns — Institute for Theoretical Physics, Cologne, Germany

The fractional quantum Hall effect is one of the paradigmatic examples of topological order in condensed matter physics. While the physics of the fractional quantum Hall effect is well understood in the lowest Landau level by means of the Haldane-Halperin hierarchy, a general method to describe the properties of quantum Hall liquids in the second Landau level is lacking. These are of particular interest, as it is believed that they may harbor exotic excitations - non-abelian anyons. In this talk, we consider a general class of model wave functions, which were recently proposed as a generalization of the Haldane-Halperin hierarchy. While these are conjectured to describe non-abelian quantum Hall liquids, many of their properties are not manifest and thus previously unknown. We determine their properties using a variety of methods. In particular, we derive the explicit conformal field theory description of the model wave functions, which reveals the non-abelian braiding statistics of the quasiparticles as well as the edge theory.

DS 11: Fundamentals of Perovskite Photovoltaics II (jointly with CPP/DS/HL)

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

Invited Talk DS 11.1 Mon 15:00 ZEU 222

Visualizing Charge Carrier Diffusion In Hybrid Halide Perovskite Thin Films — •Achim Hartschuh, Kathrin Handloser, Irene Grill, Nicolai Hartmann, Nadja Giesbrecht, Meltem Aygüler, Mathhias Handloser, Thomas Bein, and Pablo Docampo — Department of Chemistry and CeNS, LMU Munich, 81377 Munich, Germany

Organic-inorganic metal halide perovskites represent one of the most promising classes of absorber materials for future photovoltaic applications [1]. A prerequisite for the efficient extraction of photo-generated carriers is the combination of low non-radiative relaxation rates and rapid diffusive transport. We study the excited state dynamics and charge carrier transport properties in different perovskite thin films using time-resolved photoluminescence microscopy. By scanning the confocal detection with respect to the excitation spot, we visualize diffusive transport on micrometer length scales and determine the charge carrier diffusion constants and mobilities [2]. We complement these studies by transient photocurrent measurements on the same films and derived devices [3,4].

Invited Talk DS 11.2 Mon 15:30 ZEU 222

Photon recycling in hybrid lead-halide perovskite semiconductors — •Felix Deschler — University of Cambridge, Cambridge, UK

We discuss the effect of photon recycling on the externally measured radiative recombination rates in hybrid perovskites. By combining transient absorption with transient photoluminescence (PL) data, we distinguish radiative from non-radiative processes and find that the PL originates from a bimolecular process for all investigated carrier densities. We measure external photoluminescence quantum efficiencies (PLQEs) under continuous-wave and pulsed excitation. Taking into account photon recycling, we connect the externally measured radiative efficiencies with the actual internal values, and derive internal PLQEs exceeding 80%.

We map the propagation of photo-generated luminescence and charges from a local photo-excitation spot in thin films of lead triiodide perovskites using a confocal microscopy setup. We observed regenerated PL emission at distances as far as 50 micrometers away from photo-excitation. We map the internal photon distribution in the film and find that, over these distances, the peak of the internal photon spectrum red-shifts from 765 to >800 nanometers. We build a lateral-contact solar cell with selective electron- and hole-collecting contacts, using a combination of photo-lithography and electro-deposition. We used these devices as a platform to study photocurrent propagation and found that charge extraction can be achieved well beyond 50 micrometers away from the excitation.

DS 11.3 Mon 16:00 ZEU 222

Coherent Dynamics of Free Exciton Dissociation in Lead-iodide Perovskites observed by 2D Electronic Spectroscopy — •Ajay Jha[1], Hong-Guang Duan[1,2,3], Vandana Tiwari[1], Pabitra Nayak[4], Michael Thorwart[2,3], Henry J. Snaith[4], and R. J. Dwayne Miller[1,3,5] — [1]MPI-Structure & Dynamics of Matter, Hamburg, Germany — [2]Universität Hamburg,Germany — [3]CUI Hamburg, Germany — [4]University of Oxford, UK — [5]University of Toronto, Canada

Hybrid organolead halide perovskites with high carrier mobility and large dielectric constant have received considerable attention as an excellent material for low-cost efficient photovoltaics. The power conversion efficiency of perovskite based solar cells has meteorically advanced to 22.1% with excitonic dye-sensitization concept and ~15% for planar heterojunction configuration. The unprecedented success of this material demands the fundamental understanding of underlying microscopic mechanisms for photoinduced charge generation. Recent studies suggest that most photoexcitations in perovskite are free charge carriers behaving like III-V inorganic semiconductors, but the contribution of excitons has been a matter of debate. We have employed ultrafast 2D electronic spectroscopy to probe elementary optical excitation of CH3NH3PbI3 thin films. We distinctly observe the electronically coupled excitonic and free carrier transitions at room temperature. We captured an ultrafast exciton dissociation favored by low exciton binding energy of ~40 meV. The interplay of strongly coupled dominant vibrational mode to exciton dynamics will also be discussed.

DS 11.4 Mon 16:15 ZEU 222

Time Resolved Microwave Conductivity on Perovskites — •Marvin Grüne[1], Andreas Sperlich[1], Andreas Baumann[2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Organo-metal halide perovskites continue to be the star of thin film solar cells exhibiting rapidly rising power conversion efficiencies. For further improvement of these solar cells it is essential to understand the fundamental intrinsic properties like photoconductivity, recombination and charge carrier mobility. Therefore, we investigate the mixed halide perovskite layers of $CH_3NH_3PbX_3$ (X: I^-, Br^- and Cl^-) using time-resolved microwave conductivity. With this contactless measurement technique we address the charge carrier lifetime, decay kinetics and intrinsic mobility of perovskite structures with different halide substituents X. The mobility increases more than a factor of 2 in this order of substituents up to 8 cm^2/Vs. Furthermore, the influence of solvent annealing on the crystallization process of the $CH_3NH_3PbI_3$ film has been investigated, now considering temperature dependence. This crystallization method generates e.g. bigger crystal domain sizes and almost one order of magnitude higher mobilities. Due to the absence of transport layers, we can relate differences in the results to intrinsic properties of the perovskite layers. Solar cells with the investigated layer achieve up to 16% efficiency in our labs.

15 min break

Invited Talk DS 11.5 Mon 16:45 ZEU 222

Interface engineering: the route towards high efficiency and stable hybrid perovskite solar cells — •Giulia Grancini — Group for Molecular Engineering of Functional Materials, EPFL Valais Wallis, CH-1951 Sion, Switzerland

Hybrid perovskite solar cells are undoubtedly leading the photovoltaic scene with their power conversion efficiency (PCE) >22%. Tuning the material composition, i.e. by cations and anions substitution (e.g. introducing a small amount of Br) and the interfacial properties, optimizing the structural and chemical interactions and the optoelectronic processes therein have been the successful routes for a real breakthrough in device efficiency and reproducibility. However, despite the impressive PCE reported, hybrid perovskite suffer of severe instability mainly due to material degradation upon exposure to water and moisture further accelerated under local heating and UV irradiation. Diverse technological approaches have been proposed delivering appreciable improvements, but still failing by far the market requirements. Recently, we pioneered a new concept by interface engineering a multi-dimensional composite of two dimensional (2D) (HOOC(CH2)2NH3)2PbI4 / 3D-CH3NH3PbI3 perovskite molecular junction. The composite forms an exceptional gradually organized structure that yields up to 12.9% PCE. Aiming at the up-scaling of this technology, we realize 10x10 cm2 large-area solar modules by a fully printable, industrial-scale process delivering 11.2% stable devices for 9,000 hours under accelerated testing conditions, leading to a record one-year stability.

DS 11.6 Mon 17:15 ZEU 222

Characterization of perovskite solar cells: Towards a reliable measurement protocol — •Eugen Zimmermann[1], Ka Kan Wong[1], Michael Müller[1], Hao Hu[1], Philipp Ehrenreich[1], Markus Kohlstädt[2,3], Uli Würfel[2,3], Simone Mastroianni[2], Gayathri Mathiazhagan[2], Andreas Hinsch[2], Tanaji P. Gujar[4], Mukundan Thelakkat[4], Thomas Pfadler[1], and Lukas Schmidt-Mende[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Fraunhofer Institute for Solar Energy Systems ISE, Freiburg, Germany — [3]Freiburg Materials Research Center FMF, University of Freiburg, Freiburg, Germany — [4]Applied Functional Polymers, Department of Macromolecular Chemistry I, University of Bayreuth, Bayreuth, Germany

Tremendous progress on power conversion efficiency of lead halide perovskite solar cells during the last few years drastically increased the interest in research on this material. However, a so called "hysteretic" behaviour during current density-voltage (J-V) measurements is differently severe for differently prepared solar cells and strongly depends on scan parameters like scan rate, and measurement history. This challenges reliable results across different laboratories and hinders the aspect of commercialization. Here, we propose a reliable measurement protocol by introducing stabilized device characteristics obtained from an adaptive tracking of the maximum power point and the open circuit voltage, and compare such obtained values to device characteristics derived from standard and time resolved J-V measurements for varying solar cells fabricated in different laboratories.

DS 11.7 Mon 17:30 ZEU 222

Removing leakage recombination current in planar perovskite solar cells — •Kristofer Tvingstedt[1], Lidon Gil-Escrig[2], Christina Momblona[2], Philipp Rieder[1], David Kiermasch[1], Andreas Baumann[3], Henk J. Bolink[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximillian University of Würzburg, 97074 Würzburg — [2]Instituto de Ciencia Molecular, Universidad de Valencia, C/Catedrático J. Beltrán 2, 46980 Paterna, Spain — [3]Bavarian Center for Applied Energy Research 97074 Würzburg

All solar cells, including perovskites, suffer from recombination mechanisms of various types out of which leakage current usually dominates at lower voltages. Herein, we demonstrate a three order reduction of this recombination loss mechanism in planar perovskite solar cells by replacing the commonly used hole selective electrode PEDOT:PSS with a polymer arylamine hole transporting semiconductor. This renders these solar cells more useful under lower light intensity, such as end of the day and indoor conditions which we demonstrate via the extreme case of moon lighting conditions, where the cells still generates open circuit voltages of 530 mV. By this substantial leakage reduction we can be able to confirm charges to also remain in the photovoltaic device for up to 2 hours after the light has been switched off. We discuss the mechanisms behind this feature and explain why the arylamine is a superior hole selective electrode.

DS 11.8 Mon 17:45 ZEU 222

Double-layer charge selective contacts in perovskite solar cells as a key to improved efficiency and reduced hysteresis effects — •Lukas Kegelmann[1], Christian Wolff[3], Celline Awino Omondi[1], Lars Korte[1], Thomas Dittrich[1], Dieter Neher[3], Bernd Rech[1], and Steve Albrecht[2] — [1]Helmholtz-Zentrum Berlin, Inst. for Silicon Photovoltaics, Berlin, 12489, Germany. — [2]Helmholtz-Zentrum Berlin, Young Investigator Group Perovskite Tandem Solar Cells, Berlin, 12489, Germany. — [3]University of Potsdam, Soft Matter Physics, Potsdam, 14476, Germany.

Planar low-temperature processed perovskite solar cells without a mesoscopic scaffold are advantageous for a possible large-scale production but often suffer from photocurrent hysteresis, especially in the regular 'n-i-p'-structure. Here, we systematically study the influence of different low-temperature deposited electron transport materials (ETM) on planar regular solar cell characteristics. We further show that an elaborately chosen metal oxide interlayer in an ITO/metal oxide/PCBM double-layer ETM can significantly improve the device performance. J-V measurements reveal substantial reductions of hysteresis effects and enhanced power conversion efficiencies up to a champion stabilized value of 18.0 % for TiO2 interlayers. Surface photovoltage spectroscopy is used to show comparable absorber qualities on all ETMs for the fabrication process used here. Additionally, improved hole blocking for the double-layer structure is suggested by UPS and the metal oxide interlayer is considered to reduce shunt paths as it hampers direct contact between perovskite and the ITO electrode.

DS 11.9 Mon 18:00 ZEU 222

Electrical impedance spectroscopy on perovskite solar cells — •Fischer Mathias[1], David Kiermasch[1], Vladimir Dyakonov[1,2], and Andreas Baumann[2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research, 97074 Würzburg

Electrical impedance spectroscopy has shown to be a powerful technique to obtain informations about key parameters of a solar cell, like series and recombination resistance, build-in potential and the dielectric constant. Here, we performed impedance measurements over a wide temperature range from 300K down to 150K on solution processed $CH_3NH_3PbI_3$ perovskite solar cells. We compared the impedance spectra of n-i-p and p-i-n device configuration which is FTO/TiO_2/Perovskite/Spiro-MeOTAD/Au and ITO/PEDOT:PSS/Perovskite/$PC_{60}BM$/C_{60}/BCP/Au, respectively. We fit the impedance spectra by using corresponding equivalent circuits to investigate the dielectric behavior depending on the cell layout and preparation technique. We compare the extracted time constants at different frequency domains to reveal the influence from the p- and n-layer materials on the photovoltaic properties of the perovskite absorber material itself and examined charge carrier recombination behavior in dependency of illumination intensity.

DS 12: Focused Session: Inhomogeneous Materials for Solar Cells II

Although multinary compound semiconductors exhibit a variety of inhomogeneities - such as strong local concentration fluctuations, built-in vertical concentration gradients, rough interfaces, and a high density of grain boundaries - they are among the leading solar cell technologies. In this focused session, the impact of inhomogeneities on the carrier transport in solar cells shall be addressed with emphasis on material growth, characterization, and modeling. Therefore, state-of-the-art research and challenges will be highlighted for a broad range of related materials such as chalcopyrites, kesterites, perovskites, and group III-nitrides.

Organizers: Roland Scheer (MLU Halle Wittenberg), Frank Bertram (OvGU Magdeburg), and Jürgen Christen (OvGU Magdeburg)

Time: Monday 15:00–16:15 Location: CHE 89

Topical Talk DS 12.1 Mon 15:00 CHE 89

Defects in Chalcopyrites — •Susanne Siebentritt — Laboratory for Photovoltaics, Physics and Materials Science Research Unit, University of Luxembourg

Chalcopyrites (Cu(InGa)Se2) are used as absorbers in thin film solar cells. Their off-stoichiometry and their polycrystalline structure pose challenges for their semiconductor physical analysis.

The talk will present recent progress in the analysis of recombination centres and their effect on photogenerated carriers by spectral photoluminescence (PL) measurements. On the one hand side they provide information about quasi-Fermi level splitting, which indicates the amount of recombination. On the other they allow to investigate the energy positions of deep defects, which act as recombination centres. PL will be compared to results from admittance spectroscopy (AS), which can also indicate deep defects. In AS, however, it is difficult to distinguish between deep defects, barriers and other interface effects. The comparison between PL and AS indicates that the main steps are rather due to barriers than to deep defects.

Invited Talk DS 12.2 Mon 15:30 CHE 89

Growth of InGaN film and monolayer by molecular beam epitaxy — •Xinqiang Wang[1], Zhaoyin Chen[1], Xiantong Zheng[1], Xin Rong[1], Bowen Sheng[1], Bo Shen[1], Tobias Schulz[2], Martin Albrecht[2], Frank Bertram[3], and Jürgen Chirsten[3] — [1]State Key Laboratory of Artificial Microstructure and Mesoscopic Physics, School of Physics, Peking University, Beijing, 100871, China — [2]Leibniz-Institute for Crystal Growth, Berlin, Germany — [3]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, 39106 Magdeburg, Germany

InGaN, which nearly perfectly matches the solar spectrum, is a good candidate for high efficiency solar cell. However, high quality InGaN, in particular with high In content, is difficult to realize. To solve this problem, Yoshikawa et al proposed to use (InN)m/(GaN)n digital alloys instead of random InGaN alloys making the InGaN in long range ordering. This approach attracted great interest due to its potential application in devices such as solar cells. Unfortunately, the growth is difficult as well since it needs the atomical level control at either InN or GaN layer. In this talk, we will first report our effort on fabricating solar cells by using InGaN/GaN multiple quantum wells, where a positive photovoltaic efficiency temperature coefficient up to 423K have bee observed. Then, we focus on growth of InGaN films with different In compositions. An InGaN layer with In composition changed from 0-100% on the same wafer have been grown as well. Finally, we will first report manipulation of In(Ga)N monolayer by molecular beam epitaxy.

DS 12.3 Mon 16:00 CHE 89

Investigation of Carrier Transport in CuInGaSe2 by Highly Spatially, Spectrally, and Time Resolved Cathodoluminescence Microscopy — •Mathias Müller[1], Martin Müller[1], Torsten Hölscher[2], Setareh Zahedi-Azad[2], Matthias Maiberg[2], Frank Bertram[1], Roland Scheer[2], and Jürgen Christen[1] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]FG Photovoltaik, Martin-Luther-University Halle-Wittenberg, Germany

To gain a deeper understanding regarding transport of carriers and the influence of inhomogeneities, highly spatially, spectrally, and time resolved cathodoluminescence (CL) measurements have been performed on polycrystalline CuInGaSe2 (CIGSe). Absorbers with varying Cu/III-ratios (CGI: 0.73 and 0.86) and therefore varying grades of disorder were investigated.

For this purpose two separate experiments were combined. Carrier diffusion length was derived temperature dependent from spatially resolved CL measurements as was the initial carrier lifetime from time resolved CL experiments.

With decreasing temperature from 300 K to 4.5 K the diffusion length increases from 6 μm to 27 μm (CGI 0.86) and 23 μm (CGI 0.73). Simultaneously, carrier lifetime increases from 20 ns (@ 125 K) to 48 ns (@ 4.5 K) and from 3 ns (@ 125 K) to 37 ns (@ 4.5 K), respectively. The resulting mobilities follow a power law with $\mu \propto T^{-0.86}$ (CGI 0.86) and $\mu \propto T^{-0.43}$ (CGI 0.73), which reveals scattering at neutral defects as the dominant mechanism, reaching up to 340,000 cm^2/Vs at 4.5 K.

DS 13: Phase Change/Resistive Switching

Time: Monday 15:00–16:45 Location: CHE 91

DS 13.1 Mon 15:00 CHE 91

Towards Shot Noise Study of Hafnium Oxide Resistive Switching — •Donato Civita[1,2], Carlos Sabater[2], and Jan van Ruitenbeek[2] — [1]Institute of Chemistry, Graz, Austria — [2]Leiden Institute of Physics, Leiden, The Netherlands

The continuous down-scaling of memory devices led to an increased interest in the Resistive Random Access Memory (ReRAM). Such a memory device consists of an ultrathin insulating layer between two metal electrodes where the insulating layer has the resistive switching (RS) properties, i.e. the ability to reversibly change its resistance as a result of an electrical stimulus. The switching mechanism is considered to be based on the formation and dissolution of a conducting filament surrounded by the insulating matrix. However, the nature of the conducting lament is still unclear.

In the present work, we design and produce novel RS nano-devices, consisting of hafnium oxide as insulating material and platinum as material for the metal electrodes. We describe in detail the fabrication procedure and characterization of the nano-devices and their RS behavior. A novel method to investigate the RS system, the Shot Noise measurement, is presented. The Shot Noise experiments will be presented together with the results of conductance measurements, with the goal to obtain insight into the nature of the conducting filaments.

DS 13.2 Mon 15:15 CHE 91

Nonvolatile resistive switching to 10 ^6 OFF/ON resistance ratio in yttrium manganite thin films with downscaled top electrodes — •Venkata Rao Rayapati[1], Agnieszka Bogusz[1,2], Nan Du[1], Danilo Bürger[1], Ilona Skorupa[1,2], Stefan E Schulz[3], Oliver G Schmidt[1,4], and Heidemarie Schmidt[1,3] — [1]Materials systems for Nanoelectronics, Chemnitz University of Technology, 09126 Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Fraunhofer-Institut für Elektronische Nanosysteme, Abteilung Back-End of Line, Technologie-

Campus 3, 09126 Chemnitz, Germany — [4]Institute for Integrative Nanosciences, IFW Dresden, Dresden, Germany

Polycrystalline, hexagonal YMnO3 (YMO) thin films grown by pulsed laser deposition with ceramic target [1] exhibit nonvolatile unipolar resistive switching (RS). In this work, we investigate RS properties of YMO thin films with different chemical compositions on large-scale Pt and Pt/Ti bottom electrodes (BE). Circular Au and Al top electrodes (TE) of different size have been prepared by magnetron sputtering and e-beam evaporation, respectively. SET and RESET bias during RS strongly depend on ceramic target and bottom electrode. Endurance of YMO with Al TE is improved in comparison to Au TE. The observed increasing ROFF/RON ratio with decreasing size of Al TE can be related with increasing ROFF with decreasing size of Al TE due to decreased tendency for local shunting. [1] A. Bogusz et al., AIP Advances 4 (2014)

DS 13.3 Mon 15:30 CHE 91

Characterization of the early stages in the MBE-growth of phase change materials — •Marvin Kaminski[1], Marc Pohlmann[1], Matti Wirtssohn[1], Abderrafii Moktad[1], Peter Jost[1], and Matthias Wuttig[1,2,3] — [1]I. Institute of Physics, Physics of Novel Materials, RWTH Aachen University, 52056 Aachen, Germany — [2]JARA-FIT, RWTH Aachen University, Germany — [3]3JARA-Insitut Energy-efficient information technology (PGI-10), FZ Jülich, 52428 Jülich, Germany

In chalcogenide-based phase-change materials (PCMs), the switching between the amorphous and the crystalline phase is fast, reversible, and concomitant with a prominent contrast in physical properties. PCMs are, therefore, among the most promising candidates for future nonvolatile electronic memory applications. Recent developments such as the concept of interfacial phase-change materials (IPCMs), where thin layers of Sb2Te3 and GeTe are stacked as superlattices, call for highly-textured or even epitaxial films, which can be produced by sputter deposition, MOPVE, and molecular beam epitaxy (MBE). In this work, we study thin MBE-grown chalcogenide layers on Si(111). The combination of in-situ RHEED and ARHEED as well as ex-situ XRD, SEM, and AFM measurements provides insights on the early stages of the growth process. As the early stages of the growth govern the overall quality of the film to a large extent, proper understanding is crucial for further optimization.

DS 13.4 Mon 15:45 CHE 91

Accurately controllable phase transitions in pulsed laser deposition-deposited GeTe films for multi-level memory applications — •Xinxing Sun[1], Andriy Lotnyk[1], Martin Ehrhardt[1], Pierre Lorenz[1], Jürgen W. Gerlach[1], and Bernd Rauschenbach[1,2] — [1]Leibniz Institute of Surface Modification, Permoserstr. 15, D-04318, Leipzig, Germany — [2]Institute for Experimental Physics II, Leipzig University, Linnéstr. 5, D-04103 Leipzig, Germany

Multi-level storage techniques are promising for increasing storage density and for reducing energy consumption in the application of phase-change materials based memory devices. However, accurately controlling the phase transitions as well as understanding the underlying switching mechanisms are still unsolved. In this study, non-volatile optical multi-level switching in single-layer GeTe phase-change films prepared by laser ablation are demonstrated to be feasible and accurately controllable at a timescale of nanoseconds. For this purpose, an ns UV laser pump-probe setup was adapted for the investigations. This system is capable to vary the laser parameters with broad ranges. Moreover, the optical switching process and the phase transformation are correlated on the microscopic scale for understanding of the switching mechanism. It is found that each 20 ns laser pulse (wavelength: 248 nm) with a fluence of 26 mJ/cm2 excitation induced a partial crystallization, and complete crystallization was achieved by a succession of 5 such pulses. In the reverse process, a single pulse excitation at a fluence of 112 mJ/cm2 leads to re-amorphization of the film.

DS 13.5 Mon 16:00 CHE 91

Investigation of oxygen vacancy formation and migration in HfO_2 from density functional theory — •Marta Gibertini, Daniel Wortmann, Gustav Bihlmayer, Shigeru Tsukamoto, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Among the investigated storage devices, resistive random access memory (ReRAMs) are currently considered relevant because of the high-speed/high-density properties and the low energy required for the writing/rewriting cycles. A deeper understanding of the role played by point defects and dopants in the used materials is important for an optimization of those devices.

We present a density functional theory (DFT) study aimed at the investigation of the formation energies and the migration energy barriers of oxygen vacancies in Y-doped and undoped monoclinic HfO_2. We look at these properties in bulk and film systems where the formation energy is calculated also at the surface, and the dependence on the magnitude of an external electric field is studied. The nudged elastic method is applied and the DFT calculations are performed with the electronic structure code jüRS, a real-space finite-difference implementation of the projector augmented wave (PAW) method. The real-space formalism is chosen because it allows a flexible treatment of the boundary conditions and therefore it is favorable for the implementation of an external electric field. – Work is supported by DFG - SFB 917 (Nanoswitches).

DS 13.6 Mon 16:15 CHE 91

Effect of heavy ion radiation on resistive switching in HfOx based RRAM devices grown by MBE — •Stefan Vogel[1], S. U. Sharath[1], J. Lemke[1], E. Hildebrandt[1], C. Trautmann[2], and L. Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, 64287 Darmstadt, Germany — [2]Materials Research Department, Gesellschaft für Schwerionenforschung (GSI), 64291 Darmstadt, Germany

Recently, resistive random access memory (RRAM) gained a lot of attention due to its promising performances: fast switching times, high endurance, and low power consumption. RRAM devices are nonvolatile memories based on switching between a stable low resistance state (LRS) and a high resistance state (HRS) by conducting filaments which are formed and disrupted by applying voltages of different polarities. RRAM devices usually have a simple metal-insulator-metal stack structure. Hafnium oxide (HfO_2) is promising for embedded RRAM due to its established CMOS compatibility. Also, its simplicity and the possibility of 3D-stacks makes RRAM being an attractive technology for increased device density, potentially overcoming existing limitations and following Moore‘s law for floating gate metal oxide semiconductor field effect transistors. In-situ stacks of TiN/HfO_x with deficient oxygen stoichiometry were deposited by molecular beam epitaxy (MBE) using radical sources with different gases (oxygen and nitrogen). Device stacks of Pt/HfO_x/TiN were investigated towards their switching characteristics before and after heavy ion radiation utilizing Au-ions with energies of 48 MeV and fluences up to 10^{12} ions/cm^2.

DS 13.7 Mon 16:30 CHE 91

Reducing variability by introduction of thin TiO_2-layers into HfO_2 switching cells — •Alexander Hardtdegen[1], Camilla La Torre[2], Stephan Menzel[1], Rainer Waser[1,2], and Susanne Hoffmann-Eifert[1] — [1]Peter Grünberg Institute and JARA-Fit, Forschungszentrum Jülich GmbH, Jülich, Germany — [2]Institut für Werkstoffe der Elektrotechnik II, RWTH Aachen University, Aachen, Germany

Non-volatile resistive random access memory (ReRAM) cells are interesting for storage class memories, where for industrial purpose HfO_2 is typically used as oxide switching layer. The main challenge of HfO_2 is the slightly increased variability.

By designing bilayer cells combining HfO_2 with TiO_2, improvements of switching behavior can be observed. The devices switch more stable and a gradual SET with self-limiting behavior becomes visible. In contrast to this, the RESET becomes more abrupt when switching with higher current compliances. This behavior can be explained by an intrinsic stack-dependent series resistance, which can be quantified by a numerical method and also verified by physics-based compact model simulations.

In this study, the influence of the HfO_2/TiO_2 ratio is investigated in respect to the switching stability and the series resistance.

DS 14: 2D Materials Beyond Graphene II (jointly with CPP)

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

DS 14.1 Mon 16:00 REC/PHY C213

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

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

DS 14.2 Mon 16:15 REC/PHY C213

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

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

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

DS 14.3 Mon 16:30 REC/PHY C213

Direct observation of the conduction bands of single-layer WS_2 on Au(111) — •Philipp Eickholt[1], Marcel Holtmann[1], Charlotte Sanders[2], Philip Hofmann[2], and Markus Donath[1] — [1]Physics Institute, University of Münster, Germany — [2]Department of Physics and Astronomy, University of Aarhus, Denmark

In the field of 2D materials, single-layer transition metal dichalogenides, especially MoS_2, WS_2, $MoSe_2$ and $WSe2_2$, are among the promising materials due to their exceptional optical and electronic properties [1]. The key to understanding these properties is a profound knowledge of the electronic structure. While there have been many studies of the occupied electronic structure, the crucial information about the dispersion and spin structure of the conduction bands is still missing. Spin- and angle-resolved inverse photoemission (SRIPE) [2] is the ideal technique to study dispersion and spin structure of the unoccupied electronic structure. In this talk we present a SRIPE study of the conduction bands of single-layer WS_2 grown [3] on Au(111).

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

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

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

DS 14.4 Mon 16:45 REC/PHY C213

Study of the anisotropic electronic structure of $ReSe_2$ — •Ph. Eickholt[1], C. Langenkämper[1], K. Miyamoto[2], E.F. Schwier[2], J. Noky[3], M. Drüppel[3], P. Krüger[3], M. Rohlfing[3], and M. Donath[1] — [1]Physics Institute, University of Münster, Germany — [2]Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan — [3]Institute of Solid State Theory, University of Münster, Germany

Transition metal dichalcogenides (TMDCs) are heavily studied due to their fascinating optical and electronic properties and possible technical applications. $ReSe_2$ is a new material of the TMDC family. Unlike the well known MoS_2 it grows in a distorted 1T structure. Therefore it has unique anisotropic properties which can be useful in future applications [1]. To develop a fundamental understanding of the optical and electric properties we studied the occupied electronic structure of $ReSe_2$ with the help of angle-resolved photoemission (ARPES) and quasiparticle calculations.

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

DS 14.5 Mon 17:00 REC/PHY C213

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

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

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

DS 14.6 Mon 17:15 REC/PHY C213

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

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

In this work, using first principles approaches, we propose a novel strategy for engineering the level alignment in van der Waals heterostructures. In particular, we focus on the inclusion of self-assembling polar molecules (e.g. Titanyl phthalocyanine) into stacks consisting of 2D transition metal dichalcogenides (TMDCs) sheets (MoX_2 and WX_2, where X = S or Se). For structures of the type TMDC/TiOPc/TMDC we observe a shift in the frontier levels of successive TMDC layers by as much as 0.4 eV. Remarkably, for WSe_2/TiOPc/MoS_2 this allows switching between type I and type II alignment. Using multiple TiOPc layers even quantum cascades can be realized.

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

DS 14.7 Mon 17:30 REC/PHY C213

Structure determination of silicene nanoribbons on Ag(110)

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

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

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

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

DS 14.8 Mon 17:45 REC/PHY C213

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

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

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

DS 14.9 Mon 18:00 REC/PHY C213

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

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

The aim of our work is to understand the growth mechanism of MoS$_2$ on this graphene-like surface in order to exploit this knowledge to grow MoS$_2$ directly on graphene itself. Therefor MoS$_2$ flakes are grown by chemical vapor deposition and investigated by different Scanning Probe Microscopy techniques. It will be shown, that MoS$_2$ is more likely to grow at HOPG edges. These one-dimensional defects act as the growth seeds. This would constitute a serious disadvantage for the direct growth on graphene where no step edges are present. Therefore, we investigated if point defects can act as growth seeds as well. To this end, an HOPG crystal was irradiated by highly charged ions to induce quasi zero-dimensional defects [2] before the chemical vapor deposition of MoS$_2$. The first results obtained from these experiments will be presented.

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

DS 14.10 Mon 18:15 REC/PHY C213

Probing the Bandstructure of MoS$_2$ on Au(111) using Scanning Tunneling Spectroscopy — •Nils Krane, Christian Lotze, and Katharina J. Franke — Freie Universtät Berlin, Berlin, Germany

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

Here we grow MoS$_2$ epitaxially on a Au(111) surface as described in [2] and investigate it with a combined STM/AFM at low temperatures. Since STS measures the projected LDOS without information of the parallel momentum $k_\parallel$ in the Brillouin-Zone, it is not possible to assign a band gap to the K- or Γ-point. To get an insight into the band structure of MoS$_2$, we measure the decay length κ of the tunneling current, which depends on $k_\parallel$ [3]. We find a strong spatial dependence of κ. We ascribe this to the Moiré reconstruction of MoS$_2$ on Au(111), which differs between fcp- and hcp-stacking at the hollow sides. Furthermore, we investigate the band structure of quasi freestanding MoS$_2$.

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

DS 15: Focussed Session: Frontiers in Exploring and Applying Plasmonic Systems I (Joint Session of CPP, DS, HL, MM, and O, organized by DS)

With the increasing importance of plasmonics and the variety of its number of applications it becomes obvious that experimental characterization beyond the far-field optical standard methods and also theoretical tools that access the plasmonic behaviour on the atomic scale are indispensable for further development and improvement of the basic knowledge and thus, for new kinds of applications. The “Focused Session” gathers experts for unusual experimental methods (near-field studies with SNOM and EEL-TEM) and for the theoretical exploration of quantum effects in plasmonic excitations. Furthermore, new kinds of plasmonic applications (devices exploiting phase changes, alternative displays and holograms) will be introduced.

Organizers: Laura NaLiu (U Heidelberg) and Annemarie Pucci (U Heidelberg)

Time: Monday 16:30–17:15 Location: CHE 89

DS 15.1 Mon 16:30 CHE 89

Strong Coupling between Phonon-Polaritons and Plasmonic Nanorods — •Christian Huck[1], Jochen Vogt[1], Tomáš Neuman[2], Tadaaki Nagao[3], Rainer Hillenbrand[4,5], Javier Aizpurua[2], Annemarie Pucci[1], and Frank Neubrech[1,6] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Materials Physics Center (CSIC-UPV/EHU) and Donostia International Physics Center (DIPC), Donostia-San Sebastián, Spain — [3]WPI Center for Materials NanoArchitectonics, National Institute for Materials Science, Tsukuba, Japan — [4]CIC nanoGUNE and UPV/EHU, Donostia-San Sebastián, Spain — [5]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [6]4th Physics Institute, Stuttgart, Germany

We perform far-field spectroscopy of metal nanoantennas, resonant in the infrared spectral region, placed on silicon oxide (SiO$_2$) layers of different thickness. Due to strong coupling between the plasmonic excitation of the metal antenna plasmons and the surface phonon-polaritons of thin SiO$_2$ layers a splitting of the plasmonic resonance is found in the respective spectra. Although the phonon-polaritons themselves are dark excitations under normal illumination, they strongly interact with plasmon-polaritons as we detailed for a planar SiO_2 layer beneath the nanostructures. The observed splitting can result in a transparency window, corresponding to suppression of antenna scattering, respectively "cloaking" of the antenna. The effect is a kind of induced transparency in which the strength of the phonon-polariton field plays the crucial role. It represents a further tuning possibility for the optical performance of infrared devices.

DS 15.2 Mon 16:45 CHE 89

Enhanced Infrared Spectroscopy of Single Small Fine Dust Particles with Resonant Plasmonic Nanoslits — •Jochen Vogt[1], Sören Zimmermann[2], Christian Huck[1], Michael Tzschoppe[1], Frank Neubrech[1,3], Sergej Fatikow[2], and Annemarie Pucci[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Division Microrobotics and Control Engineering, University of Oldenburg, Oldenburg, Germany — [3]4th Physics Institute, University of Stuttgart, Stuttgart, Germany

Guiding the way towards dust sensing devices based on surface-enhanced infrared (IR) absorption (SEIRA), our study demonstrates the potential of plasmonic nanostructures for chemically specific identification of single tiny fine dust particles. The model system under investigation consists of individual silica spheres with diameters below 240 nm placed at defined positions in resonant plasmonic nanoslits. With dimensions far below the wavelength, direct IR spectroscopic measurements of such particles are not possible in reasonable time scales. In our SEIRA setup, the characteristic phononic particle excitations of the silica spheres are enhanced by the strong near-field of the plasmonic nanoslits, which enables the IR spectroscopic identification of individual particles. The SEIRA signal enhancement of single particles at various positions along the nanoslit structure fully corresponds to the near-field enhancement profile of these structures with the optimal position for SEIRA sensing to be located at sites towards the slit middle.

DS 15.3 Mon 17:00 CHE 89

Transverse and Longitudinal Resonances in Plasmonic Gold Tapers — Surong Guo[1], Nahid Talebi[1], Wilfried Sigle[1], Ralf Vogelgesang[2], Gunther Richter[3], Martin Esmann[2], Simon F. Becker[2], Christoph Lienau[2], and •Peter A. van Aken[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Carl von Ossietzky University of Oldenburg, Oldenburg, Germany — [3]Max Planck Institute for Intelligent Systems, Stuttgart, Germany

Conically-shaped metallic tapers are one of the most common structures with concomitant capabilities of nanofocusing and field enhancement. We distinguish two different dynamic mechanisms, reflection and phase matching, of surface plasmons excited by relativistic electrons in three-dimensional gold tapers with various opening angles from 5° to 47° which are studied both experimentally and theoretically, by means of electron energy-loss spectroscopy and finite-difference time-domain numerical calculations, respectively. We observe distinct resonances along the taper shaft independent of opening angles. We show that the origin of these resonances is different at different opening angles and results from a competition between two coexisting mechanisms. For large opening angles ($> 20°$), phase matching between the electron field and that of higher-order angular momentum modes is the dominant contribution because of the increasing interaction length between electron and the taper near-field. In contrast, reflection from the taper apex dominates at small opening angles ($< 10°$). A gradual transition of these two mechanisms is observed for intermediate opening angles.

DS 16: Layer Properties: Electrical, Optical, and Mechanical Properties I

Time: Monday 17:00–18:30 Location: CHE 91

DS 16.1 Mon 17:00 CHE 91

On the depolarization in granular thin films: A systematic Mueller-Matrix approach. — •Bruno Gompf, Maximilian Gill, Martin Dressel, and Audrey Berrier — 1. Physikalisches Institut and Research Center SCoPE, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Optical reflection or transmission measurements are usually described in the framework of Fresnel's equations, whereas the scattering of light on spherical particles is treated by Mie-theory. But what happens when strongly scattering dielectric Mie-particles form a thin film? To our eyes these granular films appear white. But how do they depolarize light? The polarization state of light is described by its Stokes vector, which can be visualized on a Poincare sphere. The interaction with the sample leads to a jump from one point of the Poincare sphere to another point (or area). Mueller-matrices allow a model-free description of this jump. Here we present systematic transmission and reflection Mueller-matrix ellipsometric measurements on strongly scattering granular BaSO4 thin films of different thicknesses. The depolarizing behavior is characterized via a comparative study of the respective differential-, product-, and sum-decomposition of the measured Mueller-matrices. The result of the different decompositions, together with the correlation effects reveals the underlying physical processes of depolarization.

DS 16.2 Mon 17:15 CHE 91

Synthesis, crystal growth and characterization of less-known vanadium-based TMDC compounds — •Konstantin Nikonov[1,3], Niels Ehlen[1], Boris Senkovskiy[1], Alexander Fedorov[1,2], Nihit Saigal[1], Wouter Jolie[1], Timo Knispel[1], Maria Brekhovskikh[3], and Alexander Grueneis[1] — [1]II. Physikalisches Institut, Universitaet zu Koeln, Germany — [2]IFW Dresden, Germany — [3]IGIC RAS, Moscow, Russia

Layered transition metal dichalcogenides are a very popular class of materials due to vast diversity of their electronic properties and layered structure, which makes it some kind of intermediate between 3D and 2D materials. Their begavior may vary from semiconducting, as in MoS_2, to metallic or semimetallic, as in VSe_2 or $ZrSe_2$. Various phenomena such as superconductivity and charge dencity waves can be observed in different TMDC under suitable conditions.

Despite long history of research, many of TMDC systems still were not studied by modern methods of solid state physics. Vanadium-based TMDC, such as VSe_2 and VTe_2 avoided close scientific attention due to difficult process of their synthesis and crystal growth.

In this work we aim to fill knowledge gap in vanadium-based systems, such as VSe_2 and VTe_2 and further investigate this group of layered materials.

DS 16.3 Mon 17:30 CHE 91

The study of interaction, nonlinear and dissipation effects in nanomembranes by investigating the dispersion relations of bending waves — •Fan Yang[1], Reimar Waitz[2], and Elke Scheer[1] — [1]Universität Konstanz, Konstanz 78457, Germany. — [2]Rational AG, 86889 Landsberg am Lech, Germany.

Deciphering the mode shapes of vibrations of nanopatterned membranes is paving the way for applications of nanoscale membranes which rely on particular properties of vibrational excitations. The mode shape of bending waves in thin membranes is measured as a function of space and time, using a phase-shift interferometer with continuous and stroboscopic light. We develop a method to separate the contribution of the excitation system from the measured amplitude in order to obtain the contribution of the membrane itself. The eigen-frequencies and the Q factor of the membrane can be obtained as well. With this method we are able to determine the dispersion relation of membrane oscillations in a frequency range from their ground mode up to 12 MHz. For membranes with an inhomogeneous stress, an algorithm to obtain a map of the lateral stress tensor components is presented. The study of the temperature dependent vibration behavior reveals an expected temperature dependence of the mechanical properties of a prestressed nanomembrane. Mechanical properties of different designed nanopattern-membranes are investigated by using our method.

DS 16.4 Mon 17:45 CHE 91

Optical Characterization of Anisotropic Thiophene-Phenylene Co-oligomer Micro Crystals by Spectroscopic Imaging Ellipsometry — •Christian Röling[1], Elena Y. Poimanova[2], and Vladimir V. Bruevich[3] — [1]Stresemannstrasse

30, 37079 Göttingen — [2]Donetsk National University, Department of Chemistry, Ukraine — [3]International Laser Center & Physics Faculty, M.V. Lomonosov Moscow State University, Vorobyevy gory, Moscow

Here we demonstrate Imaging Ellipsometry as a combination of microscopy and ellipsometry to characterize even micro-sized thin film crystals on plane surface regarding anisotropy, optical properties, crystalline domains and thickness. The semiconducting thiophene-phenylene co-oligomer 1,4-bis(5'-hexyl-[2,2'-bithiophen]-5-yl)benzene (dHex-TTPTT) crystals were grown by solvent based self-assembly technique on silicon substrate with 300 nm thermally silicon dioxide. The ellipsometric measurements were performed with an Ep4-SE (Accurion). In an ellipsometric high-contrast image of the complete sample we have localized high quality single crystals. After demonstrating the biaxial anisotropy of the crystal by using Müller-Matrix imaging ellipsometry we determined the optical axes by rotating the sample and performed spectroscopic measurements (λ = 400-700 nm) in 5 nm intervals. The optical properties were described by using a Lorentz term in the Ep4-Model. After determining the dispersion of the crystals we converted a recorded Delta and Psi-map into a 2D thickness image. Based on a quantitative analysis of the resulting thickness map we have calculated the height of a molecular layer (3.49 nm).

DS 16.5 Mon 18:00 CHE 91

Investigation of Indirect Excitons in Bulk *2H*-MoS2 Using Transmission Electron Energy-Loss Spectroscopy — •Carsten Habenicht, Martin Knupfer, Roman Schuster, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research, Dresden, Germany

Two-dimensional transition metal dichalcogenides are promising materials for applications in electronics, optoelectronics and photovoltaics among others. The design of efficient devices requires a detailed knowledge of the charge carrier dynamics in those materials, including the occurrence of excitons. We have investigated the indirect excitonic transistions in bulk *2H*-MoS2 using transmission electron energy-loss spectroscopy. The electron energy-loss spectra of *2H*-MoS2 in the (100) and (110) directions were measured for various momentum transfers up to values corresponding to the distances between the center of the Brillouin zone and their respective edges in reciprocal space. The results allow the identification of a number of indirect excitons and to a limited extent their energy-momentum dispersion. For example, an excitonic transition from a K point to an adjacent K point of the Brillouin zone were observed.

DS 16.6 Mon 18:15 CHE 91

Electronic properties of few-layer phosphorene from first-principles calculations — •Bukyoung Jhun and Cheol-Hwan Park — Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea

Phosphorene, a recently synthesized two dimensional material, has attracted a wide attention due to its numerous extraordinary physical properties such as spatially anistropic electrical and thermal conductance[1], superconductivity[2], and electronic topological transition tunable by electric field[3]. Because of the extraordinary properties, it is considered useful in opto-elctronics and electronics. We studied the electronic properties of multi-layer phosphorene in various environments by means of density-functional theory calculations. We expect the results to be helpful in interpreting experiments on the material and in designing phosphorene-based devices.

Reference

[1] Han Liu, Adam T Neal, Zhen Zhu, Zhe Luo, Xianfan Xu, David Tománek, and Peide D Ye, "Phosphorene: an unexplored 2D semiconductor with a high hole mobility," ACS nano 8 (4), 4033-4041 (2014).

[2] Y. F. Ge, W. H. Wan, F. Yang, and Y. G. Yao, "The strain effect on superconductivity in phosphorene: a first-principles prediction," New Journal of Physics 17 (2015).

[3] Q. H. Liu, X. W. Zhang, L. B. Abdalla, A. Fazzio, and A. Zunger, "Switching a Normal Insulator into a Topological Insulator via Electric Field with Application to Phosphorene," Nano Letters 15 (2), 1222-1228 (2015).

DS 17: Thermoelectric Materials

Time: Monday 17:45–19:00 Location: CHE 89

DS 17.1 Mon 17:45 CHE 89

Thermal conductivity of Half-Heusler superlattices — Paulina Komar[1,3], Niklas Reuter[1], Emigdio Chavez-Angel[1], Sven Heinz[1,3], Benjamin Balke[2], and •Gerhard Jakob[1,3] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [3]Graduate School Materials Science in Mainz, 55128, Germany

Variable designs of TiNiSn/HfNiSn superlattices (SLs) and nonperiodic multilayers were investigated to find the most effective way to reduce the crossplane thermal conductivity κ at room temperature. The latter property was determined using a differential 3ω method. The research started from investigation of the relation between κ and the SL period while keeping the ratio of the two materials in the SL period equal to unity. To obtain information exceeding that from the bare interface density, a series of films with varying layer thickness ratios was investigated. Moreover, we discuss the design of non-periodic multilayers and their influence on the thermal conductivity. For the latter materials we developed a software to simulate x-ray diffraction patterns of non-periodic structures.

The main conclusion is that the nanostructuring helps to reduce the thermal conductivity and contributes to enhanced figure of merit ZT compared to bare TiNiSn and HfNiSn films.

We gratefully acknowledge financial support by DFG (Ja821/4-2) and the Graduate School of Excellence Material Science in Mainz (GSC 266).

DS 17.2 Mon 18:00 CHE 89

Electronic and thermoelectric properties of polar LaNiO$_3$/SrTiO$_3$(001) superlattices — •Benjamin Geisler[1], Ariadna Blanca-Romero[2], and Rossitza Pentcheva[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg, Germany — [2]Department of Chemistry, Imperial College London, London, SW7 2AZ, United Kingdom

Advances in layer-by-layer fabrication techniques have made it possible to grow epitaxial transition metal oxide superlattices with atomic precision. We combine DFT+U calculations and Boltzmann transport theory to analyze the implications of the interface-dependent polar discontinuity in LaNiO$_3$/SrTiO$_3$(001) superlattices on the structural, electronic, and thermoelectric properties. While (LaO)$^+$/(TiO$_2$)^0 interfaces result in an n-type superlattice, (NiO$_2$)$^-$/(SrO)^0 interfaces lead to p-type doping. We find that significant octahedral tilts are induced in the SrTiO$_3$ region and that the La-Sr distances act as a fingerprint of the interface type. In contrast to the paradigmatic LaAlO$_3$/SrTiO$_3$ system, the electrostatic doping is mainly accommodated in the metallic NiO$_2$ layers. We explain the electronic structure within the SrTiO$_3$ band gap in terms of an orbital-selective quantization of Ni-3d-derived quantum well states. Complex cylindrical Fermi surfaces emerge which show a tendency towards nesting that depends on the interface polarity. Finally, we demonstrate that the thermoelectric response of our oxide superlattices can be selectively controlled by a targeted interface design.

Funding by the DFG within TRR 80 (G3 and G8) is acknowledged.

DS 17.3 Mon 18:15 CHE 89

Design of thermoelectrically highly efficient Heusler compounds using phase separations and nano-composites under an economic point of view — •Benjamin Balke — Johannes Gutenberg-Universität Mainz

Half-Heusler compounds are one of the most promising candidates for thermoelectric materials for automotive and industrial waste heat recovery applications. In this talk, I will give an overview about our recent investigations of phase separations in half Heusler thermoelectrics, focusing on the ternary system TiNiSn-ZrNiSn-HfNiSn. I will show how we adapted this knowledge to design a p-type Heusler compound which exhibits a ZT that is increased by 130% compared to the best published bulk p-type Heusler. I will also present how we used the phase separation to design thermoelectric highly efficient nano-composites of different single-phase materials. Since the price for Hafnium was doubled within the last 15 months, our research focused on the design of half-Heusler compounds without Hafnium. I will present a very recent calculation on ZT per € and efficiency per € for various materials followed by our latest very promising results for n-type Heusler compunds without Hafnium resulting in 20 times higher ZT/€ values. These results strongly underline the importance of phase separations as a powerful tool for designing highly efficient materials for thermoelectric applications that fulfill the industrial demands for a thermoelectric converter.

DS 17.4 Mon 18:30 CHE 89

pattern formation in the half-Heusler NiTi_{x-1}Zr_xSb_{1-y}Sn_y — •Joaquin Miranda, Thomas Gruhn, and Heike Emmerich — Material- und Prozesssimulation, Bayreuth University. Universitaetstr 30, DE 95447, Bayreuth

Domain formations offer the possibility to reduce the lattice thermal conductivity in thermoelectrics. In this view, We employed ab-initio Density Functional calculations and Monte Carlo simulations to investigate the thermoelectric NiTi_{x-1}Zr_xSb_{1-y}Sn_y presents phase separation and rich patterning when is simultaneously alloyed Ti with Zr and Sb with Sn. We found that the material undergoes multiple phase separations as the temperature is lowered. First Ti and Zr phase separated at near 650 K but Sn and Sb tend to remain homogeneously distributed until temperatures around 300 K are reached. Within this temperature range (300-650 K) it is observed a slight preference of Zr-Sn (or Ti-Sb) nearest neighbors formation. Below 300 K both neighbors are increased, giving place to a second phase separation of richer Sn regions embedded in Zr volumes and Sb regions in Ti volumes; interestingly showing a meta-crystal structure preference of neighboring Zr and Sn atoms. We discuss the relevance of these observations within the context of thermoelectrics.

DS 17.5 Mon 18:45 CHE 89

Defects in Heusler compounds for thermoelectric applications. — •Gerhard H. Fecher[1], Benjamin Balke[2], and Claudia Felser[1] — [1]Max Planck Institute - CPFS, Dresden, Germany — [2]Johannes Gutenberg University, Mainz, Germany

It turned out that semi-conducting Heusler compounds with $C1_b$ structure and 18 valence electrons are reliable materials for thermoelectric applications, in particular for generators. The materials are mostly based on Ni for n-type or Co for p-type thermoelectrics. Examples are TNiSn or TCoSb where (T =Ti, Zr, Hf) is a transition metal or a combination of transition metals e.g.: $Hf_{0.35}Zr_{0.35}Ti_{0.3}$. The latter mixture leads already to chemical disorder, as different elements share the same position of the $C1_b$ structure. Further defects are anti-site disorder caused by a swap of two different atoms (e.g.: Ti ↔Sn), off-stoichiometry by excess or deficiency of one of the elements ($TiNi_{1\pm x}Sn$) or Frenkel defects (e.g.:Ni ↔ □). First principles calculations were performed for Heusler compounds exhibiting such defects and the influence of the defects on the electronic structure was studied. The main emphasis was on the changes of the band gap and the occurrence of states inside of the gap. The effects of the different defects on the electronic transport properties will be discussed.

DS 18: Transport: Topological Semimetals 1 (jointly with MA/TT)

Time: Tuesday 9:30–11:45 Location: HSZ 201

DS 18.1 Tue 9:30 HSZ 201

Electron-hole pairing of Fermi arc surface states in a Weyl semimetal bilayer — •Paolo Michetti and Carsten Timm — Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

The topological nature of Weyl semimetals (WSMs) is corroborated by the presence of chiral surface states at the boundaries, connecting the bulk Fermi surface by Fermi arcs (FAs). We develop an analysis of the electron-hole pairing instability between the surface states of a bilayer structure realized by introducing a thin insulating spacer into a bulk WSM. We employ a minimal WSM model for the description of the surface states and a self-consistent mean-field treatment of the pairing interaction. We find that the system is unstable towards the formation of coherent electron-hole pairs, which leads to partial gapping of the FA dispersion curve and possibly to a superfluid dipolar exciton condensate, where dissipationless counter-propagating currents can be induced in the two layers. A signature of such condensate is the modifications of the peculiar quantum oscillations from surface FAs. We characterize the dependence of the single-particle energy gap and the critical temperature on the model parameters, where we emphasize in particular the linear scaling of these quantities with the separation between the Weyl points. A detrimental role is played by the curvature of the FA, although the phenomenon persists for moderately low curvature.

DS 18.2 Tue 9:45 HSZ 201

Universality and stability of the edge states of chiral nodal topological semimetals; Luttinger model for $j = \frac{3}{2}$ electrons as a 3D topological semimetal — •Maxim Kharitonov, Julian-Benedikt Mayer, and Ewelina Hankiewicz — Institute for Theoretical Physics and Astrophysics, Wuerzburg University

We theoretically demonstrate that the chiral structure of the nodes of nodal semimetals is responsible for the existence and universal local properties of the edge states in the vicinity of the nodes. We perform a general analysis of the edge states for an isolated node of a 2D semimetal, protected by *chiral symmetry* and characterized by the topological winding number N. We derive the asymptotic chiral-symmetric boundary conditions and find that there are $N+1$ universal classes of them. The class determines the numbers of flat-band edge states on either side off the node in the 1D edge spectrum and the winding number N gives the *total* number of edge states. We then show that the edge states of chiral nodal semimetals are *robust*: they persist in a finite-size *stability region* of parameters of chiral-asymmetric terms. This significantly extends the notion of 2D and 3D topological nodal semimetals. We demonstrate that the Luttinger model with a quadratic node for $j = \frac{3}{2}$ electrons is a 3D topological semimetal in this new sense and predict that α-Sn, HgTe, and possibly $Pr_2Ir_2O_7$, as well as many other semimetals described by it are topological and exhibit surface states.

DS 18.3 Tue 10:00 HSZ 201

Interband optical conductivity of the Dirac semimetal Cd_3As_2 — •D. Neubauer[1], J. P. Carbotte[2], A. A. Nateprov[3], A. Löhle[1], M. Dressel[1], and A. V. Pronin[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Department of Physics and Astronomy, McMaster University, Canada — [3]Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau, Moldova

We measured the optical reflectivity of [001]-oriented n-doped Cd_3As_2 in a broad frequency range (50 – 22 000 cm^{-1}) for temperatures from 10 to 300 K. The optical conductivity, $\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)$, is isotropic within the (001) plane; its real part follows a power law, $\sigma_1(\omega) \propto \omega^{1.65}$, in a large interval from 2000 to 8000 cm^{-1}. This behavior is caused by interband transitions between two bands, which are effectively described by a sublinear dispersion relation, $E(k) \propto |k|^{0.6}$. The momentum-averaged Fermi velocity of the carriers in these bands is energy dependent and ranges from 1.2×10^5 to 3×10^5 m/s, depending on the distance from the Dirac points. These values are in agreement with the published data on Cd_3As_2. We detect a gaplike feature in $\sigma_1(\omega)$ and associate it with the Fermi level positioned around 100 meV above the Dirac points. Finally, we compare our results with recent magneto-optical infrared data.

DS 18.4 Tue 10:15 HSZ 201

Angular-dependent magnetoresistance of 3D Dirac materials — •Henry Legg and Achim Rosch — Institute for Theoretical Physics University of Cologne Zülpicher Straße 77 D-50937 Köln Deutschland

The realisation of 3D Dirac and Weyl semi-metals has created a new playground for transport phenomena, such as the possibility to produce the chiral anomaly in a condensed matter setting. Many materials that realise a 3D Dirac dispersion are protected by crystal symmetry and therefore have multiple Dirac cones within their Brillouin zone; examples include Cd_2As_2, Na_3Bi, and $Pb_{1-x}Sn_xSe$.

In this work we show that the application of a parallel magnetic and electric field in a direction perpendicular to that connecting a pair of

Dirac cones can lead to a large positive magnetoresistance. The magnetic field leaves only an effective one-dimensional dispersion parallel to the field, due to the formation of Landau levels perpendicular to the magnetic field. The result is a large inter-nodal scattering matrix between the two Dirac cones since the Dirac nodes are close in the dimensionally reduced system. Our results are compared to recent experiments on $Pb_{1-x}Sn_xSe$.

15 min. break.

DS 18.5 Tue 10:45 HSZ 201

Quantum oscillation and Dirac fermion in $BaZnBi_2$ system — •Kan Zhao and Philipp Gegenwart — Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany

Dirac semimetals represent new quantum states of matter and have stimulated intensive studies. $AMnBi_2$(A = alkali earth/rare earth metal) is one of the established Dirac semimetals, with both antiferromagnetic order in $MnBi_4$ layer and Dirac fermion in Bi square net layer.

To investigate how the magnetism interacts with Dirac fermions, we synthesized single crystals of $SrZnBi_2$ and $BaZnBi_2$. Being isostructural to $SrMnBi_2$, $SrZnBi_2$ shows no quantum oscillation in resistivity and magnetic susceptibility up to 14 T. However, $BaZnBi_2$ shows clear multiple quantum oscillations down to 4 T in magnetic susceptibility. According to the temperature dependence of the oscillation amplitude after fast Fourier transformation (FFT), the effective electron mass is about 0.1me, comparable with that of $BaMnBi_2$. In the resistivity measurement up to 14 T at 2 K clear SdH oscillations with main oscillation frequency 168T are observed. The frequency follows a $1/|\cos(\theta)|$ dependence (θ is the angle between magnetic field and c axis), indicating a quasi 2D Fermi surface. Band-structure calculations by I. Mazin, indicate that $BaZnBi_2$ exhibits a unique structure feature and electronic structure, with a quasi Dirac band near the Fermi level. ARPES and high-field SdH measurements, to further characterize the Dirac fermions, are in progress.

DS 18.6 Tue 11:00 HSZ 201

Observation of Topological Surface States and Strong Electron/hole Imbalance in an Extreme Magnetoresistance Semimetal — •Niels Bernhard Michael Schröter[1], Juan Jiang[1,2,3,4], Shu-Chun Wu[5], Nitesh Kumar[5], Chandra Shekhar[5], Han Peng[1], Xiang Xu[6], Cheng Chen[1], Haifung Yang[7], Chan Hwang[4], Sung-Kwan Mo[3], Zhongkai Liu[2], Lexiang Yang[6], Claudia Felser[5], Binghai Yan[5], and Yulin Chen[1,2,6] — [1]University of Oxford, Oxford, UK — [2]ShanghaiTech University, Shanghai, P. R. China — [3]Advanced Light Source, Berkeley, USA — [4]Pohang Accelerator Laboratory, POSTECH, Pohang, Korea — [5]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [6]Tsinghua University, Beijing, P. R. China — [7]Chinese Academy of Sciences, Shanghai, P. R. China

The discovery of an extreme magnetoresistance (XMR) in the nonmagnetic rare-earth monopnictides LaX (X = P, As, Sb, Bi), a recently proposed new topological semimetal family, has inspired intensive research on the correlation between the XMR and their electronic structures. In this work, using ARPES to investigate the three dimensional band structure of a lanthanum monopnictide, we unraveled its topologically non-trivial nature with the observation of multiple topological surface Dirac fermions, as supported by our ab-initio calculations. Furthermore, we observed substantial imbalance between the volumes of electron and hole pockets, which rules out the electron-hole compensation as the primary cause of the XMR, putting strong constraints on future theoretical investigations.

DS 18.7 Tue 11:15 HSZ 201

Topological metal with multiple Dirac cones and nodal line — •Ashis Kumar Nandy[1], Alex Aperis[1], M. Mofazzel Hosen[2], Klauss Dimitri[2], Pablo Maldonado[1], Dariusz Kaczorowski[3], Tomasz Durakiewicz[4], Madhab Neupane[2], and Peter M. Oppeneer[1] — [1]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden — [2]Department of Physics, University of Central Florida, Orlando, Florida, USA — [3]Institute of Low Temp. & Structure Research, PAS, Wroclaw, Poland — [4]Condens. Matter and Magnet Science Group, LANL, Los Alamos, USA

The extended class of topological materials includes topological (semi) metals that support non-trivial topological surface states in the form of one-dimensional Dirac lines or Fermi-arcs connecting two Weyl points. Here we study a ternary compound using a combination of systematic theoretical calculations and detailed angle-resolved photoemission spectroscopy (ARPES) measurements. In contrast to other topological materials, our first-principles calculations suggest that the band inversion is $d-p$ type instead of the mostly observed $s-p$ type band inversion. We identify multiple Dirac fermionic states at various binding energies. A Dirac cone is computed at the Γ point about 0.5 eV above the chemical potential. Most importantly, at around 1 eV below the Fermi level our calculations reveal a surface nodal line-like feature passing through the time-reversal invariant point M. Our systematic study suggests a new family of materials for exploring the coexistence and competition of multiple fundamental fermionic quantum states.

DS 18.8 Tue 11:30 HSZ 201

***PT* Anomalous Transport in a Nodal Line Dirac Semimetal** — •Wenbin Rui, Yuxin Zhao, and Andreas P. Schnyder — Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

Recently *PT* invariant topological nodal line Dirac semimetals have attracted increasing attentions in quantum matter. Here we study the anomalous transport of the *PT* symmetric Dirac semimetals of (3+1) dimensions as responses to electromagnetic fields, for which the universal currents are originated from the parity anomaly in (2+1)-dimensional quantum field theory. Considering that the total sum of anomalous currents from soft modes spreading along the nodal loop vanishes, we design a feasible experiment to detect the effect, which is able to separate anomalous currents from distinct regions of the nodal loop.

DS 19: Fundamentals of Perovskite Photovoltaics III (jointly with CPP/HL)

Time: Tuesday 9:30–12:30 Location: ZEU 222

Invited Talk DS 19.1 Tue 9:30 ZEU 222

Investigation of hybrid organic/inorganic perovskite systems and interfaces by photoelectron spectroscopy — •Selina Olthof — University of Cologne, Germany, Luxemburgerstrasse 116, 50939 Cologne

In recent years, the interest in hybrid organic - inorganic perovskites rose at a rapid pace due to their tremendous success in the field of photovoltaics. In addition to the thin film properties of the active layer, the performance of optoelectronic devices strongly depends on the appropriate energetic alignment between the active- and adjacent layers. In order to choose adequate transport materials for the increasingly complex hybrid perovskite compositions in a non-trial-and-error fashion, it is important to understand how the induced changes in band gap relate to shifts in the valence and/or conduction band.

In this talk, I will discuss recent findings regarding measurements of the electronic structure of various hybrid perovskites, covering lead as well as tin based systems and a variety of halogens using UV-, inverse, and x-ray photoelectron spectroscopy measurements (UPS/IPES/XPS). Furthermore, using these surface sensitive techniques the alignment at interfaces between different layers can be probed in-situ as well by performing a stepwise film preparation. Looking at various bottom contacts we find that chemical interactions, band bending, and interface dipole formation play an important role. Therefore, the nature of the substrate not only determines the energetic alignment but can lead to chemical reactions and influence film formation and crystallinity.

DS 19.2 Tue 10:00 ZEU 222

Influence of air and water on the electronic structure of CH3NH3PbI3-xClx mixed halide perovskite film surfaces — •Maryline Ralaiarisoa, Fengshuo Zu, and Norbert Koch — Humboldt-Universität zu Berlin, Institut für Physik & IRIS Adlershof, Brook-Taylor-Str. 6, 12489 Berlin, Deutschland

Water and oxygen under environmental conditions reveal to be both beneficial for device performance as well as detrimental to the stability of perovskite based solar cells and films. Within this controversy, an accurate and comprehensive description of the influence of these factors is still lacking, particularly on the electronic structure of perovskite films. We investigated the effect of water and air on the ionization energy (IE) and the electronic structure of perovskite films. To this end, we used photoelectron spectroscopy to monitor the electronic structure of perovskite films following a range of procedures, including thermal post-treatment, as well as air and oxygen exposure. After air exposure, we observe changes of work function (WF) and IE similar to those after pure oxygen exposure. Furthermore, our observations indicate that even without prior ambient air exposure residual water (from processing in a typical glove-box environment) can still be present on the surface of perovskite films, even under vacuum conditions. Such water adsorption seemingly increases the WF of the perovskite films. Our results underline how environmental conditions substantially affect the electronic structure of perovskite films, which will likely impact the energy level alignment in perovskite-based photovoltaic cells.

DS 19.3 Tue 10:15 ZEU 222

Modulated surface photovoltage spectroscopy of CH3NH3Pb(I,Br)3 thin films — •Celline Awino, Thomas Dittrich, Eva Unger, and Bernd Rech — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Kekuléstr. 5, 12489 Berlin, Deutschland

The investigation of electronic properties of CH3NH3Pb(I,Br)3 and their dependence on aging and light soaking is important for better understanding of the stability of solar cells based on related materials. Modulated surface photovoltage spectroscopy allows for the ex-situ and in-situ characterization of the band gap, tail states and deep defect states in the band gap, direction of modulated charge separation and diffusion length. It has been found, for example, that the Tauc gap and the energy of exponential tail states sensitively depend on the substrate and on soaking in nitrogen atmosphere and that light soaking has strong influence on the direction and amplitude of modulated charge separation.

DS 19.4 Tue 10:30 ZEU 222

Revealing the impact of the potential distribution within high performing Lead Methylammonium Tri-Iodide solar cells with organic contact materials — •Christian Müller[1,2,3], Bernd Epding[2,3], Ramos Bwalya[2,3], Michele Sessolo[4], Lidón Gil-Escrig[4], Henk Bolink[4], Robert Lovrincic[1,3], and Wolfgang Kowalsky[1,2,3] — [1]IHF, TU Braunschweig, Germany — [2]KIP, Universität Heidelberg, Germany — [3]InnovationLab, Heidelberg, Germany — [4]Instituto de Ciencia Molecular, Universidad de Valencia, Spain

Over the last few years the power conversion efficiency of organometal-halide perovskite (such as CH$_3$NH$_3$PbI$_3$, MAPI) based solar cells has skyrocketed at an unprecedented rate to values around 22%. However, the understanding of the physical process in the solar cells drags behind the progress of efficiency. For example, the influence of the potential distribution in such cells on their performance is so far not sufficiently studied.

We focus in this work on high performing fully vacuum processed MAPI solar cells with organic contact materials [1]. We will present SKPM measurements on p-i-n and n-i-p solar cell cross sections that map the potential distribution within the device with high spatial resolution. Performing measurements under different conditions enables us to determine the influence of potential barriers at the contact interfaces and of a poling on the cell efficiency.

[1] Energy Environ. Sci., 2016, 9, p. 3456-3463, C. Momblona et al.

DS 19.5 Tue 10:45 ZEU 222

Impact of Illumination on the Electronic and Chemical Structure of Mixed Halide Perovskites — •Fengshuo Zu[1], Patrick Amsalem[1], Ingo Salzmann[1], Rongbin Wang[1,2], Maryline Ralaiarisoa[1], Stefan Kowarik[1], Steffen Duhm[2], and Norbert Koch[1] — [1]Institut für Physik,Humboldt-Universität zu Berlin,12489 Berlin,Germany — [2]FUNSOM,Soochow-University,Suzhou,China

The seemingly n-type behavior of the perovskite films is largely intriguing since these films are calculated to be bipolar conductive. For exploring the fundamental physics of the n-type behavior, we investigate the effect of white-light illumination on the electronic structure of mixed halide perovskite thin films and of CH3NH3PbI3 single crystals using X-ray and ultraviolet PES, as well as UV-Vis absorption spectroscopy. The samples are found to be strongly n-type and, upon illumination, the valence band features shift by up to 0.7 eV to lower BE. We show this effect to be correlated with initial surface band bending due to the presence of donor levels likely consisting of reduced lead (Pb0) acting as surface traps. Upon short-time illumination, this phenomenon is found to be partially reversible, for prolonged illumination, however, a high concentration of metallic Pb0 is generated inducing strong Fermi-level pinning. This effect is accompanied by the formation of PbI2 defects within the film and a deficiency of iodine in the surface region. Experiments performed on CH3NH3PbI3 single crystal reveal the presence of a relatively high concentration of reduced Pb0 at the sample surface after cleaving, likewise, strongly pinning the Fermi-level even under high intensity illumination.

15 min break

DS 19.6 Tue 11:15 ZEU 222

Giant Rashba Splitting in (CH$_3$NH$_3$)PbBr$_3$ Organic-Inorganic Perovskite — Daniel Niesner[1], Max Wilhelm[1], Ievgen Levchuk[2], Andres Osvet[2], Shreetu Shrestha[2], Miroslaw Batentschuk[2], Christoph Brabec[2,3], and •Thomas Fauster[1] — [1]Lehrstuhl für Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]I-MEET, Department of Materials Science and Engineering, FAU Erlangen-Nürnberg, Martensstr. 7, D-91058 Erlangen, Germany — [3]ZAE Bayern, Haberstr. 2a, D-91058 Erlangen, Germany

A Rashba-type spin-split band structure has been predicted for organic-inorganic perovskite semiconductors. The effect has been proposed as one of the origins of the exceptionally long carrier lifetimes in the materials, forming the basis of their successful application in opto-electronics. Using angle-resolved photoelectron spectroscopy, we investigate the band structure of (CH$_3$NH$_3$)PbBr$_3$ single crystals cleaved in ultrahigh vacuum. The orthorhombic low-temperature phase and the cubic room-temperature phase are studied. We apply a modified leading-edge method to identify the dispersion of the valence band edge. It reveals two valence band maxima, separated in k-space by 0.043 Å^{-1}. The dispersion is indicative of Rashba splitting. This interpretation is supported by the observation of circular dichroism in the orthorhombic phase. Extracted Rashba parameters of $\alpha_o = 7 \pm 1$ eV Å and $\alpha_c = 11 \pm 4$ eV Å in the orthorhombic and the cubic phase are amongst the largest reported to date.

DS 19.7 Tue 11:30 ZEU 222

Exploring the electronic band structure of (organo-)metal halide perovskite via photoluminescence anisotropy of individual nanocrystals — •Daniela Täuber[1], Mirko Goldmann[1,2], Juanzi Shi[1], Alexander Dobrovolsky[1], and Ivan Scheblykin[1] — [1]Chemical Physics, Lund University, Lund, Sweden — [2]TU Ilmenau, Germany

Understanding electronic processes in metal halide perovskites requires unraveling the origin of their electronic transitions. Light polarization studies can provide important information regarding transition dipole moment orientations. Investigating individual lead trihalide perovskite nanocrystals enabled us to detect the polarization of photoluminescence intensity and photoluminescence excitation, hidden in bulk samples by ensemble averaging. Polarization properties of $CH_3NH_3PbI_3$ crystals were correlated with their photoluminescence spectra and electron microscopy images [1]. We propose that distortion of PbI6 octahedra leads to peculiarities of the electronic band structure close to the band-edge. Namely, the lowest band transition possesses a transition dipole moment along the apical Pb-I-Pb bond resulting in polarized photoluminescence. Excitation of photoluminescence above the bandgap is unpolarized because it involves molecular orbitals delocalized both in the apical and equatorial directions of the perovskite octahedron. Trap-assisted emission at 77 K, rather surprisingly, was polarized similar to the bandgap emission.

D.T. acknowledges a personal research grant DFG-TA 1049/1-1.

[1] Täuber, D. et al., Nano Letters 16, 5087-5094, 2016.

DS 19.8 Tue 11:45 ZEU 222

Band Edge Engineering of Hybrid Halide Perovskites for Solar Cell Applications - Insights from Density Functional Theory — •Linn Leppert[1,2], Sebastian E. Reyes-Lillo[1,2], and Jeffrey B. Neaton[1,2,3] — [1]Molecular Foundry, Lawrence Berkeley National Laboratory — [2]Department of Physics, University of California Berkeley — [3]Kavli Energy NanoScience Institute at Berkeley

Efficiencies of solar cells based on hybrid halide perovskite absorbers have reached 22%, making them serious contenders to silicon solar cells. Nevertheless, the toxicity of lead, the material's instability, as well as pressing questions about the role of structural heterogeneities present challenges to its large scale fabrication and long term use. Recently it has been shown that photovoltaic properties vary significantly between different crystal facets of perovskite thin films, suggesting an appreciable effect of electric fields on the local electronic structure [1]. In this contribution, I will elucidate the coupling between electric polarization, which increases as a function of the macroscopic alignment of the organic moieties, and the band edge electronic structure. In particular the Rashba effect, an energy band splitting in k-space, increases with increasing polarization, indicating significant tunability with experimentally feasible applied fields. The effect can be tuned further by chemical substitution of the organic molecule as well as by anisotropic strain, allowing for considerable Rashba splitting even in the absence of electric fields [2]. [1] S. Leblebinci, L. Leppert, et al., Nature Energy 1, 16093 (2016). [2] L. Leppert et al., J. Phys. Chem. Lett. 7, 3683 (2016).

DS 19.9 Tue 12:00 ZEU 222

Computational serach for sulphide perovskites for solar energy conversion application — •Korina Kuhar, Mohnish Pandey, Kristian Sommer Thygesen, and Karsten Wedel Jacobsen — Center for Aromic-scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, DK * 2800 Kgs. Lyngby, Denmark

Oxide perovskites are in general known to be wide band gap semiconductors which hampers their use for visible light absorption. However, recent experiments on the synthesis of inorganic sulphide perovskites, for example BaZrS3[1] and SrZrS3[2], with band gaps of 1.7 ev and 0.8-1 eV, respectively, show that sulphur is a possible supstitution to oxygen in inorganic perovskites to lower their band gaps. Several binary, ternary and quaternary sulphides are already known to have relevant band gaps. We perform a systematic investigation of the class of ABS3 compounds in eight phases using Density Functional Theory (DFT). The screening procedure applied is based on simple criteria such as stability, band gap in the visible part of the solar spectrum, high charge mobility and small tendency of the material to form defects. Finally we report a set of sulphide perovskites we found to be stable and have interesting properties for use as solar energy conversion materials.

1. DOI: 10.1021/acs.chemmater.5b04213 2. DOI: 10.1016/j.solidstatesciences.2005.02.010

DS 19.10 Tue 12:15 ZEU 222

Towards a multiscale statistical description of hybrid perovskite materials — •Jingrui Li[1], Jari Järvi[1,2], and Patrick Rinke[1] — [1]COMP Centre of Excellence, Aalto University, Finland — [2]Department of Physics, University of Helsinki, Finland

Hybrid perovskites (HPs), in particular methylammonium lead iodide ($MAPbI_3$), have received enormous interest in recent years as promising photoactive materials in emergent photovoltaic technologies. An important feature of HPs is their structural complexity introduced by the organic cations (e.g., MA^+). At room temperature or above, the MAs will be oriented (quasi-)randomly, forcing HPs into disordered structures. The disorder affects important materials properties such as the stability and electronic structure that are crucial for the application of HPs in novel photovoltaic devices. Our previous density-functional theory (DFT) study reveals that hydrogen bonding leads to an anisotropic interaction between the MA cations and the inorganic cage. The deformed cage and the MA orientation are interdependent, analogous to a chicken-and-egg paradox [1]. From the insight of this single unit cell model, we derive a multiscale scheme for disordered $MAPbI_3$ structures, in which the interaction between neighbouring MA ions is described by a pair model. We show that the total number of relevant pairs can be reduced to only 86 and then analyse DFT results for large, geometry optimized $MAPbI_3$ supercell models in terms of their “pair-mode” distribution. With our model we can then describe disordered HPs on length scales beyond a few nanometers.

[1] J. Li and P. Rinke, *Phys. Rev. B* **94** 045201 (2016).

DS 20: Focussed Session: Frontiers in Exploring and Applying Plasmonic Systems II (Joint Session of CPP, DS, HL, MM, and O, organized by DS)

With the increasing importance of plasmonics and the variety of its number of applications it becomes obvious that experimental characterization beyond the far-field optical standard methods and also theoretical tools that access the plasmonic behaviour on the atomic scale are indispensable for further development and improvement of the basic knowledge and thus, for new kinds of applications. The “Focused Session” gathers experts for unusual experimental methods (near-field studies with SNOM and EEL-TEM) and for the theoretical exploration of quantum effects in plasmonic excitations. Furthermore, new kinds of plasmonic applications (devices exploiting phase changes, alternative displays and holograms) will be introduced.

Organizers: Laura NaLiu (U Heidelberg) and Annemarie Pucci (U Heidelberg)

Time: Tuesday 9:30–12:45 Location: CHE 89

Topical Talk DS 20.1 Tue 9:30 CHE 89

Driving nanophotonics to the atomic scale — •Javier Aizpurua — Center for Materials Physics (CSIC-UPV/EHU) and DIPC, San Sebastian, Spain

Plasmonic nanogaps are formed at the junction of two metallic interfaces and provide a great opportunity to explore atomic-scale morphologies and complex photochemical processes by optically monitoring the excitation of their intense surface plasmonic modes. In recent years, optical spectroscopy of these cavities has proven to be extremely sensitive to atomic-scale features that determine the chemistry and the optoelectronics in the gaps. In this regime, classical theories often fail to address the fine details of the optical response, and more sophisticated quantum models based on condensed matter theory techniques are needed. Additionally, theoretical approaches based on quantum electrodynamics (QED) can be properly developed to address the complex coupling of subnanometric optical cavities with electronic and vibrational states of molecules nearby. A few experimental situations in optoelectronics, molecular spectroscopy and optomechanics, where optics is proven to address the atomic scale and thus quantum effects are shown to be of paramount importance, will be described.

Topical Talk DS 20.2 Tue 10:00 CHE 89

Transverse and Longitudinal Resonances in Plasmonic Gold Tapers — Surong Guo[1], Nahid Talebi[1], Wilfried Sigle[1], Ralf Vogelgesang[2], Gunther Richter[3], Martin Esmann[2], Simon F. Becker[2], Christoph Lienau[2], and •Peter A. van Aken[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Carl von Ossietzky University of Oldenburg, Oldenburg, Germany — [3]Max Planck Institute for Intelligent Systems, Stuttgart, Germany

Conically-shaped metallic tapers are one of the most common structures with concomitant capabilities of nanofocusing and field enhancement. We distinguish two different dynamic mechanisms, reflection and phase matching, of surface plasmons excited by relativistic electrons in three-dimensional gold tapers with various opening angles from 5° to 47° which are studied both experimentally and theoretically, by means of electron energy-loss spectroscopy and finite-difference time-domain numerical calculations, respectively. We observe distinct resonances along the taper shaft independent of opening angles. We show that the origin of these resonances is different at different opening angles and results from a competition between two coexisting mechanisms. For large opening angles ($> 20°$), phase matching between the electron field and that of higher-order angular momentum modes is the dominant contribution because of the increasing interaction length between electron and the taper near-field. In contrast, reflection from the taper apex dominates at small opening angles (< 10°). A gradual transition of these two mechanisms is observed for intermediate opening angles.

Topical Talk DS 20.3 Tue 10:30 CHE 89

Nanoimaging and control of polaritons in 2D materials — •Rainer Hillenbrand — CIC nanoGUNE, San Sebastian, Spain

A promising solution for active control of light on the nanometer scale are plasmons in graphene, which offer ultra-short wavelengths, long lifetimes, strong field confinement, and tuning possibilities by electrical gating. Here, we discuss scattering-type scanning near-field optical microscopy (s-SNOM) for real-space imaging of graphene plasmons [1-3] in nanoresonators [4] and hBN-graphene heterostructures [5]. We also introduce THz near-field photocurrent nanoscopy and discuss its application for imaging acoustic graphene plasmons in a graphene-based THz detector [6]. Further, we discuss ultraslow hyperbolic volume and surface phonon polaritons in boron nitride flakes [7,8].

[1] J. Chen et al., Nature, 487, 77 (2012) [2] Z. Fei et al., Nature 487, 82 (2012) [3] P. Alonso-González et al., Science 344, 1369 (2014) [4] A. Y. Nikitin et al., Nat. Photon. 10, 239 (2016) [4] A. Woessner et al., Nat. Mater. 14, 421 (2015) [6] P. Alonso-González et al., Nat. Nanotechnol. DOI: 10.1038/nnano.2016.185 [7] E. Yoxall et al., Nat. Photon. 9, 674 (2015) [8] P. Li et al, Nano Lett. DOI: 10.1021/acs.nanolett.6b03920

15 min. break.

Topical Talk DS 20.4 Tue 11:15 CHE 89

Switchable infrared nanophotonic elements enabled by phase-change materials — •Thomas Taubner — Institute of Physics (IA), RWTH Aachen University

The strong confinement and enhancement of light when coupled to surface waves or nanoparticles is key for various applications in nanophotonics such as sensing, imaging or the manipulation of light fields. In the mid-infrared spectral range, metallic nanoantennas and materials supporting surface phonon polaritons (SPhPs) can be used as building blocks of such devices. Often, their optical functionality is only obtained at a fixed wavelength, determined by the geometric design and the material properties.

By using phase-change materials (PCMs) as tunable environment for nanophotonic resonators, their resonance frequency can be altered in a non-volatile, reversible way. PCMs offer a huge change in refractive index due to a phase transition from their amorphous to crystalline state, which can be thermally, optically or electrically triggered. We present results on thermal and optical switching, as well as addressing of individual IR resonances of both systems, metallic nanoantennas and resonators for SPhPs. SPhPs on polar dielectrics exhibit lower losses and larger Q-values compared to metallic nanoantennas, and their confinement can be even increased by adding ultrathin, switchable PCM layers. We show the all-optical, non-volatile, and reversible switching of the SPhPs by controlling the structural phase of the PCM [1], opening the door for re-configurable metasurfaces.

[1] P. Li et al., Nat. Mat. 15, 870 (2016).

Topical Talk DS 20.5 Tue 11:45 CHE 89

Nonlocal response in plasmonic nanoparticles: How much quantum? — •N. Asger Mortensen — Technical University of Denmark

Plasmonics is commonly explored and interpreted within the framework of classical electrodynamics. On the other hand, with the increasing ability to explore plasmonics in nanostructures with yet smaller characteristic dimensions, intrinsic length scales of the electron gas are anticipated to manifest in a nonlocal plasmonic response and other quantum corrections to the light-matter interactions. In nanoparticles, nonlocal response promotes frequency blueshifts and nonlocal damping of high-order modes, as has been observed in single-particle EELS. As to the quantum mechanical origin of these effects, one can quantify the degree of nonclassical effects from an energy perspective. This provides a direct link between the experimentally observed resonance blueshift and the fraction of electromagnetic energy attributed to quantum degrees of freedom.

Topical Talk DS 20.6 Tue 12:15 CHE 89

Short-range plasmonics — •Harald Giessen — University of Stuttgart, Stuttgart, Germany

Short-range plasmons with extreme light compression down to 60 nm with light wavelength of 800 nm are demonstrated. Also, the formation of orbital angular momentum of plasmons with subfemtosecond resolution is studied.

DS 21: Thin Film Characterisation: Structure Analysis and Composition II

Time: Tuesday 9:30–13:00 Location: CHE 91

DS 21.1 Tue 9:30 CHE 91

Analysis of domain formation of epitaxial chalcogenide thin films — •Marc Pohlmann[1], Marvin Kaminski[1], Matti Wirtssohn[1], Abderaffi Moktad[1], Oana Cojocaru-Mirédin[1], Peter Jost[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics, Physics of New Materials, RWTH Aachen University, 52056 Aachen, Germany — [2]Sommerfeldstr. 14

Many chalcogenide alloys can be employed in phase-change memories because their optical and electrical properties differ strongly between their crystalline and amorphous phases. Interest in highly-textured or even epitaxially-grown chalcogenide thin films is fueled by the recent discovery of the advantageous memory-switching properties of chalcogenide superlattices, so-called interfacial phase-change memories (IPCMs), as well as by the topological properties of such films. High quality thin films can be produced by molecular beam epitaxy. However, in many material systems different rotational domains lead to the formation of grain boundaries or twin defects. To reduce these defects, it is essential to understand why and how the different domains are formed.

Therefore, in this work we combined electron backscattering diffraction (EBSD) with XRD to attain a sound understanding of the local domain structure and the mechanisms of domain formation in MBE-grown chalcogenide thin films.

DS 21.2 Tue 9:45 CHE 91

Growth and characterization of VO_2 thin films deposited on various perovskite and complex oxides single crystal substrates — •Adrian Petraru[1], Gabriel Bello Waldschütz[1], Ravi Droopad[2], and Hermann Kohlstedt[1] — [1]Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel, Kiel, Germany — [2]Texas State University, Ingram School of Engineering, San Marcos, TX 78666 USA

Correlated electron materials exhibiting first-order metal-insulator phase transitions (MIT) accompanied by an abrupt change in the resistivity over several orders of magnitude have recently attracted considerable attention for applications in the field of non-volatile memories due to their sub-nanosecond transition timescale and electrical read-out scheme. Oxide multilayer heteroepitaxy combining VO_2 films and conducting/ferroelectric/dielectric films open new opportunities in creating functional devices. VO_2 thin films were deposited on various single crystal complex oxide substrates compatible with ferroelectric $PbZr_xTi_{1-x}O_3$ (PZT) and $BaTiO_3$ thin films using pulsed laser deposition method. Thus, $SrTiO_3(100)$, PZT/$SrRuO_3$ buffered $SrTiO_3(100)$, $SrTiO_3S$ buffered Si(100) substrates, NdGaO3(110), MgO(100), PZT/$SrRuO_3$ buffered $GdScO_3(110)$, and PMN-PT(001) substrates were used in combination with VO_2 films. The deposited VO_2 films were structurally charaterized by X-ray diffraction and Raman scattering spectroscopy. Electrical measurements show a change in resistance of the VO_2 across MIT ranging from 10^2 to 10^4 times.

DS 21.3 Tue 10:00 CHE 91

Microstructural properties of Ti2AlN MAX-Phase thin films, synthesized by multilayer PVD techniques — •Lukas Gröner, Eduart Reisacher, Eberhard Nold, Alexander Fromm, Frank Meyer, Chris Eberl, and Frank Burmeister — Fraunhofer IWM, Freiburg, Deutschland

Mn+1AXn phases belong to a group of ternary nitrides or carbides, where M denotes an early transition metal, A denotes mostly a group III or IVA element and X is either nitrogen or carbon. In recent years, an increasing number of investigations on the synthesis and characterization on crystalline Mn+1AXn phases have been published which focus on their suitability for industrial applications, e.g. as protective coatings. Due to the mixture of strong covalent MX bonds and weak ionic MA bonds, these materials often exhibit a high corrosion resistance as well as good electrical conductivity and thermal stability. However, these properties strongly depend on the material*s crystallinity. Ti2AlN MAX-phase thin films were synthetized on various substrates in a reactive sputter mode by a multilayer-deposition of AlN and Ti single layers under variation of the double layer thickness, followed by a subsequent annealing step. The synthesis results were investigated by elemental analysis and electron microscopy. The evolving microstructure with a preferential orientation in the texture was analyzed by polarized Raman spectroscopy and XRD. Besides temperature and annealing time, the double layer thickness turned out to be a key parameter to adjust the orientation and grain size.

DS 21.4 Tue 10:15 CHE 91

Characteristic Diffuse Scattering from Rough Lamellar Gratings — •Analia Fernandez Herrero[1], Victor Soltwisch[1], Mika Pflüger[1], Jürgen Probst[2], and Frank Scholze[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany — [2]Helmholtz-Zentrum-Berlin (HZB), Albert-Einstein Str. 15, 12489 Berlin, Germany

Lamellar-gratings are commonly-used diffractive optical elements or structural elements in state-of-the-art integrated electronic circuits. For the control of the lithographic manufacturing process a rapid inline characterization of such structures is indespensible. There are numerous reports on the determination of the geometry parameters of such gratings from optical and EUV light scattering. With shrinking structure sizes, roughness gains influence on the structure performance. Its characterization by scatterometry requires to identify the roughness contributions. For lamellar gratings, roughness is clasified as line width roughness (LWR) or line edge roughness (LER). We prepared a set of eight Si-lamellar gratings with well defined LER or LWR and a prototype grating by e-beam lithography at HZB. The samples were investigated at PTB using EUV-scatterometry, which is very sensitive to the imperfections on the structures and therefore provides a high sensitivity for roughness. We observed that each type of line roughness leads to a characteristic diffuse scattering pattern, with strong correlation between the type of roughness and the diffuse scatter angular distribution. The analysis of these diffuse scatter contributions opens a new path for the roughness characterization of line structures.

DS 21.5 Tue 10:30 CHE 91

Structure-property relationships in catalysts identified by combining data science and high-throughput experimentation — •Helge S. Stein[1], Jinjang Li[2,3], Ramona Gutkowski[4], Christina Eberling[1], Sally Jiao[5], Kirill Sliozberg[4], Christoph Schwanke[6], Karin M. Aziz-Lange[6], Lifei Xi[6], Andre D. Taylor[2,3], Wolfgang Schuhmann[4,7], and Alfred Ludwig[1,7] — [1]Institute for Materials, Ruhr-Universität Bochum — [2]Department of Chemical and Environmental Engineering, Yale University — [3]Center for Research on Interface Structures and Phenomena, Yale University — [4]Analytical Chemistry-Center for Electrochemical Sciences (CES), Ruhr-Universität Bochum — [5]Department of Chemical and Biological Engineering, Princeton University — [6]Operando Characterization of Solar Fuel Materials, Helmholtz-Zentrum Berlin für Materialien und Energie — [7]ZGH & MRD, Ruhr-Universität Bochum

The transition towards a zero-CO2-emission economy requires clean and renewably produced fuels such as hydrogen. In this contribution, catalysts for the efficient production of hydrogen through water reduction (HER) and oxidation (OER), as well as catalysts for the reverse reaction, namely oxygen reduction (ORR), will be shown. Through the implementation of versatile machine learning and statistical methods, novel structure-property correlations were discovered from a total of over 1500 synthesized compositions. These findings offer possible search strategies for the discovery of new and improved catalysts. As an outlook, high-throughput XPS analysis on Co-Fe-Mn-O will be demonstrated.

DS 21.6 Tue 10:45 CHE 91

Combining human and algorithmic analysis for the rapid identification of phase regions and crystal structures — •Helge S. Stein[1], Sally Jiao[2,1], and ALFRED Ludwig[1,3] — [1]Institute for Materials, Ruhr-Universität Bochum, — [2]Department of Chemical and Biological Engineering, Princeton University, — [3]ZGH & MRD, Ruhr-Universität Bochum

A major challenge in combinatorial materials science remains the efficient analysis of X-ray diffraction (XRD) data and its correlation to functional properties. A rapid identification of phase regions and proper assignment of corresponding crystal structures is necessary to keep pace with the improved methods for synthesizing and characterizing materials libraries. Therefore, a new modular software called htAx (high-throughput analysis of X-ray and functional properties data) is presented that couples human intelligence tasks, used for "ground-truth" phase-region identification, with subsequent unbiased verification by a peak-matching algorithm in order to efficiently analyze which phases are present in a materials library. Identified phases and phase regions may then be correlated to functional properties in an expedited manner. To demonstrate the functionality of htAx, two previously published XRD datasets of the materials systems Al-Cr-Fe-O and Ni-Ti-Cu are analyzed by htAx. The analysis of about one-thousand XRD patterns takes less than one day with htAx. The proposed method reliably identifies phase-region boundaries and robustly identifies multiple phases.

DS 21.7 Tue 11:00 CHE 91

Analysis of surface oxidation of TiON ALD films — Justyna Łobaza, •Małgorzata Kot, and Dieter Schmeisser — BTU Cottbus-Senftenberg, Konrad-Wachsmann-Allee 17, 03046 Cottbus

Titanium oxynitride (TiON) films are interesting due to their remarkable optical and electronic properties which strongly depend on the O/N ratio. However, it is known that films containing Ti are prone to oxidation in contact with the air [1]. In this work, we study the thickness of a surface oxidation layer which is inherently formed on the atomic layer deposition (ALD) grown TiON/TiN films on Si substrate. We use an Ar^+ ion bombardment source and X-ray photoelectron spectroscopy (XPS) for this analysis. We calibrate the sputter rate by using substrate signal intensity decay (here Si 2p) in the XPS spectra of the 5 nm thick TiON sample accordingly. This rate is assumed to be constant when films with a larger thickness are analyzed. We find that the surface oxidation layer is about 1 nm thick, independent on the detailed ALD parameters of the films. The TiN films found underneath are close to the stoichiometric values and have a residual O content below 5%. Finally, we compare these data to our previous results collected with synchrotron-based radiation source [2,3].

References: [1] Sowinska et al., Applied Physics Letters 100, 233509 (2012). [2] M. Sowinska et al., Applied Surface Science 381, 42-47 (2016). [3] M. Sowińska et al., Journal of Vacuum Science and Technology A, 01A12734 (2016).

15 min. break.

DS 21.8 Tue 11:30 CHE 91

Interfacial oxide formation during ALD oxide growth on reactive metals for resistive switching devices — •Stephan Aussen, Alexander Hardtdegen, Katharina Skaja, Regina Dittmann, and Susanne Hoffmann-Eifert — Peter Grünberg Institut (PGI-7) and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany

In this study we investigate the oxidation behavior of different metals (M) including Hf, Ta and Pt during atomic layer deposition (ALD) of stoichiometric oxide films (M′O) including Al_2O_3, TiO_2 and HfO_2 and the switching behavior of the resulting stacks. The 25 nm thick dense metal films with low surface roughness < 0.3 nm were grown on thermal oxidized Si wafers in an off-axis sputter tool with a base pressure $< 10^{-10}$ mbar. The hexagonal Hf films and the cubic Pt films show (002) and (111) textures, respectively. In contrast, the Ta films consist of a mixture of the α- and β-tantalum phase. All metal films were transferred under ultra-high vacuum into an ALD plasma system. 3 nm thick oxide layers were deposited at 300 °C using O_2-plasma as the oxygen source. The resulting stacks were investigated by x-ray photoelectron spectroscopy to study the oxidation of the metal surface due to the oxide deposition. In addition, complementary resistive switching experiments were performed on equivalent stacks, i.e. $Pt/M'O/MO_x/M$. The influence of the in-situ formed metal oxide interface (MO_x) on the switching behavior of the stacks is discussed.

DS 21.9 Tue 11:45 CHE 91

Analytical Electron Microscopy Study to Resolve the Phase

Morphology of Organic Solar Cell Blends — •Mona Sedighi[1,2], Markus Löffler[1], Petr Formanek[2], and Ehrenfried Zschech[3] — [1]Dresden Center for Nanoanalysis, Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden — [2]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden — [3]Fraunhofer-Institut für Keramische Technologien und Systeme (IKTS), Dresden

To increase the efficiency of bulk heterojunctions for organic photovoltaic devices (OPV), the complicated photon-to-electron conversion process has to be understood in detail. Most OPV consist of a single bulk-heterojunction active layer; the blend of electron donor (conjugated polymer) and electron acceptor (fullerene) which makes an interpenetrating network of domains, ideally on the length scale of the exciton diffusion length. Therefore, morphology of the active layer significantly contributes to the overall performance of OPV.

Obtaining insights into the morphology of the active layer requires the spatial resolution and a contrast mechanism to discriminate two phases with similar average atomic number. To tackle this challenge, we combine electron microscopy imaging with different analytical techniques; energy dispersive X-ray spectroscopy (EDX) and electron energy loss spectroscopy (EELS) in TEM. We imaged different phases of the donor and acceptor, forming ordered and non-ordered regions, depending on the way the heterojunction is fabricated.

DS 21.10 Tue 12:00 CHE 91

Quantitative Raman spectroscopy of doped and undoped multiphase TiO_2 thin films on complex substrates — •Sebastian Schipporeit[1,2,3], Dieter Mergel[1], and Volker Buck[1,2] — [1]Thin Film Technology Group, Faculty of Physics, University Duisburg-Essen — [2]CENIDE, Duisburg — [3]University of Wuppertal, School of Mechanical Engineering and Safety Engineering, Material Technology, Wuppertal

We have developed a method that allows a quantification of crystal structures in thin films on complicated substrates with Raman spectroscopy. This method was applied to pure and Nb-doped TiO_2 thin films, deposited by various coating techniques onto B270 glass. The films were deposited or post-heated between 60 °C and 650 °C Raman maps were created within areas of 30 x 30 μm in 250 nm steps. This gives the possibility to determine the spatial distribution of crystal phases within the films and to enhance the signal to noise ratio. We decompose the spectra into the two main components substrate and film, and furthermore the spectrum of the film into an amorphous content, crystalline backgrounds and, finally, the Raman peaks of the various crystal phases. Modelling the whole spectrum eliminates any arbitrary background allowing even small traces of crystalline phases to be detected. The films contain amorphous, anatase, rutile and brookite structures.

DS 21.11 Tue 12:15 CHE 91

Improved XPS Background Fitting with a Modified Tougaard Universal Cross Section Using the Example of Aluminium — •Manuel Monecke, Georgeta Salvan, and Dietrich R.T. Zahn — Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

X-ray photoelectron spectroscopy (XPS) spectra are commonly fitted in a narrow binding energy regime of several eV using either a Shirley [1] or a Tougaard [2] background. We present an improved approach for XPS background fitting using reflective electron energy loss spectroscopy (REELS) data to calculate the inelastic electron scattering cross section (IESCS). As example the photoemission spectrum of aluminium was calculated in the binding energy range from 50 to 240 eV (Al 2s and 2p). We first fit the REELS spectrum considering the contribution of elastic scattered, directly excited surface plasmon, and inelastically scattered electrons. The results of this fit are then taken as starting parameters to fit the XPS spectrum. The fit results show a much better agreement with the measured spectrum as compared to those obtained with the conventional Tougaard background. Just as important, this method reveals the presence of several satellite peaks in the region of the plasmon peaks becoming apparent due to the simultaneous fitting of the detailed IESCS for the background calculation and XPS peak functions. This sensitivity to hidden satellite peaks can become a powerful tool to gain more knowledge from XPS spectra. [1] D. Shirley, Phys. Rev. B, Vol. 5, Nr. 12 [2] S. Tougaard, Solid State Commun., Vol. 69, Nr. 9

DS 21.12 Tue 12:30 CHE 91

Präparation verschiedener Substrate mittels anodischen Vakuum-Lichtbogens zum Aufwachsen von Graphen — •Konstantin Thronberens, Sebastian Schipporeit und Volker Buck — Arbeitsgruppe Dünnschichttechnologie, Fakultät für Physik, Universität Duisburg-Essen und CENIDE, 47057 Duisburg

Graphen ist einer der interessantesten Werkstoffe der jüngeren Geschichte. Seine einzigartigen Eigenschaften, sowohl in elektrotechnischer, optischer als auch in mechanischer Hinsicht, versprechen herausragende technische Anwendungsmöglichkeiten bei Verwendung von vergleichsweise günstigem Rohmaterial. Jedoch gestaltet sich die Herstellung von Graphen in großem Maßstab als schwierig, da beim epitaktischem Aufwachsen von Graphen auch leicht unerwünschtes Graphit gebildet werden kann. Eine mögliche Lösung des Problems stellt ein Katalyseprozess dar. Als Katalysator für diesen Prozess können unter anderem Übergangsmetalle aus der Nickelgruppe wie Nickel, Platin und Palladium verwendet werden. Im Rahmen dieser Arbeit werden mit Nickel, Platin und Palladium beschichtete Saphirgläser hergestellt, die im Idealfall auch für die Verwendung als Substrat für das epitaktische Wachstum von Graphen geeignet sind. Für die Beschichtung der Saphirgläser wurde ein anodischer Vakuum-Lichtbogen verwendet, um kompakte Schichten mit einer hohen Haftung herzustellen.

DS 21.13 Tue 12:45 CHE 91

Investigation of molecular orientation in individual metal-organic nanowire by polarized Raman spectroscopy and simulation — •Yanlong Xing[1], Eugen Speiser[1], Dheeraj Singh[2], Petra Dittrich[3], and Norbert Esser[1] — [1]Leibniz-Institute for Analytical Sciences, ISAS Berlin, 12489 Berlin, Germany — [2]Department of Chemical Physics, Jacobs University, 28759 Bremen, Germany — [3]Department of Biosystems Science and Engineering, ETH Zurich, 8093 Zurich, Switzerland

To study the molecular self-organisation in metal-organic nanowires, single gold-tetrathiafulvalene (Au-TTF) nanowires were analysed using polarised Raman spectroscopy at room temperature. A first investigation was done for neutral tetrathiafulvalene (TTF) crystals. Based on the density functional theory calculation (DFT) of molecular Raman tensor and simulation of the depolarisation ratio, the orientation of TTF molecules in a single TTF crystal was revealed. The high correlation between results of the present work and that of reported single crystal data proved the efficiency of the proposed method in this work. Afterwards, both the experimental and simulation methods for TTF crystal was applied to study single Au-TTF nanowires. It was indicated that there were at least two different molecule configurations in the wire, both tilted with respected to the long axis of the wire. The 3D model of single Au-TTF wire shows a vivid image of molecular configurations in the wire. Compared to the proposed mechanism in previously reported work, this improved model can better explain the growth mechanism of Au-TTF wires with various morphologies.

DS 22: Two-dimensional materials III (jointly with HL/TT)

Time: Tuesday 9:30–13:15 Location: POT 51

DS 22.1 Tue 9:30 POT 51

Optical properties of organic/inorganic and all-inorganic lead halide perovskite nanoplatelets — •Jasmina A. Sichert[1,2], Yu Tong[1,2], Verena A. Hintermayr[1,2], Alexander F. Richter[1,2], Bernhard Bohn[1,2], Lakshminarayana Polavarapu[1,2], Carlos Cardenas-Daw[1,2], Alexander S. Urban[1,2], and Jochen Feldmann[1,2] — [1]Chair for Photonics and Optoelectronics, Department of Physics and Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität (LMU), Amalienstaße 54, 80799 Munich, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 Munich Germany

In recent years, organic/inorganic and all-inorganic lead halide perovskite have shown great potential for photovoltaics as well as for light-emitting applications. We have successfully synthesized two-dimensional methylammonium and cesium lead halide perovskite nanoplatelets of varying thickness down to one monolayer.[1,2] With decrease in crystal thickness we observed quantum-size effects and an increase in the exciton binding energy. In the extreme case of a perovskite sheet only a single unit cell thick, the screening of the exciton decreases significantly, resulting in a huge exciton binding energy of several hundred meV in the thin nanoplatelets. We conducted time-resolved photoluminescence spectroscopy to further investigate the effect of the crystal thickness on the optical properties of the nanoplatelets.

[1] Sichert et al., Nano Lett. 15, 6521-6527 (2015)

[2] Tong et al., Angew. Chem. 55, 13887-13892 (2016)

DS 22.2 Tue 9:45 POT 51

Band-gap and exciton binding-energy renormalizations due to excited carriers in monolayer TMDs — •Daniel Erben[1], Christopher Gies[1], Malte Rösner[1,2], Alexander Steinhoff[1], Matthias Florian[1], Michael Lorke[1], Tim Wehling[1,2], and Frank Jahnke[1] — [1]Insitute for Theoretical Physics, University of Bremen, Germany — [2]Bremen Center for Computational Materials Science, University of Bremen, Germany

Coulomb interaction between charge carriers in atomically thin layers of transition-metal dichalcogenides (TMDs) has been shown to be exceptionally large due to the weak screening in the thin layer itself. It causes strong renormalization effects which change the electronic properties and the optical response of the material.

We investigate excited-state optical properties of the typical monolayer TMDs MoS_2, $MoSe_2$, WS_2 and WSe_2 by solving the semiconductor Bloch equations on the full Brillouin zone using the SXCH-approximation for the Coulomb interaction. Excitonic resonances shift in absolute value and relative to each other with increasing carrier density. This effect is a result of a band-gap reduction due to many-particle renormalizations and a reduction of the binding energy due to screening of the Coulomb interaction and Pauli blocking, which we analyse and compare in detail for MoS_2, $MoSe_2$, WS_2 and WSe_2. Our calculations predict a transition from a direct to an indirect band-gap in molybdenum and tungsten disulfides in the presence of highly excited carriers. The selenides stay indirect for different excitations.

DS 22.3 Tue 10:00 POT 51

Phase separation and composition fluctuation effects on electronic and optical properties of $(BN)_{1-x}(C_2)_x$ 2D alloy — •Ivan Guilhon[1], Lara K Teles[1], Marcelo Marques[1], and Friedhelm Bechstedt[2] — [1]Grupo de Materiais Semicondutores e Nanotecnologia, Instituto Tecnológico de Aeronáutica, DCTA, 12228-900 São José dos Campos, Brazil — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, D-07743 Jena, Germany

$(BN)_{1-x}(C_2)_x$ alloys are promising materials for band gap engineering in two-dimensional electronics. Despite the importance of microstructural features, such as phase separation and composition fluctuation. The current theoretical studies of such monolayer alloys are often restricted to investigate “guessed" nonrandom structures.

Using DFT calculations combined with a statistical approach to account for disorder effects, we study the properties of these 2D alloys as a function of their average composition. A complete scenario of how thermodynamic conditions affect the distribution of atoms is provided. The solubility limits and critical temperature are studied by constructing a T-x phase diagram.

In this context, we calculate the energy gap as a function of the composition and optical absorbance spectra are predicted for different compositions. Our predictions are compared with the experimental findings. We reproduce the experimentally found absorption spectra with a two-peak pattern for intermediate carbon concentrations and identify them with phase-segregated instead of homogeneous alloys.

DS 22.4 Tue 10:15 POT 51

Electron-phonon interaction in transition metal dichalcogenides — •Nicki F. Hinsche[1], Arlette Sohanfo Ngankeu[2], Sanjoy Mahatha[2], Marco Bianchi[2], Charlotte Sanders[2], Philip Hofmann[2], and Kristian S. Thygesen[1] — [1]Center for Atomic-scale Materials Design, Technical University of Denmark, 2830 Kgs. Lyngby, Denmark — [2]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark

Atomically thin layers of Transition Metal Dichalcogenides (TMD) attract remarkable interest due to their extraordinary electronic and optical properties and are often quoted as semiconductor analogues of graphene. Possessing direct band gaps in the visible frequency range and exhibiting high electronic mobilities at room temperature, TMD's are emerging candidates for next generation electronic and optoelectronic applications [1]. By means of DFT electronic-structure and Boltzmann transport calculations [2], we discuss the impact of microscopic electron-phonon interaction onto the renormalization of the electronic structure and the phonon-limited electronic transport properties for two prototypical TMD's: TaS_2 and WS_2. Our analysis and conclusions will be drawn closely to recent experimental findings [3].

[1] F. A. Rasmussen and K. S. Thygesen. Journ. of Phys. Chem. C **13** 169 (2015) [2] N. F. Hinsche *et al.*, ACS Nano **9** 4406 (2015) [3] C. E. Sanders *et al.*, Physical Rev. B. **94** 081404 (2016)

DS 22.5 Tue 10:30 POT 51

Spin Degenerate Regimes for Single Two-Dimensional Quantum Dots on Transition Metal Dichalcogenide Monolayers — •Matthew Brooks and Guido Burkard — Department of Physics, University of Konstanz, D-78464, Germany

Strong spin orbit coupling in transition metal dichalcogenides (TMDCs) monolayers results in spin resolvable band structures about the K (K') valleys such that the eigenbasis of a 2D quantum dot (QD) on a TMDC monolayer in zero field is described by the Kramers pairs $|+\rangle = |K' \uparrow\rangle, |K \downarrow\rangle$ and $|-\rangle = |K \uparrow\rangle, |K' \downarrow\rangle$. This coupling limits the usefulness of single TMDC QDs as qubits due to the inherent difficulty of generating superposition states of the valley degree of freedom. Possible regimes of spin degenerate states overcoming the spin orbit coupling in monolayer TMDC QDs are investigated in both zero field, where the spin and valley degrees of freedom become fourfold degenerate, and in some magnetic field, localised to the K' valley. Such regimes are shown to be achieved in MoS_2, where the spin orbit coupling is sufficiently low that the spin resolved conduction bands intersect at points about the K (K') valleys and as such may be exploited by selecting suitable critical dot radii.

DS 22.6 Tue 10:45 POT 51

Electron Spin Relaxation in a Transition-Metal Dichalcogenide Quantum Dot — •Alexander Pearce and Guido Burkard — University of Konstanz, Konstanz, Germany

We study the relaxation of a single electron spin in a circular quantum dot in a transition-metal dichalcogenide monolayer defined by electrostatic gating. Transition-metal dichalcogenides provide an interesting and promising arena for quantum dot nano-structures due to combination of spin-valley physics and strong spin-orbit coupling. First we will discuss which bound state solutions in different B-field regimes can be used as the basis for qubits, at low B-fields combined spin-valley Kramers qubits and at large B-fields spin qubits. Then we will discuss the relaxation of a single electron spin mediated by electron-phonon interaction via various different relaxation channels. Rashba spin-orbit admixture mechanisms allow for relaxation by in-plane phonons arising either from the deformation potential or by piezoelectric coupling, additionally direct spin-phonon mechanisms involving out-of-plane phonons allow for relaxation. We find that the relaxation rates scale as $\propto B^4$ and $\propto B^2$ for in-plane phonons coupling via deformation potential and piezoelectric coupling respectively, while relaxation due to the direct spin-phonon coupling scales as $\propto B^2$. In the low B-field regime we also discuss the role of impurity mediated spin relaxation which will arise in disordered quantum dots.

Coffee Break

Invited Talk DS 22.7 Tue 11:30 POT 51

Influence of dark states on excitonic spectra of transition metal dichalcogenides — •Malte Selig[1,2], Dominik Christiansen[1], Gunnar Berghäuser[1,2], Ermin Malic[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden

In monolayers of transition metal dichalcogenides, excitonic effects play a significant role: Besides bright excitons, dark exciton states are formed by electrons and holes with opposite spin or constitute excitons with non-vanishing center of mass momentum well above the lightcone. Evaluating the excitonic states it turns out, that in tungsten based materials some of these dark states are energetically located below the optical accessible ones. Here, we develope excitonic Bloch equations for excitonic polarizations and densities under the influence exciton phonon interaction, adressing the strong impact of low lying dark states. We investigate the dephasing of the excitonic polarization through exciton phonon scattering [1] and the phonon mediated formation and thermalization of exciton densities. It turns out that coupling to low lying dark states is crucial for luminescence yield and lifetime. The presented results can explain several recent experimental results.

[1] M. Selig et al.,Nature Commun. 7,13279 (2016)

DS 22.8 Tue 12:00 POT 51

Transport measurements in graphene-WSe$_2$ heterostructures — •Tobias Völkl[1], Tobias Rockinger[1], Martin Drienovsky[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Universität Regensburg, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

Bringing graphene into proximity to WSe$_2$ was proposed as a way to induce a high spin orbit coupling strength in graphene, while maintaining the high intrinsic mobility of graphene. We therefore investigated the transport properties of graphene-WSe$_2$ heterostructures.

Placing graphene onto a WSe$_2$-flake resulted in mobilities around 10000 cm^2/Vs of graphene. Further a weak antilocalization behavior was observed, which indicates a high spin orbit coupling strength induced by the WSe$_2$.

Higher mobilities around 100000 cm^2/Vs were achieved by encapsulation of graphene between WSe$_2$ and hBN. In these samples no weak antilocalization behavior could be observed. We attribute this to a transition from diffusive to the quasiballistic regime. Also a feature dependent on the sample width arises in the low magnetic field range. We attribute this to a magneto size effect which further indicates quasiballistic behavior.

DS 22.9 Tue 12:15 POT 51

Electrical behavior of the oxidation of atomically thin HfSe$_2$ under ambient conditions — •Christopher Belke, Hennrik Schmidt, Benedikt Brechtken, Johannes C. Rode, Dmitri Smirnov, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover

12 years after the discovery of graphene [1], two-dimensional materials are of rising importance in the research and development section. An example for those layered materials are TransitionMetalDichalcogenide (TMD) with the chemical formula MX$_2$, where M is a transition metal and X a chalcogenide [2]. Some materials are very fragile in ambient conditions. One of them is the n-type semiconductor hafnium diselenide (HfSe$_2$) [3]. During the fabrication the samples were prepared under nitrogen atmosphere or were covered with PMMA. An increasing resistance was measured while the sample was oxidized under ambient conditions, as well as a change of the electric field effect was observed.

[1] A. K. Geim et al., Nature Materials, **6**, 183 (2007)

[2] A. K. Geim, and I. V. Grigorieva, Nature **499**, 419 (2013)

[3] M. Kang et al. APL **106**, 143108 (2015)

DS 22.10 Tue 12:30 POT 51

***ab initio* study of the transport properties in bulk and monolayer MX$_3$ (M = Ti, Zr, Hf and X = S, Se) compounds.** — •Yasir Saeed — Qatar Environment and Energy Research Institute (QEERI), Hamad Bin Khalifa University (HBKU), Qatar Foundation, P.O. Box 5825, Doha, Qatar

Two dimensional (2D) materials are best candidates for thermoelectric application due to their low thermal conductivity which is key property to achieve high efficiency for their usage in the filed of energy harvesting. Owing to that, here we present a study on electronic as well as thermal transport of bulk and monolayer MX$_3$ compounds (M = Ti, Zr, and Hf and X = S and Se) are investigated by by density functional theory and semi-classical Boltzmann theory. The bandgap amounts to rather similar value for bulk and monolayer, only the shape of band near Fermi level changes slightly, which results in a modified effective mass. We found that monolayer MX$_3$ compounds are good TE materials than bulk. Also p-type monolayer TiS$_3$ has twice large PF at 600 K than its room temperature value. However, monolayer Zr/HfSe$_3$ compounds showing promising behavior as a n-type TE materials at elevated high temperature of 600 K. In-plane tensile strain is also possible to tune the bandgap to increase S and disorder the monolayer lattice to minimize κ, therefore turns out to be a highly efficient approach for creating high performance TE materials.

DS 22.11 Tue 12:45 POT 51

Nonlinear Hall voltage from magnetic hot-spots — •Karina A. Guerrero Becerra, Andrea Tomadin, Andrea Toma, Remo Proietti Zaccaria, Francesco De Angelis, and Marco Polini — Istituto Italiano di Tecnologia, via Morego 30, I-16163 Genova, Italy

Electromagnetic simulations have recently shown that specifically designed plasmonic nanostructures are able to enhance and localize an oscillating magnetic field within a micro-meter area. These magnetic hot-spots, generated by forcing the plasmonic resonances of planar nanostructures to generate displacement currents of coil-type shape, have been shown to operate in the NIR [A. Nazir, *et. al.* Nano. Lett., 14, 3166-3171 (2014)] and in the MIR [S. Panaro, *et. al.* Nano. Lett., 15, 6128-6134 (2015)] frequency regions. Operating frequencies can be extended towards the THz regime. Here we propose that magnetic hot-spots might be probed through transport measurements by exploiting the response of the 2D electron gas (2DEG) hosted in a graphene bar, placed within the hot-spot area. We study the response of the 2DEG, being subject to the oscillating in-plane electric field of the radiation driving the coil-type resonance, and to the localized magnetic field induced by it. We found that the response of the graphene 2DEG drives a rectification effect giving rise to a measurable Hall-like dc voltage, being sensitive to the operational frequency of the hot-spot. We discuss the conditions under which the predicted dc voltage is experimentally accessible, within the range of frequencies from THz to MIR. We show that the electric and magnetic fields within the hot-spot launch graphene plasma waves.

DS 22.12 Tue 13:00 POT 51

Exchange Interaction for Quantum Dots in TMDCs — •Alessandro David, Andor Kormanyos, and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We study the properties of double quantum dots in Transition Metal Dichalcogenides (TMDCs) where trapped electrons comprise not only the usual spin and valley degrees of freedom, but also a spin-orbit splitting in the spectrum. The spin-orbit coupling splits the four-fold spin and valley degeneracy into two Kramers pairs with correlated spin and valley states. We consider two different situations where the spin-orbit splitting is either much larger or comparable to the tunneling. Our aim is to use such systems filled with only two electrons for quantum information processing. In the case of large spin-orbit splitting, it turns out that there is a fourfold degenerate ground state (well separated from higher states) where, with a simple redefinition of Pauli matrices, we can obtain a CNOT gate in the same way it was obtained in the quantum computer proposed by Loss and DiVincenzo. In the case of small spin-orbit splitting, we have to consider a 16 dimensional subspace, but it is still possible to obtain a unitary evolution operator, that also depends on the value of spin-orbit splitting.

DS 23: Organic Semiconductors (jointly with CPP/HL)

Time: Tuesday 9:30–13:15 Location: POT 251

DS 23.1 Tue 9:30 POT 251

Femtosecond time-resolved spectroscopy of an acceptor-donor-acceptor oligomer film — •Ephraim Sommer[1], Antonietta De Sio[1], Elena Mena-Osteritz[2], Peter Bäuerle[2], and Christoph Lienau[1] — [1]Institut für Physik, Carl-von-Ossietzky Universität Oldenburg — [2]Institut für Organische Chemie II und Neue Materialien, Universität Ulm

Conjugated oligomers are gaining increasing popularity for application in organic solar cells as photoactive materials thanks to their high production reproducibility and device efficiencies [1]. However, a detailed understanding of the initial charge transfer in such systems is missing. Recently, in polymer based active materials it was found that coherent vibronic coupling plays an important role in this process [2]. This raises the question whether this also holds for oligomers. To answer this, we investigate a novel A-D-A-type oligomer by pump-probe and 2D electronic spectroscopy with femtosecond time resolution. Upon selective excitation of the donor unit, we observe strong peak-shifts of the exciton signals as a most dominant feature at early times. Moreover, the signal shows long lived vibrational oscillations. Such a peak shift cannot be explained within a vibronically coupled dimer model including only one dominant vibrational mode like in [2]. Our preliminary results suggest that the photoinduced charge transfer may occur via a conical intersection between the donor and acceptor potential energy surfaces. We will discuss theoretical modelling aimed at validating this idea.

[1] R. Fitzner et al., Adv. Funct. Mater., 12, (2015)

[2] A. De Sio et al., Nat. Commun., 7, (2016)

DS 23.2 Tue 9:45 POT 251

Polariton bottleneck dynamics in organic microcavities — •Felix Lemke, Hartmut Fröb, and Karl Leo — IAPP, TU Dresden, Germany

Organic molecules are known to be promising candidates for strong coupling experiments due to their large exciton binding energy. Simultaneously, organic materials reveal large inhomogeneously broadened absorption spectra, complicating the investigation. Even so, small organic molecules have advantages in processing, stability (to ambient conditions and high optical excitation) and lifetime.

In this work we will present a method to investigate the microcavity polariton properties utilizing the oligomer Bu4-Ph4-DIP. We perform angle-resolved streak camera measurements and compare the data with a rate-equation model. Simulation and measurement agree very well. From this, we can see directly the influence of the polariton bottleneck, which proofs, that our system is in the strong coupling regime. Moreover, we can extract the characteristic time constants and gain an insight into the polariton dynamics.

DS 23.3 Tue 10:00 POT 251

Charge-exciton quenching in organic transistors — •Wouter Koopman[1,2], Stefano Toffanin[2], and Michele Muccini[2] — [1]Universität Potsdam, Potsdam, Deutschland — [2]CNR-ISMN, Bologna, Italien

Organic Light-Emitting Transistors (OLETs) possess a huge potential for the design of highly integrated multifunctional optoelectronic systems and intense nanoscale light sources, such as the long-searched-for electrically pumped organic laser. In order to fulfill these promises, the efficiency and brightness of the current state-of-the-art devices have to be increased. The dominating quenching process limiting the external quantum efficiency in OLETs is charge-exciton interaction. A comprehensive understanding of this quenching process is therefore of paramount importance. The present talk reports a systematic investigation of charge-exciton interaction in organic transistors employing time-resolved photoluminescence electro-modulation (PLEM) spectroscopy on the picosecond timescale. The results show that the injected charges reduce the exciton radiative recombination in two ways: (i) charges may prevent the generation of excitons and (ii) charges activate a further non-radiative channel for the exciton decay. Moreover, the transient PLEM measurements clearly reveal that not only trapped charges, as it is was already reported in literature, but rather the entire injected charge density contributes to the quenching of the exciton population. Finally, lessons for the design of high-efficiency OLET are disused.

DS 23.4 Tue 10:15 POT 251

Investigating the doping efficiency of organic semiconductors by thermoelectric measurements — •Bernhard Nell[1], Markus Krammer[2], Karin Zojer[2], and Koen Vandewal[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, Dresden, Germany — [2]Institute of Solid State Physics, Technische Universität Graz, Graz, Austria

We use thermovoltage (Seebeck effect) and temperature-dependent conductivity measurements on doped organic semiconductors to determine the dominating type of charge carriers introduced by the dopant and to gain insight into the position of the transport level with respect to the Fermi level. The investigation of fullerene dopants with a high degree of fluorination in various amorphous host materials allows us to tune the energy level offset between host and dopant and to study their influence on Fermi level position and overall doping efficiency systematically. Combining thermoelectric measurements with Kinetic Monte Carlo simulations gives further insight into the influence of Coulomb interactions on the trapping of mobile charge carriers in doped organic semiconductors. We find that at low doping concentrations a high amount of charge carriers is immobilized in trap states, leading to a reduced doping efficiency. Upon increasing the doping concentration, the trap states are subsequently passivated and an increased doping efficiency can be observed. Furthermore the doping efficiency is increased upon fluorination of the dopant molecules and we find a correlation between the energy level offset and the doping efficiency, at the same molar concentration.

DS 23.5 Tue 10:30 POT 251

Vibronic coherence in a reference organic photovoltaic blend — •Antonietta De Sio[1], Ephraim Sommer[1], James Lim[2], Susana F. Huelga[2], Martin B. Plenio[2], Giulio Cerullo[3], and Christoph Lienau[1] — [1]Institut für Physik, Universität Oldenburg, Germany — [2]Institut für Theoretische Physik, Universität Ulm, Germany — [3]Department of Physics, Politecnico di Milano, Italy

The microscopic mechanisms underlying charge separation in organic solar cells are still highly debated. Although recent theoretical work [1] suggests that vibronic couplings may lie at the origin of efficient charge generation in such systems, clear experimental evidence on the role of vibronic coherence for charge separation is still lacking. Here we use ultrafast two-dimensional electronic spectroscopy with 10-fs time resolution to investigate the initial dynamics of excitons and polaronic species in P3HT and P3HT:PCBM thin films with different acceptor concentration. Our experimental results, supported by theoretical simulations, show that strong vibronic coupling favors exciton delocalization and accelerates charge separation even in presence of disorder, resulting in long-lived coherent oscillatory dynamics of strongly correlated excitons and polaron pair states, mutually coupled to a dominant vibrational mode. These results allow us to gain fundamental new insights into the initial dynamics of charge separation and may open up new perspectives for optimizing devices [2,3].

[1] Tamura et al, JCP 137, 22A540, 2012. [2] Falke et al, Science 344, 1001, 2014. [3] De Sio et al, Nat.Commun. 2016 in press.

DS 23.6 Tue 10:45 POT 251

Crystalline Packing Motifs in Pentacene-like Organic Semiconductors — •Michael Klues and Gregor Witte — Fachbereich Physik, Universität Marburg, Germany

While the impact of chemical modifications on the molecular electronic system can be well computed, the influence on solid state properties is hardly predictable. In fact already slight chemical modifications, like the introduction of heteroatoms or small side groups, often lead to dramatically changed crystal structures and thereby rather different charge carrier mobilities or exciton binding energies. Within a comparative study of various pentacene-like organic semiconductors, based on a Hirshfeld analysis [1] we reveal correlations between molecular properties and packing motives. By choosing molecules with nearly identical geometrical dimensions the complexity of intermolecular interactions is considerably reduced and effects of electrostatic potentials, hydrogen bonds and atom sizes can be carved out. Thereby, we attain a simple rule for predicting the occurrence of herringbone packing motifs and point out the relevance of hydrogen bonds for parallel molecular arrangements as found previously for partially fluorinated

HBC. [2] Furthermore we suggest a route to increase intermolecular orbital overlap by integration of large heteroatoms in the periphery of aromatic systems which yields an improved charge carrier mobility in the case of DNTT.

[1] M.A Spackman; D. Jayatilaka, CrystEngComm, 11, 19, (2009)

[2] T. Breuer et al., Phys. Chem. Chem. Phys., (2016), DOI: 10.1039/C6CP06126E

Coffee Break

DS 23.7 Tue 11:30 POT 251

Strongly reduced inhomogeneous broadening of molecular aggregates in hybrid nanostructure system — •Xuan Trung Nguyen[1], Antonietta De Sio[1], James Lim[2], Alexandra Markovic[3], Julia Witt[3], Gunther Wittstock[3], Susana Huelga[2], Martin Plenio[2], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]Institut für Theoretische Physik and IQST, Universität Ulm, Germany — [3]Institut für Chemie, Carl von Ossietzky Universität Oldenburg, Germany

The applications of nanostructures based on organic molecular aggregates range from solar cells to all-optical switching. These aggregates are often modeled as disordered systems that exhibit inhomogeneously broadened absorptive line shapes. In such a system, disorder localizes the exciton wavefunction and leads to limited exciton transport efficiency, which is important in devices like solar cells. By using linear and non-linear spectroscopy, we show that the inhomogeneous broadening of a model J-aggregate cyanine dye is strongly reduced in the presence of an ultrathin gold layer and the resulting optical spectra display almost perfect Lorentzian line shapes. Supported by theoretical simulations, we explain the experimental results in terms of increased delocalization of the exciton wavefunction due to electronic coupling to surface plasmon polaritons supported by the aggregate-gold. This coupling can average out the disorder effect and thus increase the exciton transport efficiency.

DS 23.8 Tue 11:45 POT 251

The Influence of Molecular Packing on Charge-Transfer States at the Pentacene/Perfluoropentacene Interface — •Andre Rinn[1], Tobias Breuer[1], Julia Wiegand[2], Michael Beck[2], Jens Hübner[2], Michael Oestreich[2], Gregor Witte[1], and Sangam Chatterjee[3] — [1]Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany — [3]Institute of Experimental Physics I, Justus-Liebig University Giessen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany

We study different model systems of intermixed and layered heterostructures of pentacene and perfluoropentacene by means of time resolved photoluminescence spectroscopy to investigate the impact of molecular packing at the interface on the optical properties. We assign the different PL signals visible in the heterostructures to their respective origin and find an increase in the PL intensity of the charge-transfer signal for pi-stacking at the interface. Significantly slower carrier dynamics are measured for the charge-transfer states when compared to bulk exciton emission which are quenched by singlet exciton fission.

DS 23.9 Tue 12:00 POT 251

Three-dimensional confinement and exciton-polaritons in open organic microcavities — •Simon Betzold[1], Marco Dusel[1], Jürgen Ohmer[2], Utz Fischer[2], Christof P. Dietrich[1], and Sven Höfling[1,3] — [1]Technische Physik, Universität Würzburg — [2]Institut für Biochemie, Universität Würzburg — [3]SUPA, School of Physics and Astronomy, University of St Andrews

Frenkel excitons, characteristic of organic semiconductors, possess large binding energies making them stable at room temperature, rendering polariton experiments at ambient air conditions possible. Organic materials further exhibit very large oscillator strengths and thus strongly interact with a cavity field. Since organic materials are very sensitive to the deposition of semiconductor layers on top of them, we use an open cavity system, which makes non-invasive investigation possible. Open cavities are tunable systems and comprise a bottom semiconductor distributed Bragg reflector (DBR) with the active material (the organic semiconductor) on top and a concave top DBR separated by a micrometer sized air gap. This configuration allows a 3D photonic confinement and brings unprecedently high quality factors into reach.Here, we show the versatility of open cavities by performing reflectivity and photoluminescence measurements in Fourier imaging configuration and exemplary investigate the strong exciton-photon coupling between a fluorescent protein and the dielectric cavity. We emphasize that the open cavity approach can easily be extended to more complex systems like photonic lattices and active regions including 2D monolayer materials or hybrid organic-inorganic bilayers.

DS 23.10 Tue 12:15 POT 251

Improving lasing properties of a hybrid OLED/microcavity structure — •Stefan Meister, Robert Brückner, Markas Sudzius, Hartmut Fröb, and Karl Leo — IAPP, TU Dresden, Germany

Organic materials have many advantages which can be utilized in different kinds of devices such as light-emitting diodes, solar cells, or even lasers. Some examples are the spectrally separated broad absorption and emission spectra, the possibility to build very thin and flexible devices, and the fact of having an intrinsic four-energy-level-system.

The goal of realizing an electrically driven organic solid state laser is so far well beyond reach. As a first step, we incorporate an OLED into a microcavity (MC) consisting of two Distributed Bragg Reflectors (DBR). These devices are investigated electrically and with a micro-photoluminescence setup to determine the optical functionality. The optical measurements further allow to compare it to standard organic MCs. These insights are analyzed and addressed with the help of photolitography to improve the quality of the metal layers. Further, different very thin (60nm - 0.15mm) encapsulation methods are tested to allow measurements under ambient conditions.

DS 23.11 Tue 12:30 POT 251

High temperature stable single carrier hole only devices — •Shahidul Alam[1,2], Peter Fischer[3], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena) Friedrich-Schiller-Universität Jena Philosophenweg 7a 07743 Jena, Germany — [2]Institute of Organic and Macromolecular Chemistry Friedrich-Schiller-Universität Jena Humboldtstr. 10 07743 Jena, Germany — [3]Institut für Werkstofftechnik, TU Ilmenau, Gustav-Kirchhoff-Str. 6, 98693 Ilmenau, Germany

Thin hole transport layers (HTL) are crucial elements in organic semiconductor based devices. Metal oxides are an encouraging material class for this purpose. Metal oxides can be used to modify either of the two contacts in a device for improved wettability as well as chemical and electronic compatibility of the contacts with the organic layer. Several materials like NiO, V2O5, WO3 and MoO3 have demonstrated encouraging prospective for performing as efficient charge transport layers. Among them molybdenum oxide (MoO3) attracted extensive interest due to its superior performance. In order to evaluate charge transport properties of annealed semiconductor films, devices are required to be stable at high annealing temperature. Whereas PEDOT:PSS has generally proper charge injection and extraction properties, these may drastically change upon heating above certain temperature. In this work, we show that a MoO3 interlayer can efficiently substitute PEDOT:PSS as hole transport layer within single carrier hole only devices (SCHD), because of its better stability at high annealing temperature.

DS 23.12 Tue 12:45 POT 251

Tuning the conductivity in organic-based charge-transfer materials: A combined NEXAFS and electrical transport study — •Antonia Morherr[1], Sebastian Witt[1], Alisa Chernenkaya[2], Katja Medjanik[2], Gerd Schönhense[2], Harald O. Jeschke[3], Roser Valentí[3], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe Universität, 60438 Frankfurt am Main — [2]Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz — [3]Institut für theoretische Physik, Goethe Universität, 60438 Frankfurt am Main

Single crystals of the novel charge transfer complexes phenanthrene- and picene/TCNQ-F$_x$ (x=0,2,4) were grown by physical vapor transport [1] and investigated by electrical transport measurements, near-edge X-ray absorption spectroscopy (NEXAFS) and density functional theory calculations. The electrical conductivity and the mobility of the samples increase with increasing acceptor strength. The activation energy of the complexes was studied by temperature dependent measurements and compared to the electrical band structure investigated by NEXAFS [2]. The results were compared to the DFT calculations for the electrical band structure and simulated NEXAFS spectra.

[1] A. Morherr et al., Physica B 496, 98-105 (2016)

[2] A. Chernenkaya et al., J. Chem. Phys. 145, 034702 (2016)

DS 23.13 Tue 13:00 POT 251

Three-dimensional photonic confinement of imprinted pillars in an organic Tamm-plasmon structure — •Marco Dusel[1], Simon Betzold[1], Christof P. Dietrich[1] und Sven Höfling[1,2] — [1]Technische Physik, Julius-Maximilians-Unversität Würzburg, Am Hubland, 97074 Würzburg — [2]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, UK

The fluorescence of organic solids at room temperature is governed by the radiative decay of Frenkel excitons that are characterized by large exciton binding energies and short Bohr radii compared to inorganic semiconductors. Due to their very large oscillator strength, organic materials further strongly interact with light, in particular in microcavities.

So far, photonic confinement within the cavity plane has mainly been achieved by tailoring the dielectric part of the cavity. Here, we present a novel technology that enables 3D photonic confinement within the active organic layer of a Tamm-plasmon structure (metal-clad cavity) by laterally imprinting pillars. The fabricated pillars have diameters ranging from 7 to 20 μm and heights between 2 and 4 μm. The developed technology enables far more complicated photonic potentials including coupled pillars, chains and lattices.

DS 24: Fundamentals of Perovskite Photovoltaics IV (jointly with CPP/HL)

Time: Tuesday 14:00–16:00 Location: ZEU 222

Invited Talk DS 24.1 Tue 14:00 ZEU 222

Ultrafast transient absorption spectroscopy of organic-inorganic hybrid perovskites on mesoporous titanium dioxide in contact with hole transport materials — •Thomas Lenzer — Universität Siegen, Physikalische Chemie, Adolf-Reichwein-Str. 2, 57076 Siegen

Organic-inorganic hybrid perovskites, such as methylammonium lead iodide, are particularly promising for applications in solar light harvesting and optoelectronics. We present our recent results on the carrier dynamics of such materials using ultrafast pump - supercontinuum probe spectroscopy in the 260-1600 nm range. The perovskite systems are investigated over a wide range of carrier densities. Slow carrier recombination processes, "phonon bottlenecks" during carrier cooling and confinement effects in low-dimensional perovskite structures are identified. We investigate electron injection processes from the perovskite into the mesoporous titania scaffold and estimate the relative contributions of electron transport pathways in the perovskite and titanium dioxide. We also discuss the hole transfer from the perovskite into triarylamine-based hole transport materials (HTMs).

DS 24.2 Tue 14:30 ZEU 222

Identification of charge transport limiting factors in perovskite-based solar cells by Time-of-Flight measurements — •Irene Grill[1,2], Meltem Aygüler[1,2], Nadja Giesbrecht[1,2], Pablo Docampo[1,2], Thomas Bein[1,2], Matthias Handloser[3], and Achim Hartschuh[1,2] — [1]Department of Chemistry & CeNS, LMU Munich — [2]Nanosystems Initiative Munich (NIM) — [3]Toptica Photonics AG

Hybrid perovskites represent one of the most promising absorber materials for future photovoltaic applications due to the recently achieved high PCE values [1]. In this work, we determine the transport time of photoinduced charges in between the top- and bottom-electrode in perovskite thin film solar cells upon pulsed laser excitation, using Time-of-Flight (ToF) photocurrent measurements. To extract the influence of the individual layers on the transport characteristics and to identify limiting factors we carried out additional ToF studies on the respective absorber layer of the photovoltaic device in a lateral architecture. The results of the single film measurements are discussed in terms of crystal size and orientation. The direct comparison of the data obtained for the individual layers and the photocurrent transients of the final device under working conditions permits the identification of limiting factors for inter-facial and intra-film charge transport simultaneously to allow for the optimization of both the fabrication techniques [2,3] and device architecture. [1] M. Saliba et al., Energy Environ. Sci. 2016, 9, 1989. [2] I. Grill et al., Sol. Energ. Mat. Sol. Cells 2016, accepted. [3] A. Binek, I. Grill et al., Chem. Asian J. 2016, 11, 1199.

DS 24.3 Tue 14:45 ZEU 222

Fill factor optimization strategies in efficient, stable triple cation perovskite solar cells — •Martin Stolterfoht, Christian Wolff, Yochai Amir, Andreas Paulke, and Dieter Neher — Institute of Physics and Astronomy, University of Potsdam, Potsdam-Golm, Germany

Perovskite solar cells (PSCs) now compete with their inorganic counterparts in terms of power conversion efficiency. To advance this technology even further, more insights into the physical mechanisms that define the bias dependence of the photocurrent are required. In this work, we varied the organic electron/hole transport layers (ETL/HTL) thickness in efficient triple cation PSCs and studied the charge carrier recombination and transit through the device. Using resistance dependent photovoltage (RPV), we identify the transit time through the transport layers as key figure of merit for maximizing the fill factor (FF) and the overall photovoltaic performance. The results are complemented by intensity dependent photocurrent measurements which elucidate the role of the HTL thickness on the bias dependence of the recombination losses and recombination order. By optimizing the transit time through the HTL (undoped PTAA) we demonstrate efficiencies under solar AM1.5G conditions of up to 20.4% with high FFs of 80%. The reported cells also exhibit excellent stability under light illumination and stability in air, even without encapsulation. However, further improving the FF via a continuous reduction of the HTL leads to significant open-circuit voltage losses which highlights the challenge to simultaneously optimize the FF and open-circuit voltage.

DS 24.4 Tue 15:00 ZEU 222

Optical phonons in methylammonium lead halide perovskites and implications for charge transport — •Michael Sendner[1,2], Pabitra K. Nayak[3], David A. Egger[4], Sebastian Beck[1,2], Christian Müller[1,2,5], Bernd Epding[2,5], Wolfgang Kowalsky[1,2,5], Leeor Kronik[4], Henry J. Snaith[3], Annemarie Pucci[1,2], and Robert Lovrincic[2,5] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab, Heidelberg — [3]Clarendon Laboratory, University of Oxford — [4]Department of Materials and Interfaces, Weizmann Institute of Science — [5]Institut für Hochfrequenztechnik, TU Braunschweig

Recent reports indicated that the mechanical and electronic properties of lead-halide perovskites are strongly affected by the lattice vibrations. Herein we report far-infrared spectroscopy measurements of $CH_3NH_3Pb(I/Br/Cl)_3$ thin films and single crystals at room temperature (RT) and a detailed quantitative analysis of the spectra. We find strong broadening and anharmonicity of the lattice vibrations for all three halide perovskites, which indicates dynamic disorder of the lead-halide cage at RT. We determine the frequencies of the transversal and longitudinal optical phonons, and use them to calculate, via appropriate models, the static dielectric constants, polaron masses, electron-phonon coupling constants, and upper limits for the phonon-scattering limited charge carrier mobilities. Within the limitations of the model used, we can place an upper limit of 200 $cm^2V^{-1}s^{-1}$ for the RT charge carrier mobility in $MAPbI_3$ single crystals.
See also: Sendner et al., Materials Horizons, 3, pp 613-620, 2016.

DS 24.5 Tue 15:15 ZEU 222

Advances in Vapour Deposition of Metal-Halide Perovskite Thin-Films for Solar Cells — •Juliane Borchert, Jay B. Patel, Henry J. Snaith, and Michael B. Johnston — Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX13PU, UK

Hybrid metal-halide perovskite materials are promising absorber materials both for use in single junction and tandem solar cells. A particular focus in recent research has been on the fabrication of perovskite absorber layers from solution. Alternatively, perovskite thin-films can also be deposited using co-evaporation in vacuum. This method offers several benefits. The obtained films show high uniformity over large surface areas. Thus the technique is well suited to the fabrication of large-area planar heterojunction solar cells. Additionally, the uniform film thickness makes the evaporated films ideal for precision characterisation of the optical properties of metal halide perovskite materials. Furthermore, the vapour deposition is solvent-free, which makes it compatible with a wide range of substrates and interlayers. This is for example advantageous in the fabrication of tandem solar cells. Here we present current advances in the understanding of the influence that different process variables have on the quality of the obtained films, as well as the application of co-evaporated perovskite absorber layers in devices.

DS 24.6 Tue 15:30 ZEU 222

Carrier Recombination Analysis in Perovskites Using Time-Resolved Photoluminescence — •Liudmila Kudriashova[1], Philipp Rieder[1], Kristofer Tvingstedt[1], Andreas Sperlich[1], Georgy Astakhov[1], Andreas Baumann[2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Despite the incredible progress of perovskite-based photovoltaics, many aspects of charge carrier recombination in organometal halide perovskites still remain unclear, inhibiting the targeted production of high-performance solar cells. Under solar cell operating conditions photoluminescence (PL) in perovskites is mainly caused by recombination of free photogenerated charge carriers. Hence the time-resolved photoluminescence (TRPL) is a powerful tool to reveal the complex charge carrier behaviour in perovskite films. Here, we implement the combination of several kinetic models for TRPL in $CH_3NH_3PbI_3$ and $CH_3NH_3PbI_{3-x}Cl_x$ films to extract the characteristic recombination rates and estimate the trap concentration. We obtain trap densities in the range of $10^{15} - 10^{16}$ cm^{-3} and show that PL decay drastically depends on interfaces between the perovskite and conducting layers. Currently controversial aspects, such as different recombination pathways, origin of trap states, and the effect of photon recycling, are discussed. In summary, TRPL analysis enables the calculation of trap density and clarifies the origin of defects, which is crucial for the further development of perovskite-based photovoltaics.

DS 24.7 Tue 15:45 ZEU 222

Monolithic serial interconnection of perovskite solar cells using laser ablation — •Felix Schneider[1], Christof Schultz[1], Rutger Schlatmann[1,2], Steve Albrecht[3], and Bert Stegemann[1] — [1]HTW Berlin - University of Applied Sciences, Wilhelminenhofstr. 75a, 12459 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, PVcomB, Schwarzschildstr. 3, 12489 Berlin, Germany — [3]Helmholtz-Zentrum Berlin, Institut für Silizium-Photovoltaik, Kekuléstraße 5, 12489 Berlin, Germany

Based on recent work on serial interconnection of thin film solar cells by laser ablation, the proper laser parameters for scribing planar, inverted perovskite solar cell samples were determined. A device design with the layer sequence ITO/PTAA/perovskite/PCBM/Ag was used in which the P1 scribes the ITO, the P2 separates the perovskite and the selective contact layers and the P3 the metal electrode. As a result, successful P1 to P3 laser scribes with sufficiently small area losses, i.e. small dead areas, were obtained. Degradation due to humidity of the perovskite layer during laser scribing was avoided by complete laser processing in nitrogen atmosphere. Detailed characterization of the sample composition by energy dispersive x-ray spectroscopy, the morphology by atomic force microscopy as well as of the electrical functionality of the P2 scribes will be provided. The influence of laser-induced material modifications in the vicinity of the laser scribes on the module performance will be discussed.

DS 25: Gaede Prize Talk (jointly with O)

Time: Tuesday 15:30–16:00 Location: WIL C307

Invited Talk DS 25.1 Tue 15:30 WIL C307

STM-induced light emission: from molecular LED to sub-nanometric optical microscopy. — •Guillaume Schull — Institut de Physique et Chimie des Materiaux de Strasbourg, UMR 7504 (CNRS - Universite de Strasbourg), Strasbourg, France

The electric current traversing the junction of a scanning tunneling microscope (STM) may generate a local emission of light. During the last years, we have used this method to study the intrinsic luminescence properties of individual molecules. This work has progressed in two directions. On one side we have used the ability of the STM to manipulate matter with atomic-scale precision to form single-molecule light emitting devices. Composed by individual molecular wires suspended between the tip and the sample of the STM, these devices generate an emission of light whose color, intensity and bandwidth can be controlled with high precision. On the other side, we used the intrinsic resolution of the STM to performed sub-molecularly resolved vibronic spectroscopy of molecules separated from a metallic surfaces by a thin insulating layers. These results constitute an important step towards photonic measurements with atoms-scale resolution.

DS 26: Metallic Nanowires on Semiconductor Surfaces (jointly with O)

Time: Tuesday 18:30–20:30 Location: P1C

DS 26.1 Tue 18:30 P1C

Quasi-one-dimensional plasmons in Si(hhk)-Au: a crossover of dimensions — •Timo Lichtenstein[1], Zamin Mamiyev[1], Marvin Detert[1], Julian Aulbach[2], Jörg Schäfer[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Physikalisches Institut and RCCM, Universität Würzburg

For future plasmonic devices one-dimensional (1d) plasmons offer unique properties: an inherently predetermined direction, a wavelength much shorter than those of photons, and an almost linear dispersion. Au induced wires on regularly stepped Si(hhk) are a playground for quasi-1d structures. Therefore, they were prepared at coverages where the surfaces host single or double atomic gold chains parallel to the steps. This allows studying the influence of spacing and wire width. The wire quality was checked with spot profile analysis in low energy electron diffraction, in combination with an electron energy loss spectrometer providing both high energy and momentum resolution it gave access to the plasmon dispersion. Although 1d metallicity is observed, the plasmon dispersion strongly depends on two-dimensional properties: the lateral distribution of the 1d electron density within one terrace (intrawire correlation) and the spacing of the wires (interwire correlation). We obtained effective widths considerably smaller than the terrace width. A quantitative description is possible by a modified wire array plasmon model, claiming extensions of theory. Also, STM gives a modulated DOS of comparable width. Both the chain type as well as the terrace size seem to be of influence.

DS 26.2 Tue 18:30 P1C

Au-chains grown on Ge(100): A detailed SPA-LEED and EELS-LEED study — •Timo Lichtenstein, Zamin Mamiyev, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover

Ge(100) is known as a substrate for self-organized growth of one-dimensional quantum wires by adsorption of Au, highly interesting for future plasmonic devices. In this study, the morphology has been investigated by means of spot profile analysis low energy electron diffraction. Using LEED in combination with an energy electron loss spectrometer we measured the plasmon dispersion relation with both high energy and momentum resolution. First, we systematically measured the properties on variously prepared surfaces. From G(S)- and H(S)-analyses on ex-situ chemically treated Ge-samples followed by multiple in-situ Ar^+-sputtering and high-temperature annealing cycles, we were able to obtain surfaces with a terrace width of around 100 nm and low roughness After the growth of the Au-wires, this analysis favors a giant missing row structure. For Au coverages higher than 0.7 ML low-dimensional plasmon modes appear in the loss spectra. Their dispersion relation increases linearly for parallel momentum $> 0.1\,\text{Å}^{-1}$, but deviates from the typical dispersion of a quasi-one-dimensional plasmon for $< 0.1\,\text{Å}^{-1}$. These effects are possibly attributed to the strong electronic correlations of the system due to the Luttinger-liquid-like behavior inside the wires as well as the strong coupling between. Peak widths and heights of the plasmon excitations in the loss spectra reveal a low excitation probability and very short lifetimes.

DS 26.3 Tue 18:30 P1C

Tin nanowires on vicinal Si(111) surfaces — •Monika Jäger, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

Si(111) surfaces covered by 0.3 ML Sn are known to form a $\sqrt{3}\times\sqrt{3}$ reconstruction and reveal a Mott transition upon cooling below 70 K [1]. This system is now confined to a wire like one-dimensional structure using vicinal Si(111) substrates and investigated by means of STM and LEED.

Adsorption of Sn at 900 K gives rise to a refacetting of the Si(557) surface into a local (223) orientation with an average spacing of 1.58 nm similar to the isoelectronic Pb/Si(557) system (e.g. [2]). This change in orientation ist compensated by wider (111) terraces exhibiting a $\sqrt{3}\times\sqrt{3}$ reconstruction. In order to improve the long-ranged ordering, Si(223) surfaces are used additionally as a substrate. On both vicinal surfaces, the (223)-orientated parts consist of $4\frac{2}{3}\times 0.332$ nm wide (111) terraces which show a 0.75 nm periodicity along the terraces. This is consistent with the ×2 features seen in LEED measurements. Furthermore, the electronic structure is probed at different temperatures by STS.

[1] S. Modesti et al., PRL **98**, 126401 (2007).
[2] C. Brand et al., Nat. Comm. **6**, 8118 (2015).

DS 26.4 Tue 18:30 P1C

Quantitative LEED studies on Si(111)-(5×2)-Au — •Andreas Alexander[1], Frederic Timmer[1], Joachim Wollschläger[1], Kaori Seino[2], and Friedhelm Bechstedt[2] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

The (5×2)-Au reconstruction on Si(111) has been in the focus of research for nearly 50 years now. Lately, in particular as a prototype for one-dimensional (1D) metallic chain structures. In order to understand the physical properties accompanying these 1D chains a profound knowledge of the atomic structure is needed. Historically, a plethora of atomic structures (EBH [1],AN [2],KK [3]) with varying Au coverages were discussed. More recently Shirasawa et al. [4] were able to show that Surface X-ray Diffraction experiments favor the KK-model slightly. Due to the higher surface sensitivity of Low Energy Electron Diffraction (LEED) as compared to SXRD we carried out quantitative LEED experiments in order to assess this observation.

[1] S. Erwin et al., Phys. Rev. B **80**, 155409 (2009)
[2] T. Abukawa and Y. Nishigaya, Phys. Rev. Lett. **110**, 036102 (2013)
[3] S. G. Kwon and M. H. Kang, Phys. Rev. Lett. **113**, 086101 (2014)
[4] T. Shirasawa et al., Phys. Rev. Lett. **113**, 165501 (2014)

DS 26.5 Tue 18:30 P1C

Gold-induced Surfaces on Stepped Germanium: Growth and Characterization — •Tim Wagner, Julian Aulbach, Ralph Claessen, and Jörg Schäfer — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg

Adsorption of gold atoms on stepped Ge(hhk) surfaces leads to the formation of atomic wires via self-organization. Inspired by interesting physics such as spin chains on the step edges of similar gold-induced Si(hhk) surfaces [1], we establish recipes for the preparation of several gold-induced Ge(hhk) surfaces. Therefore, the preliminary sputter and anneal treatment of the stepped Ge(335), Ge(557) and Ge(553) substrates as well as the adsorption procedure of gold atoms provided by an electron beam evaporator have been optimized to achieve well-ordered surfaces. Due to the adsorption of gold atoms some Ge(hhk) surfaces undergo a refacetting in order to form a stable gold-induced surface. Based on scanning tunneling microscopy and low energy electron diffraction we determine the formation of surface reconstructions on the atomic scale on the Ge(hhk)-Au surfaces. In particular, we have characterized these surfaces regarding the formation of atomic wire structures, such as those formed by the Au and Ge atoms, and will present first indications for the occurence of superstructures.

[1] J. Aulbach et al., Nano Lett. 16(4) (2016).

DS 27: 2D Materials beyond Graphene (jointly with O)

Time: Tuesday 18:30–20:30 Location: P2-EG

DS 27.1 Tue 18:30 P2-EG

Effect of different sulfur environment on sulfurization of MoO3 into MoS2 nanoflakes — •Prabhat Kumar, Megha Singh, and Gade B Reddy — Thin Film Laboratory, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016

In present work, Molybdenum disulfide (MoS2) nanostructured thin films (NTFs) were synthesized by sulfurizing MoO3 NTFs in three different non-conventional methods (named methods 1-3). Method 1 uses sulfur vapors, second utilizes H2S/Ar gas and third adopts plasma of H2S/Ar gas. The effect of sulfurizing ambient on its efficiency to convert MoO3 into MoS2 has been studied. And parameters such as crystallinity, purity, uniformity and stoichiometry control have been basis of this study. The samples showed uniform nanoflakes (NFs) structures throughout sample, revealed by SEM, same as their precursor MoO3. XRD and Raman disclosed crystalline MoS2 in all three methods, however the degree of crystallinity was greater in case of sulfurization in H2S/Ar plasma ambient. HR-TEM revealed formation of core-shell nanostructures comprising of MoO2 in core and MoS2 making shell. Quantitative analysis of sulfurized films carried out by XPS, shows the presence of MoS2 in methods 1,2 and 3 with percentage found to be 18%, 87% and ~100% respectively. Plasma ambient has resulted in high quality of MoS2 NTFs based on parameters such as crystallinity and stoichiometry control. Hydrogen sulfide plasma provides reducing environment as well as source of reactive sulfur species for sulfurization. The advantage of using plasma is reduced temperature and time.

DS 27.2 Tue 18:30 P2-EG

X-ray absorption spectroscopy studies on transition metal dichalcogenide heterointerfaces — •Florian Rasch[1], Sage Bauers[2], Danielle Hamann[2], Gavin Mitchson[2], Kyle Hite[2], Javier Herrero-Martín[3], Manuel Valvidares[3], David Johnson[2], Bernd Büchner[1], and Jorge Hamann-Borrero[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Dresden, Germany — [2]Department of Chemistry and Materials Science, University of Oregon, Eugene, Oregon, United States — [3]ALBA Synchrotron Light Source, Cerdanyola del Vallès, Barcelona, Spain

Transition metal dichalcogenides (TMD) are layered quasi 2D materials that exhibit exciting physical phenomena such as superconductivity (SC) and charge density waves (CDW), which strongly depend on the TMD dimensionality. In order to study the effect of dimensionality on the electronic properties of TMD a series of ferecrystal heterostructures with chemical formula $[(\mathrm{MSe})_m\,/(\mathrm{TSe}_2)_n]_k$ (M = Sn, Pb, Bi and T = V, Nb, Ti) were synthesized with precise control of the dimensionality, i.e. m and n. Additionally, study of the charge transfer (CT) into the dichalcogenide layer is possible by changing the M cation. Here we present a X-ray absorption spectroscopy (XAS) study at the transition metal $\mathrm{L}_{2,3}$ edges for $(\mathrm{PbSe})_1/(\mathrm{VSe}_2)_n$ (with n = 1, 3), as well as $(\mathrm{MSe})_1/(\mathrm{NbSe}_2)_1$ and $(\mathrm{MSe})_1/(\mathrm{TiSe}_2)_1$ (with M = Sn, Pb, Bi) heterostructures at temperatures below and above T_{CDW}. Our experiments clearly show strong changes of the transition metal XAS spectra by changing the M ion. Moreover, X-ray magnetic circular dichroism reveals weak magnetism for samples containing Ti and V.

DS 27.3 Tue 18:30 P2-EG

Synthesis and Spectroscopy of Bismuthene — •Felix Reis[1], Gang Li[2,3], Lenart Dudy[1], Maximilian Bauernfeind[1], Stefan Glass[1], Werner Hanke[3], Ronny Thomale[3], Jörg Schäfer[1], and

Ralph Claessen[1] — [1]Physikalisches Institut and RCCM, Universität Würzburg, Würzburg, Germany — [2]Institute for Solid State Physics, Vienna University of Technology, Vienna, Austra — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Würzburg, Germany

The search for quantum spin Hall materials with large band gap has become one of the major research thrusts of solid state physics. Despite other approaches, graphene with its honeycomb lattice geometry always fascinated the community. Here, we report the realization of so-called "bismuthene", which is synthesized on the wide-bandgap substrate SiC(0001). Scanning tunneling microscopy imaging clearly displays the honeycomb structure. Using tunneling spectroscopy, we find a huge bulk gap of $\sim 800\,\mathrm{meV}$, with the Fermi level positioned well inside this gap. Interestingly, metallic edge states are observed when the bismuthene film edge is approached. A comparison of angle-resolved photoemission measurements and density functional theory band structure calculations is a further manifestation of the formation of bismuthene. To understand the empirical electronic properties, a detailed theoretical analysis is performed. A low-energy effective model demonstrates that the substrate not only stabilizes bismuthene, but plays a crucial role in the formation of the observed huge band gap, which is driven by the large on-site spin-orbit coupling.

DS 27.4 Tue 18:30 P2-EG

Thermodynamic stability, electronic and optical properties of graphene oxide dependence on oxidation level. — •Ivan Guilhon[1], Lara K Teles[1], Marcelo Marques[1], Friedhelm Bechstedt[2], Jürgen Fürthmuller[2], and Silvana Botti[2] — [1]Grupo de Materiais Semicondutores e Nanotecnologia, Instituto Tecnológico de Aeronáutica, DCTA, 12228-900 São José dos Campos, Brazil — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, D-07743 Jena, Germany

Graphene oxide is a two-dimensional material with potential applications in ultra-thin electronic, optoelectronic and sensor devices. It is an intermediate compound in the graphene synthesis through chemical route. Despite the fact that the chemical composition of such system have strong influence on its electronic and optical process, these interesting features have not been investigated until now.

We propose a statistical model for graphene oxide based on the cluster expansion of the disordered system based on the generalized quasi-chemical approximation (GQCA). Epoxide and hydroxyl groups are considered. Thermodynamic stability of the system is investigated and the known tendency of the system to decompose into highly oxidized domains and pristine graphene is explained and discussed in the light of binodal and spinodal decomposition. We calculate the energy gap as a function of the degree of oxidation considering composition fluctuation effects in the whole composition range, showing tunable electronic properties in a wide range interval. Optical absorbance spectra are predicted for different chemical compositions.

DS 27.5 Tue 18:30 P2-EG

Low Temperature Scanning Tunneling Spectroscopy on MoS_2 nanoflakes on Au(111) — •Daniela Dombrowski[1,2] and Carsten Busse[1,2] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster

We perform low temperature scanning tunneling spectroscopy at 5 K of MoS_2 nanoflakes grown on Au(111) by a combination of physical and chemical vapour deposition. We find a band gap of approx. 1.9 eV and pronounced peaks, originating from the MoS_2 bands. The Shockley-surface state at 0.5 eV is present on the bare gold surface, but absent below the MoS_2 islands.

Furthermore, we take advantage of the spatial resolution of scanning tunneling spectroscopy to measure the influence of the moiré superstructure arising from the lattice mismatch between the MoS_2 layer and the underlying gold substrate. We observe a significant shift of the valence band edge, whereas the conduction band remains almost unchanged, hence leading to a variation of the gap energy induced by the moiré pattern.

Finally, we find a new state right above the valence band, which is associated with the edge of the MoS_2 flakes.

DS 27.6 Tue 18:30 P2-EG

Structural dynamics of TMDC heterostructures studied by femtosecond electron diffraction — •Daniela Zahn, Thomas Vasileiadis, Lutz Waldecker, and Ralph Ernstorfer — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Vertical heterostructures of two-dimensional (2D) crystals offer intriguing new perspectives for the fabrication of novel nanodevices [1]. Especially for optoelectronic devices, it is important to understand their relaxation dynamics after optical excitation, which are governed by the interplay of electronic and phononic coupling across the interface and electron-phonon coupling in the individual materials. One experimental technique that can directly observe the structural response to photoexcitation is femtosecond electron diffraction [2]. The evolution of the atomic mean-square-displacement can be experimentally accessed by means of the Debye-Waller effect. Our focus lies on heterostructures with staggered (type II) band alignment, which exhibit photo-induced charge separation across the interface. We present results on bulk WSe_2/WS_2 heterostructures revealing sub-picosecond transfer of hot charge carriers across the interface and intralayer energy transfer from the charge carriers to the lattice on a timescale of few picoseconds in both materials. The results suggest that the equilibration between the two materials is carried out primarily by hot charge carrier transfer while vibrational coupling plays a minor role.

[1] A. Geim, I.V. Grigorieva, Nature 499, 419-425 (2013).

[2] L. Waldecker, R. Bertoni, R. Ernstorfer, JAP 117, 044903 (2015).

DS 27.7 Tue 18:30 P2-EG

Growth of ultrathin MoS_2 films - Temperature dependency — •Vanessa Zeuner, Lukas Madauss, and Marika Schleberger — Universität Duisburg-Essen, Deutschland

Molybdenum disulfide (MoS_2) is an important representative of transition metal-dichalcogenides (TMDCs).With a direct bandgap it is an interesting candidate for a variety of electronic and optoelectronic applications. Therefore, the growth of large area, two dimensional films is investigated. We synthesized the MoS_2 films by chemical vapour deposition on SiO_2/Si substrates and used MoO_3 and S powders as the reactants. The influence of the temperature during the process on the morphology of the two dimensional MoS_2 flakes is studied.

DS 27.8 Tue 18:30 P2-EG

Electronic Structure of surface-doped FeTe bulk crystals and epitaxial FeTe thin films on Bi_2Te_3 — •Fabian Arnold[1], Jonas Warmuth[2], Jan Fikáček[3], Matteo Michiardi[1], Marco Bianchi[1], Jan Honolka[3], Tim Wehling[4], Philip Hofmann[1], and Jens Wiebe[2] — [1]Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark — [2]Department of Physics, Hamburg University, Hamburg, Germany — [3]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [4]Institut für Theoretische Physik, Universität Bremen, Bremen, Germany

The realization of unconventional superconductivity in iron-based superconductors (SCs) has attracted growing attention in the physics community in the recent years, especially after the discovery of high temperature superconductivity in systems involving thin layers. Iron-chalcogenides have the simplest crystal structure in this materials class which turns them into good candidates for fundamental studies of the electronic structure and its relation to the superconductivity. It is especially interesting that for strongly correlated high-Tc SC materials like Fe-based SCs, a transition to the SC phase upon chemical doping is observable. Here we present an angle-resolved photoemission spectroscopy study of bulk FeTe and thin films of FeTe grown on the topological insulator Bi_2Te_3 [1,2], surface-doped with alkali atoms, and compare to ab-initio calculations. Interestingly, there is almost no change in the electronic structure upon surface doping. [1] S. Manna et al., arXiv:1606.03249 (2016), Nat. Commun. (in press). [2] T. Hänke et al., arXiv:1606.09192 (2016), Nat. Commun. (in press).

DS 27.9 Tue 18:30 P2-EG

Near-surface dynamics of hot carriers in $2H$-MoS_2: momentum-dependent relaxation and spin- and valley-polarized excitation — •Hauke Beyer, Petra Hein, Gerald Rohde, Ankatrin Stange, Marcel Behrendt, Kerstin Hanff, Lexian Yang, Kai Rossnagel, and Michael Bauer — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany

Time- and angle-resolved photoelectron spectroscopy (trARPES) is employed to study different aspects of ultrafast near-surface carrier dynamics in $2H$-MoS_2. Momentum-dependent population and relaxation processes within the conduction-band energy landscape are monitored following photoexcitation with 395 nm laser pulses. Our results indicate that surface-localized defect states play a key role in the final

depopulation of the conduction band [1]. Furthermore, we are able to selectively address K and K' valleys in the trARPES experiment using circularly polarized 590 nm laser pulses owing to the lack of inversion symmetry in the top layer of 2*H*-MoS_2. Similar to recent trARPES results reported for 2*H*-WSe_2 [2], dichroism is observed in excited state intensity as well as dynamics.
[1] P. Hein et al., Phys. Rev. B **94**, 205406 (2016).
[2] R. Bertoni et al., arXiv:1606.03218.

DS 27.10 Tue 18:30 P2-EG

Ultra-thin Bi2Te3 films on semiconductor substrates — •Mert Taşkin and Oğuzhan Gürlü — Istanbul Technical University, Department of Physics, Maslak, 34469, Istanbul, Turkey

Bi2Te3 has a rhombohedral crystal structure and it consists of quintuple layers (QLs) along c-axis. QLs bind with van der Waals interaction. Consequently, the crystal can be cleaved from this interface and the resulting Te1 terminated (0001) surface can be investigated with scanning probe techniques. Bi2Te3 was shown to be a topological insulator (TI) besides being a thermoelectric material; yet, the knowledge on the electronic structure of this material at ultra-thin limit is still incomplete. Before making any attempt at an application with Bi2Te3 in the 2D limit, it is quite important to understand its general physical properties. We modified chemical vapor deposition (CVD) technique to grow ultra-thin Bi2Te3 films on semiconductor/metal-oxide surfaces. In this process we obtained ultra-thin films and micro-particles of Bi2Te3. The heights of obtained Bi2Te3 films are measured to be a few QLs. The radius of Bi2Te3 micro-particles are 1-5 micrometers. Here the structural and spectroscopic characteristics of these ultra-thin films will be discussed.

DS 27.11 Tue 18:30 P2-EG

The interaction of the calcium-intercalated silicene (CaSi2 - R15) surface with a H2 molecule, a DFT study — •Pingo Mutombo, Petr Brázda, Martin Ondráček, and Lukáš Palatinus — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, CZ-16200, Prague, Czech Republic

First-principles calculations have been used to investigate the silicene intercalated CaSi2-R15 compound and discuss the adsorption of H2 at its silicon-rich surface. We assess the stability of the surface by calculating the surface energy. We further determine the band structure of the compound, the surface work function, and charge redistribution both inside the compound and near the surface. It was found that there is a charge transfer from Ca to Si atoms. Moreover, the silicene-related Dirac cone shifts from high symmetric point of the hexagonal Brillouin zone and moves below the Fermi level,due the presence of the Ca atoms. DFT calculations suggest that a hydrogen molecule undergoes a dissociative adsorption on the topmost Si atoms, indicating a high reactivity of the silicene surface layer.

DS 27.12 Tue 18:30 P2-EG

Structural modifications of 2D hexagonal boron nitride caused by ion irradiation — Lara Bröckers, •Henry Bohnen, and Marika Schleberger — Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany

Single layers of hexagonal boron nitride (hBN) – often called *white graphene* – are a two-dimensional insulating material, which is interesting as a building block for heterostructures with graphene or other 2D semiconducting materials. Its atomic structure is similar to the structure of graphene. That makes it interesting to test if one can cause the same structural modifications of hBN by ion irradiation, as shown for graphene.[1,2] Therefore we irradiated ultrathin hBN layers with swift heavy ions under grazing incidence. We investigated the efficiency (i.e. number of ions needed to create one folding on average) for different number of layers and different substrates. As a result we found a higher efficiency for the folding of thicker layers hBN in comparison to graphene.

[1] Akcöltekin S. et al. *Applied Physics Letters* 98 (2011) 101063
[2] Ochedowski O. et al. *NimB*, 340 (2014) 39-43.

DS 27.13 Tue 18:30 P2-EG

Nanostructuring 2D Materials by Ion Irradiation — •Andre Maas[1], Roland Kozubek[1], Lukas Madauss[1], Ursula Ludacka[2], Mukesh Kumar Tripathi[2], Henning Lebius[3], Marko Karlusic[4], Jani Kotakoski[2], and Marika Schleberger[1] — [1]Universität Duisburg and Cenide, Fakultät für Physik, 47048 Duisburg, Germany — [2]Universität Wien, Boltzmanngasse 5, 1090 Vienna, Austria — [3]CIMAP, (CEA-CNRS-ENSICAEN-UCN), blvd Henri Becquerel, F-14070 Caen, France — [4]Ruder Bošković Institute, Bijenićka cesta 54, 10000 Zagreb, Croatia

To fully exploit the colossal technological potential of 2D materials, methods to introduce defects in a controlled way are a key factor. We have investigated energetic ion irradiation induced defects and nanostructures in 2D materials like graphene and single layer MoS2. We show that apart from the well-known binary collisions caused by singly charged keV projectiles, the dense electronic excitation triggered by highly charged ions as well as swift heavy ions may be used to create various characteristic nanostructures each of which may be fabricated by choosing the proper irradiation conditions.

Our experiments, including optical spectroscopy techniques and atomic resolution STEM, reveal unique morphologies such as closed bilayer edges with a given chirality, nanopores of round shape as well as chemical modifications like hydrogenation of the 2D material. By controlled variation of ion parameters like kinetic energy, charge state, angle of incidence, etc., this wide spectrum of modifications in 2D materials can be accessed.

DS 27.14 Tue 18:30 P2-EG

Investigation of sputter processes on metalic surfaces and 2D-Materials using Time-of-Flight mass spectroscopy — •Stephan Sleziona[1], Philipp Ernst[1], Matthias Herder[2], Andreas Wucher[2], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, AG Schleberger, Germany — [2]Universität Duisburg-Essen, AG Wucher, Germany

We have investigated the sputtering processes and ionization probability of metallic surfaces (Indium and Molybdenum) irradiated by two different kinds of ions. We used highly charged ions (HCI), i.e. Xe^{30+} Ions (E_{pot}= 15 keV and E_{kin}= 180 keV) , and singly charged Ar-Ions with kinetic energy of E_{kin}= 4 keV. While the interaction of the latter with the solid is dominated by nuclear stopping the interaction of HCIs consist partly of electronic stopping, too. To study the differences, the Indium surface was irradiated by both types of ions and Time-of-Flight (ToF) mass spectra were recorded. In order to do so we optimized the spatial positions of the Argon-Gun, the HCI source,the spectrometer, and the laser, which was used to post-ionize secondary neutral particles . In addition, the operating voltages and timings of the different components were optimized. With this new set-up we obtained ToF spectra which show a significant difference between the two types of ions. Most recently we used this technique to investigate sputter processes of 2D-Materials.

DS 27.15 Tue 18:30 P2-EG

Influence of the Charge Density Wave Order on Quasiparticle Excitations in 2*H*-$NbSe_2$ — •Eva-Maria Liebhaber[1], Olof Peters[1], Michael Ruby[1], Kai Rossnagel[2], Benjamin W. Heinrich[1], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany. — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany.

The transition metal dichalcogenide (TMDC) 2*H*-$NbSe_2$ is a layered material with interesting properties of strongly correlated electrons at low temperatures. A superconducting phase with a critical temperature of $T_{c,SC} \approx 7.2\,K$ coexists with a threefold symmetric charge density wave (CDW) with $T_{c,CDW} \approx 33\,K$. Although the material has been studied intensively for a long time, the exact interplay between superconductivity and CDW order is still under debate. Recently, Soumyanarayanan *et al.* observed a quantum phase transition from the familiar triangular CDW to a stripe charge order which they assigned to local strain caused by subsurface defects [1].
Here, we investigate the influence of the different CDW phases on the quasiparticle excitation spectra using low temperature scanning tunneling spectroscopy with superconducting tips. The quasiparticle spectra show variations with the periodicity of the CDW as well as on the atomic scale.

[1] A. Soumyanarayanan *et al.*, *Proceedings of the National Academy of Sciences* **110**, 1623-1627 (2013).

DS 27.16 Tue 18:30 P2-EG

Structural analysis of PTCDA domains on an epitaxial hexagonal boron nitride (hBN) monolayer via SPA-LEED and STM — •Christine Brülke[1], Timo Heepenstrick[1], Moritz Sokolowski[1], and Sergey Subach[2] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstraße 12, 53115 Bonn, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52452 Jülich, Germany

Epitaxial monolayers of hBN on metal surfaces are of interest as two-dimensional insulating substrates as well as templates for the formation of epitaxial layers of organic molecules. Here, we report a structural analysis of one monolayer of PTCDA on hBN/Cu(111) by spot profile analysis low energy electron diffraction (SPA-LEED) and scanning tunneling microscopy (STM). hBN grows on the Cu(111) surface in an incommensurate structure with a lattice mismatch of 2.0 % (at 100 K) corresponding to an unstrained hBN layer. The films show rotational mosaicity, however, the majority of the hBN domains are in or close to alignment with the unit cell vectors of the Cu(111) surface (± 2°).

On this hBN layer PTCDA molecules form ordered domains with a herringbone structure with lattice constants a = (19.8 ± 0.3) Å and b = (12.4 ± 0.2) Å. This yields a size of the unit cell that deviates by 3.1 % and 2.2 % from that in the (102) plane of the α and β bulk crystals, respectively. The majority of PTCDA domains are statistically distributed in their azimuthal orientation. There is only a small preference for domains that are oriented along the unit cell vectors of the hBN layer.

DS 27.17 Tue 18:30 P2-EG

Deposition of biphenylthiols on Au(111) by Electrospray Ionization — •Patrick Stohmann[1], Sascha Koch[1], Antoine Hinaut[2], Thilo Glatzel[2], Ernst Meyer[2], and Armin Gölzhäuser[1] — [1]Department of Physics, Universität Bielefeld, Universitätsstrasse 25, 33615 Bielefeld, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

When aromatic self-assembled monolayers (SAMs) are electron-irradiated, intermolecular cross-linking leads to the formation of Carbon Nano Membranes (CNM) with molecular thickness [1]. The preparation of SAMs requires clean surface conditions for the formation of well-defined molecular structures as well as for the analysis via scanning probe techniques. However, thermal evaporation under UHV conditions may lead to the fragmentation of molecules during the sublimation while the formation of wet-prepared SAMs may suffer from polluting adsorbates on the bare surface. Here we present the study of biphenylthiols on Au(111), prepared by Electrospray Ionization (ESI). ESI allows for the introduction of organic molecules in vacuum under controlled conditions on atomically clean surfaces and was successfully applied in previous experiments [2]. The molecular deposition on the surface is investigated by means of scanning tunneling microscopy (STM) and nc-atomic force microscopy (NC-AFM) combined with Kelvin probe force microscopy (KPFM). [1] A. Turchanin et al., A. Gölzhäuser, Adv. Mater., 2009, 21, 1233-1237 [2] A. Hinaut et al., E. Meyer, Beilstein J. Nanotechnol., 2015, 6, 1927-1934

DS 27.18 Tue 18:30 P2-EG

Spectroscopic Mapping and Imaging Ellipsometry applied to Conducting, Semi-Conducting and Insulating 2D-Materials — Sebastian Funke[1], Ursula Wurstbauer[2,3], Aleksandar Matkovic[4], Avery Green[5], and •Peter H. Thiesen[1] — [1]Accurion GmbH, Stresemanstraße 30, 37079 Göttingen, Germany — [2]Walter Schottky Institute and Physics-Department, TU München, Garching 85748, Germany — [3]Nanosystems Initiative Munic 80799, Germany — [4]Centre for Solid State Physics and New Materials, Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — [5]College of Nanoscale Science and Engineering, State University of New York, 253 Fuller Road, Albany, New York 12203

The poster will present the localization and characterization of Graphene Monolayer flakes and similar thicknesses regions of insulating hexagonal boron nitride (hBN) and on semiconducting transition metal dichalcogenide Molybdenum disulphide (MoS2).

Matkovic et al. characterized monolayers of graphene by spectroscopic imaging ellipsometry (SIE). The resulting Fano resonance modelling for the dispersion of Graphene can be used to search for flakes of graphene on different substrates, based on the spectroscopic mapping of the ellipsometric angles Δ and Ψ. This ellipsometric flakesearch is less dependent from the substrate compared to e.g. conventional light microscopy.

DS 27.19 Tue 18:30 P2-EG

Imaging Mueller Matrix Ellipsometry for the Characterization of Microstructured Anisotropic Thin-Film Samples — Matthias Duwe[1], Sebastian Funke[1], Christian Röling[1], •Peter H. Thiesen[1], Aday J. Molina-Mendoza[2], and Andres Castellanos-Gomez[3] — [1]Accurion GmbH, Stresemannstr. 30, 37079 Göttingen, Germany — [2]Universidad Autonoma de Madrid. Departamento de Fisica de la Materia Condensada. Campus Universitario de Cantoblanco, 28049 Madrid, Spain — [3]IMDEA Nanoscience, C/ Faraday 9, Campus Universitario de Cantoblanco, 28049 Madrid, Spain

Imaging ellipsometry (IE) is an established technique for the characterization of structured thin-film samples with lateral resolutions down to the micron scale. In most cases, however, imaging ellipsometers featuring microscopic resolution only yield the ellipsometric angles Δ and Ψ. Thus, these ellipsometers mainly have been applied to isotropic samples so far. Here, we present imaging Mueller matrix ellipsometry (IMME) with high microscopic lateral resolution capable of measurements at a variable angle of incidence. By operating Accurion*s imaging ellipsometer EP4 (PCSA configuration) in a rotating-compensator mode, the ellipsometer yields Mueller matrix micrographs for the upper 3x4 matrix elements of the sample. We applied this imaging Mueller matrix ellipsometer to the characterization of microscopic flakes of anisotropic 2D-materials, such as black phosphorus.

DS 27.20 Tue 18:30 P2-EG

Lateral heterostructures of MoS2 and carbon nanomembranes — •Antony George[1], Christof Neumann[1], Zian Tang[1], Andreas Winter[1], Uwe Hübner[2], Michael Mohn[3], Ute Kaiser[3], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, D-07743 Jena, Germany — [2]Leibniz-Institut für Photonische Technologien e.V., 07745 Jena, Germany — [3]Electron Microscopy Group of Material Science, Ulm University, 89081 Ulm, Germany

Atomically thin two dimensional (2D) materials are promising for future ultrathin electronic and optoelectronic devices. In order to realize such devices, it is highly desired to connect/stitch different 2D materials laterally. Here, we present our recent results of the fabrication of lateral heterostructures of molecular thin carbon nanomembranes (CNMs) with MoS2 by electron beam assisted crosslinking. To this end, MoS2 single layer crystals grown by chemical vapour deposition (CVD) were transferred onto gold films on mica substrates. Then, self-assembled monolayers of 4*-nitro-1, 1*-biphenyl-4-thiol (NBPT) were grown on the areas between the MoS2 crystals. Electron beam irradiation was employed to crosslink the SAM molecules with each and with the edges of the MoS2 crystals. The formed CNM-MoS2 lateral heterostructures were transferred onto new solid and holey substrates and characterized by complementary methods including Raman spectroscopy, atomic force microscopy (AFM), helium ion microscopy (HIM) and high resolution transmission electron microscopy (HRTEM).

DS 28: Focussed Session: Oxide Semiconductors for Novel Devices I

Wide band gap semiconducting oxides such as the group-III sesquioxides find potential application in e.g. UV- or deep UV-sensors, transparent photovoltaic devices, power electronics or quantum well infrared photo detectors. This session sets a focus on growth of binary bulk material and thin films, the physical properties of these and their surface, properties of heterostructures and interfaces and the fabrication and performance of demonstrator devices.

Organizers: Oliver Bierwagen (PDI Berlin) and Holger von Wenckstern (U Leipzig)

Time: Wednesday 9:30–13:00 Location: CHE 89

Topical Talk DS 28.1 Wed 9:30 CHE 89

Self-consistent hybrid functional calculations: Electronic and optical properties of oxide semiconductors — •Daniel Fritsch[1], Benjamin Morgan[1], and Aron Walsh[1,2] — [1]Department of Chemistry, University of Bath, BA2 7AY Bath, UK — [2]Department of Materials, Imperial College London, SW7 2AZ London, UK

Owing to limitations of existing approximate exchange-correlation functionals, band gaps of semiconductors and insulators are often severely underestimated in density functional theory calculations. Considerable improvements are possible by including a fraction of Hartree-Fock exchange, constructing a so-called “hybrid” functional. The precise proportion of Hartree-Fock exchange is typically treated as an empirical parameter chosen from intuition and experimental calibration.

A recent self-consistent hybrid functional [1] removes this empiricism and offers a new approach for parameter-free hybrid functional investigations. Moreover, it provides a better starting point for many-body perturbation calculations based on the *GW* approximation. Applying this approach to a range of oxide semiconductors, we report on the electronic and optical properties, and compare them to other theoretical and experimental data [2].

[1] J. H. Skone, M. Govoni, and G. Galli, Phys. Rev. B **89**, 195112 (2014).
[2] D. Fritsch, B. Morgan, and A. Walsh, Nanoscale Research Letters **12**, 19 (2017).

DS 28.2 Wed 10:00 CHE 89

High-throughput screening of transparent conducting oxides — •Christopher Sutton[1], Robert J. N. Baldock[2], Luca M. Ghiringhelli[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Transparent conducting oxides (TCOs) are a well-developed and commercialized class of wide-bandgap semiconductors that are crucial for the function of many electronic devices. Recent experimental work has demonstrated bandgap engineering in ternary $(Al_xGa_yIn_z)_2O_3$ over 3 eV by adjusting the ratio of In/Ga and Ga/Al. The phase diagram for ternary and quaternary $(Al_xGa_yIn_z)_2O_3$ (where $x+y+z=2$) are examined using DFT-based cluster expansion models combined with fast stochastic optimization techniques (nested sampling) to efficiently search (meta)stable configurations for many different crystal structures. A new semi-grand-ensemble implementation enables exploration of ternary and quaternary $(Al_xGa_yIn_z)_2O_3$. With an extensive search over configurational space, statistical learning is performed for the bandgaps and stabilities to identify structure-property relationships between the targeted properties (e.g., optical transparency) and the fundamental chemical and physical parameters that control these properties.

DS 28.3 Wed 10:15 CHE 89

Pressure-dependent elastic properties of Ga_2O_3 in the α and β phase from first principles — •Konstantin Lion, Dmitrii Nabok, Pasquale Pavone, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin D-12489 Berlin

The structural and elastic properties of the monoclinic β and the hexagonal α phase of the transparent conducting oxide Ga_2O_3 are investigated from first principles using the full-potential all-electron code `exciting` [1]. The full stiffness tensor at fixed pressure of both phases is calculated using the tool `ElaStic` [2]. All eigenvalues of the stiffness tensor at zero pressure are positive and therefore both phases are considered elastically stable at equilibrium according to the Born stability criterion. The bulk moduli at $p = 0$ GPa for both phases, $B_0^\alpha = 218.48$ GPa and $B_0^\beta = 169.38$ GPa, are calculated as a linear combination of second-order elastic constants and show good agreement with previous results [3]. We also investigate the behavior of the stiffness tensor under load. The removal of band degeneracies and changes in the electronic band structure of both phases are investigated under the influence of different kinds of strain.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[2] R. Golesorkhtabar *et al.*, Comp. Phys. Commun. **184**, 1861 (2013).
[3] J. Furthmüller *et al.*, Phys. Rev. B **93**, 115204 (2016).

DS 28.4 Wed 10:30 CHE 89

***Ab-initio* lattice dynamics of Ga_2O_3 polymorphs with an emphasis on polar phonon modes** — •Rut Waldenfels, Dmitrii Nabok, Pasquale Pavone, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Gallium oxide is a promising material for novel opto-electronic devices, due to its large band gap and its remarkable high carrier mobilities. Understanding electron-phonon interactions and in particular polaronic effects is essential for describing transport properties in polar materials. In this work, we perform a comparative study of the lattice dynamics of the two most stable polymorphs of Ga_2O_3, the α and β phase, using density-functional theory. We include non-analytical contributions to the dynamical matrix which allow for the full description of polar phonon modes. For these modes, we calculate the dependence of frequencies and eigenvectors on the wave-vector direction. We investigate which modes have the strongest impact on the electronic structure by calculating mode effective charges and average long-range coupling constants.

DS 28.5 Wed 10:45 CHE 89

Anisotropic thermal conductivity in Ga2O3 — •Mitdank Rüdiger[1], Handwerg Martin[1,3], Galazka Zbigniew[2], and Fischer Saskia F.[1] — [1]AG Novel Materials, Institut für Physik der Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2 , 12489 Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

The monoclinic crystal structure of β-Ga2O3 causes a significant anisotropy of the thermal properties. The temperature-dependent values of the thermal diffusivity D in [010] and [001] direction as well as thermal conductivity values λ in [100], [010] and [001] direction using Mg-doped insulating monoclinic β-Ga2O3 bulk crystals were measured by the 2-Omega-method [1,2]. The measurements were carried out by using the same sample. The room temperature values for the thermal conductivity in the main crystal axes are determined to λ[100] = 11+-1 W/(mK), λ[010] = 29+-2 W/(mK) and λ[001] = 21+-2 W/(mK). For the diffusivity we found D[100] = 3,7+-0,4 mm*/s, D[010] = 9,6+-0,5 mm*/s and D[001] = 7,1+-0,4 mm*/s. The anisotropy factor is the same and independent of temperature. We found D[010]/D[001] = λ[010]/λ[001] = 1,4+-1. The temperature dependence of the thermal diffusivity and conductivity is in accord with phonon-phonon-Umklapp-scattering for T > 150 K.

[1] Handwerg et al., SST 31, 125006 (2016) [2] A. T. Ramu and J. E. Bowers, Rev. Sci. Instr. 83 ,124903 (2012)

15 min. break.

Topical Talk DS 28.6 Wed 11:15 CHE 89

Exceptional Points in Oxide Bulk and Metamaterials — •Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, D-04103 Leipzig

The spectral dispersion of exceptional points (singular optic axes) is measured for (monoclinic and thus biaxial) β-Ga_2O_3 bulk material in the absorption regime. Also we show that exceptional points exist in fully transparent, optically 'effectively' biaxial, anisotropic microcavities, fabricated using an uniaxial cavity material with its axis inclined to the Bragg mirror growth direction. Here the lack of time reversal symmetry is mediated by the mode broadening, i.e. the photon escape from the – in principle – open cavity system. As a consequence the eigenmodes are generally elliptically polarized, and completely circularly polarized eigenmodes are expected in certain directions. Via geometric and chemical composition design degrees of freedom, the spectral and angular position of these chiral modes can be rationally designed. Thus circularly polarized emission becomes possible without the use of spin injection or internal or external magnetic fields.

DS 28.7 Wed 11:45 CHE 89

Dielectric function and band structure of α Ga_2O_3 — •Martin Feneberg[1], Anderson Janotti[2], Maciej D. Neumann[3], Norbert Esser[3], Luis Artus[4], Ramon Cuscó[4], Tomohiro Yamaguchi[5], and Rüdiger Goldhahn[1] — [1]Otto-von-Guericke Universität Magdeburg — [2]University of Delaware — [3]Leibniz-Institut fur Analytische Wissenschaften - ISAS - e.V. — [4]ICTJA-CSIC, Barcelona — [5]Kogakuin University

Polytypes of gallium oxide are a very promising class of materials for electronic device applications. It is possible to stabilize α-Ga_2O_3 by mist chemical vapor deposition on sapphire substrates. However, the optical properties of this metastable corundum-like phase have not yet been investigated thoroughly. Spectroscopic ellipsometry at room temperature has been applied to determine the ordinary ($\varepsilon_\perp$) dielectric function of α-Ga_2O_3. This corresponds to an electric field direction perpendicular to the optical axis (0001), which is the growth direction of the thin (about 400nm) α-Ga_2O_3 films. A high energy spectral range up to 20eV has been investigated using synchrotron radiation. Several high-energy transitions have been resolved, which are consistent with ab-initio calculations of the dielectric function that include the solution of the Bethe-Salpeter equation, i.e. Coulomb interaction between electrons and holes. The calculations suggest that α-Ga_2O_3 is an indirect semiconductor with its valence band maximum between Γ and K points of the Brillouin zone. Strong direct absorption onsets at around 5.3 and 6.2eV are found, only slightly higher in energy than the predicted band gap.

Topical Talk DS 28.8 Wed 12:00 CHE 89

Kinetics and thermodynamcis of binary and ternary oxides during molecular beam epitaxy — •Patrick Vogt and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5–7, 10117 Berlin, Germany

Group-III and IV oxide semiconductors such as Ga_2O_3, In_2O_3, and SnO_2 may be efficiently n-type doped and have generated much interest due to their wide band gaps, optical transparency in the visible, as well as deep ultra-violet (DUV) regime of light. Alloying binary to ternary systems, combines their properties depending on their metal (Me) concentration, facilitates band gap engineering, and enables the growth of heterostructures, for applications such as transparent electronics, power transistors, or DUV detectors.

This talk presents a comprehensive understanding of the reaction kinetics and thermodynamics of oxides grown by plasma-assisted molecular beam epitaxy (MBE). The defined growth surface chemistry during MBE makes it an ideal system for studying fundamental growth processes. Knowing the reaction behavior of materials allows the systematic manipulation of their crystal and electronic characteristics depending on all growth parameters. Semi-empirical macroscopic kinetic growth models are presented predicting the Me incorporation and desorption of the mentioned compounds. These models may be generalized for other oxide systems and give information about the underlying reaction mechanisms these compounds are based on.

The findings are qualitatively applicable to other growth techniques such as pulsed laser- and metal-organic vapor phase deposition.

DS 28.9 Wed 12:30 CHE 89

Tin Assisted Growth of ϵ-Ga_2O_3 on c-plane Sapphire — •Max Kracht[1], Alexander Karg[1], Jörg Schörmann[1], and Martin Eickhoff[1,2] — [1]I. Physikalisches Institut, Justus Liebig Universität, Gießen, Germany — [2]Institut für Festkörperpysik, Bremen,Germany

Gallium oxide can crystallize in different polymorphs. The most common phase β-Ga_2O_3 is a promising material for high power devices and has therefore been widely studied. Although most physical properties such as the large band gap ($\approx 5eV$) are expected to be comparable for the different polymorphs , high quality material is needed to study their characteristics in detail. For example theoretical studies predict a high spontaneous polarization in ϵ-Ga_2O_3 , which would allow the realization of heterostructures with a two dimensional electron gas with high sheet carrier densities . This work focuses on the growth of gallium oxide on c-plane Al_2O_3 by plasma assisted molecular beam epitaxy. In the metal-rich growth regime gallium sub-oxide Ga_2O, which evaporates at growth temperature, is formed. With the addition of a small tin flux (flux ratio Ga/Sn = 10000) we can suppress this sub-oxide-etching and expand the growth window to more metal-rich conditions. Under these conditions phase pure ϵ-Ga_2O_3 is formed. A growth model for this tin assisted growth mode is presented.

DS 28.10 Wed 12:45 CHE 89

Transport properties of the In_2O_3 surface electron accumulation layer — •Alexandra Papadogianni, Julius Rombach, and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

In_2O_3 is a natively n-type transparent semiconducting oxide with unique properties attractive for several applications. Particularly interesting is its surface electron accumulation layer (SEAL), which enables gas-sensing applications. The SEAL electrical transport properties will be the main focus of this talk.

We study single-crystalline In_2O_3 thin films grown by plasma-assisted molecular beam epitaxy (PA-MBE) on insulating buffer layers achieved by doping with Ni as a new compensating acceptor, in order to remove potential interface conductance. This provides us with a model system of reduced complexity, with the electrical conductivity of these films essentially consisting of two parallel contributions: the bulk of the film and SEAL. To further modulate either the SEAL or the bulk in a targeted way and disentangle their contributions to the overall conductivity, we "turn off" the SEAL by an oxygen-plasma treatment and the bulk by Ni-doping. As a result, this enables us to study the temperature dependent transport properties of each individual conductive system.

DS 29: Organic Thin Films I

Time: Wednesday 9:30–13:15 Location: CHE 91

DS 29.1 Wed 9:30 CHE 91

Photochromic self-assembled monolayers of phosphonate diarylethene switches on polar ZnO surfaces — •Qiankun Wang[1], Giovanni Ligorio[2], Björn Kobin[3], Stefan Hecht[3], Emil J. W. List-Kratochvil[2], and Norbert Koch[1] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin — [2]Institut für Physik, Institut für Chemie & IRIS Adlershof, Humboldt-Universität zu Berlin — [3]Department of Chemistry, Humboldt-Universität zu Berlin

Photochromic molecular switches are attractive components in multifunctional devices, such as phototransistors and optical memories. By inserting a molecular switch interlayer into these devices, they can be used to modulate the charge injection properties by forming photoswitchable charge traps or charge barriers under the stimulation by external light. Here, we investigate the interfacial chemical and switchable properties of the phosphonic-acid diarylethene (PA-DAE) switch in form of a self-assembled monolayer (SAM) on ZnO(0001) and ZnO(000-1) surfaces by photoelectron spectroscopy. The observed work function increase is attributed to the introduced surface dipole moment; the binding modes of the phosphonate linker were retrieved from the deconvolution of core level (O 1s) spectra. Upon appropriate illumination with ultraviolet and visible light, we observe a 0.7 eV energy level shift at the onset of the highest occupied molecular orbitals (HOMO) level of the switches, which might be used to reversibly switch the energy level alignment at the ZnO/PA-DAE interface in device structures.

DS 29.2 Wed 9:45 CHE 91

Donor-acceptor mixtures of diindenoperylene (DIP) and hexafluoro-tetracyanonaphtoquinodimethane (F6TCNNQ) studied by Polarization Modulation Infrared Reflection-Absorption Spectroscopy (PMIRRAS). New insights into the signatures of charge-transfer interactions. — •Giuliano Duva, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Probing intermolecular interactions in donor:acceptor (D:A) binary mixtures of organic semiconductors (OSC) [1] requires high sensitivity techniques to overcome the intrinsic limitation of having a limited amount of material and typically a weak signal. A widely used technique for studying the effects of charge-transfer (CT) interactions on molecular vibrations is Fourier-transform IR spectroscopy (FTIR) [2]. However, interference from atmospheric water and the possibly low oscillator strength of some modes may severely limit the amount of reliable information that can be extracted from the final spectrum. We present a new approach for the study of mixtures of OSCs employing PMIRRAS as high-sensitivity technique to overcome the above limitations. Supported by the structural characterization of the films via X-ray scattering, we identify and discuss the spectral signatures of CT in correlation with the formation of D:A co-crystals. [1] A. Hinderhofer et al. Chem. Phys. Chem. 13 (2012). [2] D. Nanova et al. Org. Electr. 13 (2012).

DS 29.3 Wed 10:00 CHE 91

Coherent absorption in organic thin-film layered structures — •Tony Henseleit, Tim Wagner, Markas Sudzius, Hartmut Fröb, and Karl Leo — IAPP, Dresden, Deutschland

Development of strongly absorbing materials and devices has been a long-standing research field. Many of these efforts are based on a intriguing concept of perfect coherent absorption, which (assuming, that all required conditions are set up correctly) leads to a perfect conversion of optical energy to some form of an internal energy within the optically active material.

In this study, we focus on coherent absorption in layered thin-film structures with an organic absorbing material. The structures consist of a high optical quality dielectric distributed Bragg reflector and thermally evaporated layer of small organic molecules on it. We demonstrate both experimentally and numerically, that careful control of the resonator design and optical properties of an absorbing layer, allows to reduce amount of reflected light to the minimum and, therefore, to enhance absorption efficiency of thin organic layer up to almost 100 percent.

DS 29.4 Wed 10:15 CHE 91

Determination of the molecular orientation in thick organic emission layers — •Christian Hänisch — IAPP, TU Dresden

The orientation of the transition dipole moment of light emitting molecules in organic thin films of up to 150nm is determined via angular resolved photoluminescence spectroscopy.

DS 29.5 Wed 10:30 CHE 91

Influence of bulk heterojunction morphology on performances of organic solar cells — •Vladislav Jovanov, Hirwa Hippolyte, Arne Müller, Nivedita Yumnam, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

The bulk heterojunction morphology of solution processed organic solar cells can be determined by using atomic force microscopy phase imaging as we have demonstrated in our previous studies. The energy dissipated in the cantilever tip interaction with the film surface depends on the material that is present at the surface. Consequently, phase contrast is observed if different materials are forming the film surface. In this study, we have investigated the influence of a bulk heterojunction morphology on the electrical properties of organic solar cells. We have chosen a blend mixture of polymer PTB7 (donor) and fullerene PC[60]BM (acceptor) deposited from DCB/DIO solution as a materials system. In the first step, we have measured the morphologies of bulk heterojunction for different concentrations of the polymer and fullerene material. The determined structure is correlated to the electrical properties of solar cells such as short circuit current, fill factor and series resistance. The results show that bulk heterojunction morphology is crucial not only for the dissociation of generated excitons, but also for the transport of the free charge carries. Finally, we discuss the optimal organization of polymer and acceptor material.

DS 29.6 Wed 10:45 CHE 91

The growth of α-6T on different silver surfaces — •Thorsten Wagner, Ebrahim Ghanbari, Andrea Navarro-Quezada, and Peter Zeppenfeld — Johannes Kepler University, Linz, Austria

The combination of photoelectron emission microscopy (PEEM) and differential (optical) reflectance spectroscopy (DRS) is used to compare the growth of the prototype organic semiconductor α-sexithiophene (α-6T) on different silver surfaces, namely the Ag(111), the Ag(110), and the vicinal Ag(441) surface.

An unpolarized Hg lamp was used as excitation source for the photoelectrons. For all three substrates, the transient of the mean intensity obtained with PEEM follows the same trend: The first layer decreases the emission barrier for the photoelectrons and, hence, increases the electron yield. The deposition of additional molecules just decreases the electron yield, because the electron exclusively excited from the silver substrate have to pass through the molecular layers which do not further alter the emission barrier. In all three cases, at least an equivalent of two monolayers has to be deposited before nucleation of 3D crystallites is observed in PEEM.

After being reflected at the sample surface, the light of a white LED was split by a prism into its two linearly polarized components (pol-DRS). For the isotropic Ag(111) surface, the spectra obtained for s and p polarized light do not differ qualitatively. For the Ag(110) surface, the optical spectra indicate an orientation of the α-6T molecules along the [001] direction. On the Ag(441) surface, the molecules align parallel to the steps, i.e., along the $[1\bar{1}0]$ direction.

DS 29.7 Wed 11:00 CHE 91

How molecular quadrupole moments affect the energetics in organic thin films — •Martin Schwarze[1], Christopher Gaul[2], Katrin Ortstein[1], Frank Ortmann[2], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials, TU Dresden, 01069 Dresden, Germany — [2]Institute for Materials Science and Dresden Center for Computational Materials Science, TU Dresden, 01069 Dresden, Germany

The efficiency of organic semiconductor devices crucially depends on the precise energy level alignment of different organic layers. In most organic semiconductors, the ionization energy (IE) and the electron affinity (EA) of single molecules determine the electronic levels in organic devices and, therefore, their optimization is usually based on the IE and the EA of neat materials. However, these values can change substantially with the film morphology, at interfaces or in blends of different molecules.

By photoelectron spectroscopy, we obtain the IE of neat films at different molecular orientations and of blends with varying mixing ratios for a variety of small molecule materials. The changes of the IE, as a function of molecular orientation and mixing ratio, scale directly with the magnitude of the molecular quadrupole moments, as obtained by density functional theory simulations. By adjusting the mixing ratio of two different donor molecules, namely ZnPc and F4ZnPc, such electrostatic effects can be exploited in organic solar cells to tune the open-circuit voltage [1].

[1] Schwarze et al., Science 352, 1446 (2016)

15 min. break.

DS 29.8 Wed 11:30 CHE 91

Correlation of Structure, Morphology, and Spectroscopic Properties of Polymorphic, Textured Squaraine Thin Films — •Frank Balzer[1], Heiko Kollmann[2], Martin Silies[2], Matthias Schulz[3], Arne Lützen[3], Christoph Lienau[2], and Manuela Schiek[2] — [1]University of Southern Denmark, Sønderborg, Denmark — [2]University of Oldenburg, Germany — [3]University of Bonn, Germany

The dihydroxy anilino squaraine 2,4-bis[4-(*N*,*N*-diisobutylamino)-2,6-dihydroxyphenyl]squaraine (SQIB) crystallizes into at least two polymorphic structures: a monoclinic and an orthorhombic phase. Spin-coated thin films are, depending on the annealing temperature, highly textured with two distinct morphological features, which are assigned to the two polymorphic forms. These features exhibit different absorption spectra with characteristic spectral signatures of molecular excitons with oblique transition dipole alignment and large Davydov splitting. The monoclinic form shows a blue-shifted absorption compared to the monomer band, while the absorption profile of the orthorhombic form is red-shifted. The transitions of the excitonic states for each polymorph are polarized mutually perpendicular, probed by polarization-resolved confocal spectro-microscopy. X-ray diffraction reveals a strong out-of-plane orientation. Crystalline domains are distributed with random in-plane orientation on the samples. Their local in-plane orientation is deduced from spectro-microscopy recordings as well as from polarized light microscopy.

DS 29.9 Wed 11:45 CHE 91

Combined structural and optical real-time study on growth of a charge transfer complex — •Valentina Belova, Alexander Hinderhfer, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Molecular arrangement and structure formation in binary mixed thin film organic semiconductors being in a close correlation with intermolecular interaction [1] directly influence device functionality [2]. We present a real-time investigation of structure evolution during growth (by organic molecular beam deposition OMBD) of a small-molecule donor:acceptor pair (diindenoperylene DIP : N,N0-1H,1H-perfluorobutyl-cyanoperylenediimide PDIF-CN2 [Polyera ActivInk N1100]) combining X-ray scattering methods with differential reflectance spectroscopy (DRS) in the visible range. We found strong changes in the structural and optical properties upon mixing of donor and acceptor molecules that evidence the complex formation. A strong influence of substrate temperature was observed. DRS was performed during film growth in order to establish the correlation between changes in optical spectra due to the intermolecular coupling and structural/mixing behavior. The analysis is complemented with atomic force microscopy (AFM), ellipsometry, photoluminescence and UV-Vis absorption. [1] J. Dieterle et al. J. Phys. Chem. C, 2015, 119 (47) 26339; [2] A. Opitz et al. Phys. Status Solidi A 2009, 206 (12) 2683

DS 29.10 Wed 12:00 CHE 91

Evaluation of in-operando potential distributions in OLEDs combining experimental and drift-diffusion studies — •Maybritt Kühn[1,2], Christof Pflumm[3], Wolfram Jaegermann[1,2], and Eric Mankel[1,2] — [1]Technische Universität Darmstadt, Institute of Materials Science — [2]InnovationLab GmbH, Heidelberg — [3]Merck KGaA, department OLED-Physics, Darmstadt

Nowadays organic light-emitting diodes are widely used as displays in smart phones. As these devices consist of several functional layers it is not only important to know the driving voltage of the whole device but also the potential distributions within the single layers. Therefore we present a combined experimental and drift-diffusion study to determine in operando transport properties of the single layers. Two types of OLEDs that only differ in the emission layer but obviously exhibit different potential distributions are investigated. If the emission layer consists of TH-A a shift of the onset voltage in case of layer thickness variation can be observed while using TH-B, an isomer to TH-A, the onset voltage remains unchanged. The voltage development per layer is determined from IV curves of a set of devices with varying layer thickness. Empirically the voltage development can be described with a power law. Using the drift-diffusion model the current density dependent development of the coefficient and the exponent of the power law can be well described. With the model the mobility, the carrier injection mechanism into the respective layer and the barrier height are determined. Furthermore we are able to show that an electric field at or close to the contact is necessary to describe the TH-A behaviour.

DS 29.11 Wed 12:15 CHE 91

Direct Micropatterning of Organic Thin Films by Electron Beam Processing — •Marie Hoffmann, Elisabeth Bodenstein, Björn Meyer, Falk Winckler, Matthias Schober, and Christoph Metzner — Fraunhofer FEP, Winterbergstr. 28, 01277 Dresden

The patterning of organic layers becomes more and more important especially for applications in solar cells and organic electronics. Organic light-emitting diodes (OLEDs) offer numerous advantages compared to commercially used LCD technology for displays and lighting, e.g. no backlight is needed and the feasibility of very thin, flexible displays is given. The improvement of OLED displays regarding efficiency, lifetime and resolution is an ongoing effort. One of the major challenges is the realization of very small structure sizes. Current patterning methods like thermal evaporation through fine metal masks, printing or lift-off techniques have been demonstrated, however, deficiencies regarding the flexibility of new applications are still existing and desired structure sizes could not be achieved jet. Therefore a method for direct patterning by using electron beam technology has been investigated. Penetrating electrons heating a multilayer system locally lead to a structured evaporation of the organic material. In the current work several experiments and investigations of electron beam processing of organic layers were performed. The process window for a careful adjustment of defined material properties could be narrowed through additional simulation calculations. First results will be shown and the technology assessed to its prospective usability.

DS 29.12 Wed 12:30 CHE 91

Structural Properties of Thin Films of Phenacenes — •Jan Hagenlocher[1], Alexander Hinderhofer[1], Kera Satoshi[2], and Frank Schreiber[1] — [1]Eberhard Karls Universität, Tübingen — [2]Institute for Molecular Science, Okazaki, Japan

We studied the structural properties of the high band gap organic semiconductors Picene, [6]Phenacene and [7]Phenacene which exhibit high conductivity. X-ray reflectivity, grazing incidence X-ray diffraction and atomic force microscopy were applied to study the influence of a small length difference between the molecules on the crystallographic structure and morphology of the resulting mixed thin film. The compounds employed are well suited since they consist of different numbers of benzene rings fused together in a zig-zag pattern and differ only in length. It was found that the crystallographic structure remains unchanged upon mixing but the wetting behaviour, the morphology and especially the films roughness changes significantly. Different explanations are discussed and further explored using real-time X-ray reflectivity and analysis of terrace coverage of individual islands. Additionally, the optical properties of the thin films were investigated with UV-Vis spectroscopy.

DS 29.13 Wed 12:45 CHE 91

Cyano-phenyl porphyrin on Cu(111): A STM, XPS and DFT study — •Juan Carlos Moreno-López[1], Alisson Ceccatto Dos Santos[2], Michael Lepper[3], Hubertus Marbach[3], Henry P. Pinto[1], and Abner De Siervo[2] — [1]Yachay Tech University, School of Physical Sciences and Nanotechnology, 100119-Urcuquí, Ecuador — [2]Universidade Estadual de Campinas, Instituto de Fisica "Gleb Wataghin" CP 6165, CEP 13081-970, Campinas, SP, Brazil. — [3]Lehrstuhl für Physikalische Chemie 2, Universität Erlangen-Nürnberg, Germany

The study of organic molecules on surface gained increasing interest during the last years in the research community. Studies of individual organic molecules and studies of self-assembled networks with complex interactions have shown the plausible technological applications of organic molecules on diverse fields, such as: molecular machines, molecular electronics, gas storage in molecular porous networks, etc. With this background we studied cyano-functionalized porphyrins, namely 2H-tetrakis-(p-cyano)-phenylporphyrin (2HTCNPP) on Cu(111). In this work, we performed a thorough study, by means of Scanning tunneling microscopy (STM), X-ray photoelectron Spectroscopy (XPS) and Density-functional theory (DFT) calculations, in order to gain insight into the adsorption behavior of 2HTCNPP on Cu(111) and its evolution after the deposition of Pd atoms as well as its behaviour after thermal treatment.

DS 29.14 Wed 13:00 CHE 91

Influence of radiative efficiency and dipole orientation on optimal layer thicknesses of monochrome OLEDs for maximum EQE — •Paul-Anton Will, Cornelius Fuchs, Reinhard Scholz, Simone Lenk, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Germany

For realizing highly efficient organic light-emitting diodes (OLEDs), the light-emitting molecule has to meet several requirements. Among chemical, energetic, and optical characteristics two crucial properties are the radiative efficiency η_{rad} and the emissive dipole orientation described by the anisotropy factor a. While the first is already close to its maximum for commonly used emitter molecules, a lot of research is currently ongoing to understand and control the dipole orientations of organic molecules. However, the external quantum efficiency (EQE) of OLEDs depends on the optical enviroment of the emitting molecules. As known, the Purcell effect leads to an effective radiative efficiency η^*_{rad} for emitters in a cavity. In this work, we show how the radiative efficiency η_{rad} and the anisotropy factor a influence the optimal layer thickness of monochrome OLEDs to reach maximum EQE. We find that for emitters with $\eta_{\mathrm{rad}} < 100\,\%$ the product of η^*_{rad} and the outcoupling efficiency η_{out} needs to be optimized, instead of solely optimizing η_{out}. When doing so, the EQE of planar OLEDs with highly oriented molecules but imperfect radiative efficiency can be pushed further. In this way, the full potential of planar OLEDs can be exploited.

DS 30: Two-dimensional materials IV (jointly with HL/TT)

Time: Wednesday 9:30–13:15 Location: POT 51

DS 30.1 Wed 9:30 POT 51

Landau-Quantized Graphene: A Tunable Nonlinear Optical Material in the THz Range — •Jacob C. König-Otto[1,2], Yongrui Wang[3], Alexey Belyanin[3], Claire Berger[4,5], Walt A. de Heer[4], Milan Orlita[6,7], Alexej Pashkin[1], Harald Schneider[1], Manfred Helm[1,2], and Stephan Winnerl[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Technische Universität Dresden, Germany — [3]Texas AM University, USA — [4]Georgia Institute of Technology, USA — [5]CNRS-Universitè Alpes, France — [6]LNCMI, Grenoble, France — [7]Charles University in Prague, Czech Republic

Finding nonlinear optical materials for the THz and mid-infrared regimes is not straightforward. State-of-the-art devices with a high third-order optical susceptibility are often processed as complex multi-quantum-well structures designed to feature one specific resonance frequency. In our work we study Landau-quantized graphene as a tunable and simple to produce nonlinear material. To this end we perform time-integrated degenerate four-wave mixing (FWM) experiments at a photon energy of 78 meV resonant to the transitions between the Landau levels LL_{-1}, LL_0 and LL_1 at a magnetic field of roughly 4 T. We can recover expected scaling of the FWM-signal with the incident fields and the resonance behavior. The value of the third-order surface susceptibility in this material is in agreement with our calculations based on the density matrix formalism. We find the order of $\chi^{(3)}$ of Landau-quantized graphene to be competitive with more complex and elaborated solutions.

DS 30.2 Wed 9:45 POT 51

Ballistic transport in 2D periodically modulated graphene — •Andreas Sandner[1], Martin Drienovsky[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]NIMS, 1-1 Namiki, Tsukuba, Japan

Embedding graphene into a heterostructure with hexagonal boron nitride was shown to be an efficient way of achieving a high bulk mobility. The encapsulated graphene is protected in any further top-down fabrication procedure and pronounced commensurability features could be observed in 2D antidot lattices [1].

Here, we want to introduce a new method for periodical modulation of the carrier density, employing a few layer graphene patterned bottom gate. The bottom gate is defined by etching a 2D hole array into the few layer graphene and adapts perfectly to the commonly used stacking method for van der Waals heterostructures. By tuning the local bottom gate and the global back gate voltage, we can switch between the unipolar and bipolar transport regime.

We fabricated patterned bottom gates with lattice periods down to 150 nm and observe pronounced commensurability peaks that can be nicely compared to experiments with hard-wall graphene antidot lattices. We report on the difference between the unipolar and the bipolar regime, as well as the influence of the magnitude of the imposed superlattice potential.

[1] A. Sandner et al., Nano Lett. **15**, 8402 (2015)

DS 30.3 Wed 10:00 POT 51

Commensurability oscillations in electrostatically modulated graphene — •Martin Drienovsky[1], Jonas Joachimsmeyer[1], Takashi Taniguchi[3], Kenji Watanabe[3], Ming-Hao Liu[2], Klaus Richter[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Institut für Theoretische Physik, Universität Regensburg, Germany — [3]National Institute for Material Science, Tsukuba, Japan

We report on the first experimental observation of commensurability oscillations (COs) [1] in a 1D periodic graphene superlattice. Employing a locally acting few layer graphene patterned bottom gate (FLG PBG) and a dry van-der-Waals stacking method we prepare high mobility graphene-boron nitride heterostructures, where the ballistic length exceeds several periods of the modulation. The potential landscape can be tuned by the striped FLG PBG and a global back gate in such a way that a small, periodic and unipolar potential perturbation is generated. The magnetoresistance exhibits well pronounced COs at predicted magnetic field positions for electrostatic modulation, both for the electron and hole transport regime. Our measurements confirm strong robustness of the COs in graphene with respect to temperature [2], as they remain visible up to 155 K.

[1] D. Weiss et al., Europhys. Lett. 8, 179 (1989) [2] A. Matulis and F. M. Peeters, Phys. Rev. B 75, 125429 (2007)

DS 30.4 Wed 10:15 POT 51

Intrinsic mobility due to electron-phonon interaction in black phosphorus. — •Sergey Brener, Alexander Rudenko, and Mikhail Katsnelson — Radboud Universiteit, Niederlanden

Flexural and in-plane thermal fluctuations in crystalline membranes affect the band structure of the carriers, which has an effect on transport properties of 2D systems. I consider a specific example of one-layer black phosphorus, which is a highly anisotropic material, and present our recent results on intrinsic carrier mobility. In contrast to graphene, where the mobility is determined by two-phonon (flexural) scattering, in black phosphorus one-phonon (in-plane) processes dominate.

DS 30.5 Wed 10:30 POT 51

Strain-induced commensurability oscillations in graphene — •Jonas Joachimsmeyer[1], Martin Drienovsky[1], Takashi Taniguchi[2], Kenji Watanabe[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

We realized a periodic strain modulation in a graphene/hexagonal boron-nitride (hBN) heterostructure by transferring it onto a prepatterned 1D superlattice etched into hBN. The transfer was performed using a dry van-der-Waals pick-up technique. This method yields a high mobility graphene device with a mean free path exceeding the period of the corrugation.

We conducted magnetotransport experiments in this corrugated graphene monolayer with a period of 150 nm. The modulation leads to a periodic strain which in turn gives rise to an effective periodic pseudopotential with half of the period of the corrugation [1], i.e. 75 nm. Due to the periodic potential we observe commensurability oscillations (COs) [2] in the longitudinal magnetoresistance, however superimposed by Shubnikov-de Haas (SdH) oscillations. Since both oscillations show different temperature dependences we increased the temperature up to 80 K. While the SdH oscillations get suppressed the COs still remain visible.

[1] Burgos, R., and Lewenkopf, C., arXiv:1610.04068 (preprint 2016).

[2] Ye, P. D., Weiss, D., et al., Semicond. Sci. Technol. 10, 715 (1995).

DS 30.6 Wed 10:45 POT 51

Temperature switchable type of conductivity in hybrid conjugated polyelectrolyte/graphene two-dimensional nanocomposites — •Viktor Brus[1], Marc Gluba[1], Cheng-Kang Mai[2], Stefany Fronk[2], Jörg Rappich[1], Norbert Nickel[1], and Cuillermo Bazan[2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekulèstr. 5, 12489 Berlin, Germany — [2]Center for Polymers and Organic Solids, Department of Chemistry and Biochemistry, University of California at Santa Barbara, Santa Barbara, CA, 93106, USA

We found that a submonolayer of CPE-PyrBIm4 on CVD-grown graphene forms a novel two-dimensional hybrid material that exhibits preferential transport of holes or electrons as a function of temperature. Doping efficiencies increase with the increase of the temperature used to anneal the heterobilayers and a decrease of the CPE-PyrBIm4 film thickness. The switching of the conductivity type of the thin CPE-PyrBIm4/graphene heterobilayer composite occurs when graphene is not strongly overcompensated. Moreover, the conversion of the conductivity type is reversible. Doping mechanisms under consideration include charge transfer from electron rich structural units in the CPE-PyrBIm4 backbone and/or field-effect doping as a result of interfacial electrostatic effects from adjacent ionic functionalities. This effect shows the unique and complex nature of electrical properties of the novel heterobilayer hybrid organic-inorganic CPE-PyrBIm4/graphene nanocomposite material and enhances interest in further investigations.

DS 30.7 Wed 11:00 POT 51

Interlayer screening in n-doped bilayer and trilayer transition metal dichalcogenides — •Andor Kormányos[1], Viktor Zólyomi[2], and Guido Burkard[1] — [1]University of Konstanz, Germany — [2]Manchester University, United Kingdom

We derive an effective Hamiltonian based on the k.p approach that describes the dispersion at the band edges of the conduction band of bilayer and trilayer transition metal dichalcogenides (TMDCs). This model is then used to consider n-doped bilayer MoS_2 placed in uniform external electric field. We discuss the charge re-distribution between the layers due to the electric field and calculate the bandgap that opens at the K-point of the Brillouin zone in self-consistent Hartree approximation. We point out the relation between the induced band-gap and the quantum capacitance and briefly discuss the relevance of our results to recent photoluminiscence experiments in double gated bilayer MoS_2.

Coffee Break

DS 30.8 Wed 11:45 POT 51

Driven Hofstadter Butterflies — •Martin Wackerl[1] and John Schliemann[2] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Institut für Theoretische Physik, Universität Regensburg

Periodically driven quantum systems offer a great way of tuning band structures or Chern numbers. The first part will be about graphene illuminated with circular polarized light. The external driving is introduced via the Floquet formalism and the main focus will be on the deformation of the band structure of graphene. Afterwards we will give a short introduction to the Hofstadter butterfly and unify it with the Floquet formalism. We will show how the Hofstadter spectrum gets distorted when tuning the light intensity, photon energy, and polarization. The last part is about the influence of polarized light to the distribution of ground state Chern numbers of the Floquet-Hofstadter spectrum.

DS 30.9 Wed 12:00 POT 51

Resonant scattering off adatoms in monolayer graphene — •Susanne Irmer, Denis Kochan, and Jaroslav Fabian — University of Regensburg, Regensburg, Germany

We present a theoretical investigation of resonant scattering off adatoms on graphene. Resonant scattering is an important feature of adatoms as it leads to resonant enhancement of the impact of proximity effects such as local magnetic moments or spin-orbit coupling [1,2,3]. We investigate the three different adsorption positions of hollow, top, and bridge employing effective realistic tight-binding models and the T-matrix formalism. The developed resonance conditions are useful for quantum transport models as well as studies of spin relaxation in graphene with adatoms.

This work was supported by the DFG SFB 689 and GRK 1570, and by the European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

[1] D. Kochan, M. Gmitra, and J. Fabian, Phys. Rev. Lett. 112, 116602 (2014)

[2] J. Bundesmann, D. Kochan, F. Tkatschenko, J. Fabian, and K. Richter, Phys. Rev. B 92, 081403 (2015)

[3] D. Kochan, S. Irmer, and J. Fabian, arXiv:1610.08794

DS 30.10 Wed 12:15 POT 51

Experimental realization and characterization of an electronic Lieb lattice — •Marlou Slot[1], Thomas Gardenier[1], Peter Jacobse[1], Guido van Miert[2], Sander Kempkes[2], Stephan Zevenhuizen[1], Cristiane Morais Smith[2], Daniel Vanmaekelbergh[1], and Ingmar Swart[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, Netherlands — [2]Institute for Theoretical Physics, Utrecht University, Netherlands

Geometry, whether on the atomic or nanoscale, is a key factor for the electronic band structure of materials. For example, the honeycomb geometry leads to Dirac-type bands where the charge carriers behave as massless particles. Theoretical predictions are triggering the exploration of novel 2D geometries, such as graphynes, Kagomé and the Lieb lattice. The latter is the 2D analogue of the 3D lattice exhibited by perovskites; it is a square-depleted lattice, which is characterised by a band structure featuring Dirac cones intersected by a topological flat band. Whereas photonic and cold-atom Lieb lattices have been demonstrated, an electronic equivalent in 2D is difficult to realize in an existing material. Here, we report an electronic Lieb lattice formed by the surface state electrons of Cu(111) confined by an array of CO molecules positioned with a scanning tunneling microscope. Using scanning tunneling spectroscopy and wave-function mapping, we confirm the characteristic electronic structure of the Lieb lattice. The experimental findings are corroborated by muffin-tin and tight-binding calculations. At higher energy, second-order electronic patterns are observed, which are equivalent to a super-Lieb lattice.

DS 30.11 Wed 12:30 POT 51

Interlayer Configuration in Twisted Bilayers of Folded Graphene — •Johannes C. Rode, Christopher Belke, Hennrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

Twisted bilayer graphene (TBG), i.e. stacks of two graphene sheets in arbitrary rotational misalignment, exhibit rich electronic spectra[1,2] which are highly dependent on the interlayer twist angle in general[3] as well as details in stacking configuration like lattice commensuration and corrugation[4] in particular. We here examine the latter TBG properties coming from the morphological side: TBG are prepared via Atomic Force Microscope, folding ribbons out of monolayer sheets. In the recently proposed picture of a thermally activated growth process[5], here measured quantities like interlayer distance and shape of the folded edge are found to hold novel information about angle-dependent interlayer configuration and provide insight about interaction in van der Waals bound materials.

[1] H. Schmidt; J. C. Rode; D. Smirnov; R. J. Haug,
Nat. Comm. **5**, 5742 (2014).

[2] J. C. Rode; D. Smirnov; H. Schmidt, R. J. Haug,
2D Materials **3**, 035005 (2016).

[3] J. M. B. Lopes dos Santos; N. M. R. Perez; A. H. Castro Neto, Phys. Rev. Lett. **99**, 25682 (2007).

[4] E. J. Mele, Phys. Rev. B **81**, 161405(R) (2010).

[5] J. Annett; G. L. W. Cross, Nature **535**, 271-275 (2016).

DS 30.12 Wed 12:45 POT 51

Multi-scale approach for strain-engineering of phosphorene — Daniel Midtvedt[1] and •Alexander Croy[2] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany

A multi-scale approach for the theoretical description of deformed phosphorene is presented. This approach combines a recently developed valence-force model [1] to relate macroscopic strain to microscopic displacements of atoms and a tight-binding model [2] with distance-dependent hopping parameters to obtain electronic properties. The resulting self-consistent electromechanical model is suitable for large-scale modeling of phosphorene devices. We demonstrate this for the case of an inhomogeneously deformed phosphorene drum, which may be used as an exciton funnel [3].

[1] D. Midtvedt and A. Croy, Phys. Chem. Chem. Phys. 18, 23312 (2016). [2] A. N. Rudenko, S. Yuan, and M. I. Katsnelson, Phys. Rev. B 92, 085419 (2015). [3] P. San-Jose et al, Phys. Rev. X 6, 031046 (2016).

DS 30.13 Wed 13:00 POT 51

Evolution of electronic structure of few-layer phosphorene from angle-resolved photoemission spectroscopy of black phosphorous — •Niels Ehlen[1], Boris Senkovskiy[1], Alexander Fedorov[1,2,3], Andrea Perucchi[4], Paola Di Pietro[4], Antonio Sanna[5], Gianni Profeta[6], Luca Petaccia[4], and Alexander Grüneis[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]IFW Dresden, Germany — [3]St. Petersburg State University, Russia — [4]Elettra Sincrotrone Trieste, Italy — [5]Max Planck Institute of Microstructure Physics, Halle, Germany — [6]Department of Physical and Chemical Sciences/SPIN-CNR, University of L'Aquila, Italy

A complete set of tight-binding parameters for the description of the quasiparticle dispersion relations of black phosphorous (BP) and N-layer phosphorene with $N = 1 \ldots \infty$ is presented. The parameters, which describe valence and conduction bands, are fit to angle-resolved photoemission spectrocopy (ARPES) data of pristine and lithium doped BP. We show that zone-folding of the experimental three-dimensional electronic band structure of BP is a simple and intuitive method to obtain the layer-dependent two-dimensional electronic structure of few-layer phosphorene. Zone-folding yields the band gap of N-layer phosphorene in excellent quantitative agreement to experiments and *ab-initio* calculations. A combined analysis of optical absorption and ARPES spectra of pristine and doped BP are used to estimate a value for the exciton binding energy of BP.

DS 31: 2D Materials Beyond Graphene III (jointly with O)

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

DS 31.1 Wed 10:30 WIL A317

Band structure and excitons of monolayer and bulk ReSe$_2$: A many-body view — •Jonathan Noky[1], Matthias Drüppel[1], Philipp Eickholt[2], Thorsten Deilmann[3], Koji Miyamoto[4], Peter Krüger[1], Markus Donath[2], and Michael Rohlfing[1] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Physikalisches Institut, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [3]Center for Atomic-Scale Materials Design (CAMD), Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark — [4]Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan

Transition metal dichalcogenides (TMDCs) are a fascinating new class of semiconductors, which attracted a lot of interest in the past few years. They are promising materials for new optical and electronic devices on the nanoscale. Here, we focus on one of the less studied members of this group: ReSe$_2$. In contrast to other TMDCs, it grows in a distorted $1T$ structure, which leads to new anisotropic properties.

We present electronic and excitonic spectra for both monolayer and bulk ReSe$_2$ within many-body perturbation theory (MBPT). For this, we apply the GW-BSE (Bethe-Salpeter equation) approach within the efficient LDA+GdW approximation [1]. Our results on the quasiparticle band structure are complemented with experimental ARPES data. Based on the band structure we investigate the excitons. The lowest four states show distinct dipolar characteristics, which is in contrast to many other TMDCs.

[1] M. Rohlfing, Phys. Rev. B. **82**, 205127 (2010)

DS 31.2 Wed 10:45 WIL A317

Fabrication and characterization of coupled TMDC heterostructures — •Borja V. Pano[1,2], Bastian Miller[1,2], Alexander W. Holleitner[1,2], and Ursula Wurstbauer[1,2] — [1]Walter Schottky Institute and Physics-Department, Technical University Munich, Am Coulombwall 4a, 85748 Garching — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 Munich, Germany

Atomically thin transition metal dichalcogenides (TMDC) have emerged as an exciting class of two-dimensional (2D) semiconductors with unique electronic and optoelectronic properties, and are of interest for both fundamental research and novel device applications.

We investigate heterostructures of four different TMDC monolayers (MoS$_2$, WS$_2$, MoSe$_2$, WSe$_2$). Due to the formation of a type II band alignment between the layers and the strong Coulomb binding energy in 2D TMDC, these devices open a promising path for studying long-lived interlayer excitons, where bound electrons and holes are localized in different layers.

A polymer-based dry transfer technique is used to vertically stack micromechanical cleaved monolayers with angle alignment of the crystal axes. We characterize the heterostructures through optical and atomic force microscopy, Raman and photoluminescence spectroscopy. We observe strong signatures of interlayer coupling.

We acknowledge the financial support by the DFG and the excellence cluster Nanosystems Initiative Munich (NIM).

DS 31.3 Wed 11:00 WIL A317

Switchable white graphene: electrochemical surface science of the boron nitride nanomesh — •Stijn Mertens — TU Wien, Institut für Angewandte Physik, Wiedner Hauptstraße 8-10/134, 1040 Vienna, Austria — KU Leuven, Chemistry Department, Celestijnenlaan 200F, 3001 Leuven, Belgium

On Rh(111), a monolayer of hexagonal boron nitride (h-BN) forms a so-called nanomesh superstructure [1] with a 3.2-nm lattice constant and strong electronic corrugation, useful for trapping atoms and molecules [2,3].

We show by electrolyte-to-vacuum transfer experiments and thermal desorption spectroscopy that hydrogen underpotential deposition (H upd) [4] leads to submonolayer quantities of hydrogen intercalated between the h-BN overlayer and Rh(111). In situ STM reveals that this lifts the corrugation of the nanomesh and is fully reversible under potential control. Copper upd is used to quantify the defect density in the nanomesh, and to determine the electrochemical window where the nanomesh is stable. Dynamic contact angles of an electrolyte drop show that the microscopic change within the 2-dimensional material leads to a macroscopic effect related to a 10% change in adsorption energy [4]. The static friction on the other hand, which can be extracted by extending the Young equation for non-equilibrium effects, remains unchanged for the surface in the two states.

[1] Corso et al., Science 303 (2004) 217. [2] Berner et al. Angew. Chem., Int. Ed. 46 (2007) 5115. [3] Dil et al. Science 319 (2008) 1824. [4] Mertens, Greber et al. Nature 534 (2016) 676.

DS 31.4 Wed 11:15 WIL A317

In-situ LEEM investigation of the growth of hexagonal boron nitride on metal surfaces — •Janina Felter, Markus Franke, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and Jülich Aachen Research Alliance (JARA)-Fundamentals of Future Information Technology, Germany

Hexagonal boron nitride (hBN) is a prominent and frequently studied member of the family of two-dimensional (2D) materials. Due to its structural and electronic properties, in particular its insulating nature, it is of highest interest as part of hetero-epitaxial systems in conjunction with other 2D materials or organic thin films. However, the production of high quality hBN monolayers and organic thin films on hBN necessitates a deep understanding of nucleation and growth of these materials. Here, we present a detailed in-situ and real-time study of the growth of hBN monolayers on Cu(111) using Low-Energy Electron Microscopy (LEEM). We correlate the results with structural information obtained by μLEED and discuss the influence of substrate temperature, growth rate and movement of step edges.

DS 31.5 Wed 11:30 WIL A317

Time-of-Flight Secondary Ion and Neutral Mass spectrometry of particles ejected from 3D and 2D materials during irradiation with highly charged and swift heavy ions — •Philipp Ernst[1], Florian Meinerzhagen[1], Matthias Herder[2], Stephan Sleziona[1], Andreas Wucher[2], and Marika Schleberger[1] — [1]University Duisburg-Essen, AG Schleberger, Germany — [2]University Duisburg-Essen, AG Wucher, Germany

We have studied the ionization probability for strontium titanate bombarded by energetic ions, i.e. swift heavy ions (SHI) and highly charged ions (HCI). Strontium titanate is a dielectric and as such is known to be very sensitive to both, SHI and HCI irradiation, which result in characteristic surface modifications [1,2]. Therefore, it has been postulated that both projectile types trigger similar mechanisms leading to these modifications. To test this hypothesis, we compare time-of-flight mass spectra taken during irradiation with SHI at different electronic stopping powers (dE/dx) and with HCI with varying potential energy (^{129}Xe ions with a potential energy from E_{pot} 4.5 up to 59 keV by constant kinetic energy E_{kin}), respectively. Both, emitted secondary ions (SIMS) and secondary neutrals (SNMS), were detected in order to determine differences of the ionization probability. To further test if the spatial distribution of the energy deposition (HCI a few nm, SHI up to tens of microns) does play a role, exemplary measurements with a 2D dielectric have been performed.

[1] F. Meinerzhagen, et al. Rev. Sci. Instr, 87 (2016) 013903.

[2] F. Aumayr, et al. J. Phys. Condens. Matter, 23 (39) (2011).

DS 31.6 Wed 11:45 WIL A317

A monolayer of MoS_2 on Au(111) as a decoupling layer for single molecules — •Christian Lotze, Nils Krane, Robert Steyrleuthner, Robert Bittl, Jan Behrends, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin

Thiophene based molecules are commonly used for semiconducting devices like solar cells or light emitting diodes. In order to optimize these, a detailed understanding of the molecules electronic structure and the environmental influence on the latter is of great interest.

Scanning tunneling spectroscopy (STS) allows to address individual molecules in a precisely known surrounding. However, it bears the drawback that it requires a conductive substrate. Deposition of organic molecules on a metal substrate leads to strong hybridization of the electronic states. Preservation of the molecular character requires the inclusion of thin band-gapped materials.

Here, we present STS experiments performed on 2,5-bis(3-dodecylthiophen-2-yl)thieno[3,2-b]thiophene-n (BTTT-n; n=1,2) molecules adsorbed on a single layer molybdenum disulfide (MoS_2) on Au(111). We show that it acts as an effective decoupling layer. Differential conductance spectra of the molecules exhibit a multitude of sharp characteristic peaks, that are connected to the highest occupied molecular orbital. We propose that these originate from a surprisingly effective excitation of vibronic resonances by the tunneling electrons.

DS 31.7 Wed 12:00 WIL A317

Surface-confined Mott transition in the strongly correlated compound 1*T*-$TaSe_2$ — •Florian Diekmann, Christian Sohrt, Kerstin Hanff, Lars-Philip Oloff, Arndt Quer, Matthias Kalläne, and Kai Rossnagel — Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany

The surface associated modification of the electronic structure of 1*T*-$TaSe_2$ in the commensurate charge density-wave (CDW) state is examined by utilising photon energy dependent X-Ray photoemission spectroscopy. In particular, the CDW-induced splitting of the Ta $4f$ core levels is probed over a wide range of photon energies from 80 eV to 6 keV corresponding to a variation of the information depth from extreme surface to effective bulk sensitivity. The measured depth-dependent core-level splitting corroborates the idea of a surface-confined Mott transition due to a modified CDW at the surface [1,2].

[1] L. Perfetti *et al.*, Phys. Rev. Lett. **90**, 166401 (2003).

[2] C. Sohrt *et al.*, Faraday Discuss. **171**, 243 (2014).

DS 31.8 Wed 12:15 WIL A317

Insights into structure and binding of micron-sized hexagonal boron nitride islands on Ir(111) — •Marin Petrović, Michael Horn-von Hoegen, and Frank-J. Meyer zu Heringdorf — Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany

Single-layer hexagonal boron nitride (hBN) islands have been synthesized on Ir(111) via chemical vapor deposition (CVD) of borazine at various temperatures. By using low-energy electron microscopy (LEEM) as the main experimental tool, two types of hBN islands were identified which differ in their shape (triangular and trapezoidal) and in their rotational registry with respect to the iridium. Moreover, photoemission electron microscopy (PEEM) and IV-LEEM spectroscopy measurements show that the two island types exhibit different work functions and interaction strengths with iridium, which is proposed to be the origin of their divergence in shape and growth modes. In addition, it is found that for CVD synthesis above ≈950 °C additional boron islands are formed on the iridium surface, which is a result of increased decomposition of hBN and significant solubility of boron in iridium at high temperatures.

DS 31.9 Wed 12:30 WIL A317

Intervalley scattering dynamics in MoS_2 imaged by two-photon photoemission with a high-harmonic probe — •Robert Wallauer, Johannes Reimann, Nico Armbrust, Jens Guedde, and Ulrich Hoefer — Fachbereich Physik und Zentrum für Materialwissenschaften Philipps-Universität, 35032 Marburg, Germany

We will report on the application of time- and angle-resolved two-photon photoemission (2PPE) with a high-harmonic probe for the investigation of the electron dynamics of MoS_2 in momentum space. For this purpose, we combined a high-repetition rate high-harmonic source with tunable femtosecond pump pulses and a 3D (k_x, k_y, E) electrostatic electron spectrometer. At our high-harmonic photon energy of 23.5 eV we essentially probe only the first layer, which is not necessarily equal to a bulk sample.

We used this setup to study the electron dynamics in the conduction band of MoS_2 after optical excitation with different pump photon energies. Thereby we showed that optical excitation above the A exciton resonance at 1.8 eV with 2.05 eV pump pulses results in an immediate occupation of the conduction band at K followed by an ultrafast transfer to the conduction band minimum at Σ [1]. Subsequently, the occupation at both high-symmetry points decays slowly on a ps timescale. We will present new data for pump photon energies in the range of 1.8 - 2.1 eV and show how the dynamics of this transfer depend on the excess energy above the exciton resonance.

[1] R. Wallauer et al., Appl. Phys. Lett. 109, 162102 (2016).

DS 31.10 Wed 12:45 WIL A317

Theoretical aspects in the investigation of intrinsic magnetic order in monolayer FePS3 — •Pilkwang Kim[1], Jae-Ung Lee[2], Sungmin Lee[1,3], Ji Hoon Ryoo[1], Soonmin Kang[1,3], Tae Yun Kim[1], Cheol-Hwan Park[1,4], Je-Geun Park[1,3], and Hyeonsik Cheong[2] — [1]Department of Physics and Astronomy, Seoul National University (SNU), Seoul 08826, Korea — [2]Department of Physics, Sogang University, Seoul 04107, Korea — [3]Center for Correlated Electron Systems, Institute for Basic Science (IBS), Seoul 08826, Korea — [4]Center for Theoretical Physics, Seoul National University (SNU), Seoul 08826, Korea

It has been a while since Onsager established that there can be a phase transition at a finite temperature in the two-dimensional (2D) Ising system. However, experimental verification of such long-range magnetic order has been mostly limited to the magnetism arising from extrinsic effects such as defects and chemical dopants. Bulk iron phosphorus trisulfide (FePS3) is a van der Waals material with an Ising-type antiferromagnetic order. In this presentation, we discuss the results of our first-principle calculations on the electronic structure and vibrational spectrum of monolayer FePS3. The calculations are compared with the experimental Raman spectra that exhibit several new peaks emerging below the Néel temperature. We demonstrate that the drastic changes in the Raman spectra can be understood in terms of the zone-folding effects, which suggests that monolayer FePS3 exhibits intrinsic anti-ferromagnetic order.

DS 32: Focussed Session: Oxide Semiconductors for Novel Devices II

Wide band gap semiconducting oxides such as the group-III sesquioxides find potential application in e.g. UV- or deep UV-sensors, transparent photovoltaic devices, power electronics or quantum well infrared photo detectors. This session sets a focus on growth of binary bulk material and thin films, the physical properties of these and their surface, properties of heterostructures and interfaces and the fabrication and performance of demonstrator devices.

Organizers: Oliver Bierwagen (PDI Berlin) and Holger von Wenckstern (U Leipzig)

Time: Wednesday 14:45–17:45 Location: CHE 89

Topical Talk DS 32.1 Wed 14:45 CHE 89
Defect induced magnetic or optical properties in gallium-based oxides — •Laurent Binet and Didier Gourier — Chimie-ParisTech, Paris, France

Gallium based oxides such as Ga2O3 and ZnGa2O4 are wide-gap transparent conducting oxides, which have been receiving a growing interest. Indeed, their electrical, optical and magnetic properties can be tuned by intrinsic defects or doping.

In Ga2O3, the magnetic interaction between the delocalized electron spins released by intrinsic shallow donors and the gallium nuclear spins results in an original memory effect, the so-called bistable conduction electron spin Resonance, which is based on a bistable dynamic nuclear polarization. This effect appears in the magnetic resonance of the conduction electrons as the possibility of switching between two different resonance states by acting on the external magnetic field, the microwave power or the temperature.

In ZnGa2O4, which shares some common features with Ga2O3, intrinsic defects are able to store a fraction of the excitation energy of Cr3+ dopants, which is responsible of a long persistent luminescence of Cr3+ in the red-near infrared. This unprecedented property can be applied to in vivo optical imaging of tumours.

DS 32.2 Wed 15:15 CHE 89
Photo- and electroluminescence of chromium doped β-Ga_2O_3 — •Andreas Fiedler, Zbigniew Galazka, and Klaus Irmscher — Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin, Germany

Chromium doped β-Ga_2O_3 single crystals were grown by the Czochralski method. The Cr doping produces a greenish coloration of the crystal, which results from two broad absorption bands centered at wavelengths of about 450 nm and 600 nm, respectively. Similar absorption bands are well know from Al_2O_3:Cr (ruby) and assigned to Cr^{3+} on Al site. This suggest that in the β-Ga_2O_3:Cr crystals Cr prefers Ga site occupation in the Cr^{3+} oxidation state. In analogy to ruby, we also see the characteristic red photoluminescence (PL) line due to an intra-center transition of Cr^{3+}. The PL line of ruby at 694.3 nm is shifted to 695.6 nm in β-Ga_2O_3:Cr due to the different ligand field. The PL was characterized between 4.2 K and 300 K. With increasing temperature an increasing broadening of the PL peak occurs. The excited state has a lifetime of $160\,\mu$s at room temperature, which makes it possible to generate a population inversion. In contrast to ruby, our β-Ga_2O_3 is semiconducting, hence an electroluminescence can be generated by electron impact excitation, which shows two transitions at 695.1 nm and at 696.2 nm. The beat frequency of these transitions is 0.7 THz, which is in the so called terahertz gap. This may be used for a terahertz laser, which opens a new field of applications for β-Ga_2O_3 beside the power devices and the photo detectors.

Topical Talk DS 32.3 Wed 15:30 CHE 89
Vacancy defects and electrical compensation in gallium oxide — •Filip Tuomisto — Aalto University, Espoo, Finland

Ga_2O_3 has recently generated significant interest and high quality growth (both thin-film and bulk) has been achieved with several techniques. Its distinctive feature compared to other transparent semiconducting oxides is the high transparency all the way to UV thanks to a wide 4.9 eV band gap. Hence this material has potential applications in future UV devices and high power electronics. n-type doping is achieved with Sn and Si, and highly resistive material can be produced by doping with Fe and Mg. p-type doping is yet to be achieved. Ga vacancies have been shown to act as efficient compensating centers in n-type material. In order use Ga_2O_3 as a semiconductor in electronics, detailed understanding and control of defects and doping are required. In this work, we analyze the formation mechanisms of Ga vacancies with positron annihilation spectroscopy in Ga_2O_3 thin films. We show that the choice of substrate, growth conditions and n-type dopant all have a dramatic effect on the efficiency of Ga vacancy formation and hence on the electrical properties of thin-film Ga_2O_3.

DS 32.4 Wed 16:00 CHE 89
Localized defect states and charge trapping in Al_2O_3 films prepared by atomic layer deposition — •Karsten Henkel, Malgorzata Kot, and Dieter Schmeisser — BTU Cottbus-Senftenberg, Angewandte Physik-Sensorik, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

The evaluation of the electronic structure and intrinsic defect mechanisms in Al_2O_3 thin films is essential for their effective use in applications with desired functionality such as surface passivation schemes for solar cells [1]. We present a comparative study of different Al_2O_3 films grown by atomic layer deposition (ALD) [2]. The layers were deposited on different substrates using the same aluminum precursor (TMA, trimethylalumium) and employing different process parameters (thermal-ALD, plasma-enhanced-ALD, substrate temperature). These films were characterized by resonant photoelectron spectroscopy and by electrical measurements (capacitance-voltage). For all films investigated intrinsic defect states within the electronic band gap were observed including excitonic, polaronic, and charge-transfer defect states, where their relative abundance is subject of the choice of ALD parameters and of the used substrate. The spectroscopic assigned in-gap defect states are related with electronic charges as determined in the electrical measurements. [1] G. Dingemans and W.M.M. Kessels, J. Vac. Sci. Technol. A 30, 040802 (2012). [2] K. Henkel, M. Kot, D. Schmeißer, J. Vac. Sci. Technol. A 35, (2017), accepted.

15 min. break.

Topical Talk DS 32.5 Wed 16:30 CHE 89
Integration of Oxide Semiconductors with Traditional Semiconductors - A New Twist — •Scott Chambers — Pacific Northwest National Laboratory, Richland, Washington, USA

Over the past two decades, a significant amount of research has been carried out on the integration of oxides with Si and various III-V semiconductors, most notably GaAs. In much of this work, the emphasis has been on the development of new gate dielectrics. However, other efforts have looked into the discovery and utilization of novel functional oxides as more active components in devices. In contrast, Ge has received relatively little attention. Yet, Ge has many highly desirable properties, including high electron and hole mobilities and a small bandgap. The latter is of particular interest for visible light harvesting applications, such as water splitting.

In this talk, I will present our recent work on the MBE growth and properties of SrZrxTi1-xO3 (SZTO) on p-Ge(001), a system with considerable potential as a photocathode for the hydrogen evolution reaction associated with water splitting. As-grown SZTO is typically n-type due to the formation of oxygen vacancies resulting from the low O2 partial pressure required to prevent oxidation of the Ge substrate during MBE growth. I will present our investigation of band alignment at the n-SZTO/p-Ge heterojunction via high-energy-resolution x-ray photoemission spectroscopy (XPS), along with preliminary results on water chemistry with the SZTO surface by means of ambient-pressure XPS and in situ photoelectrochemistry.

DS 32.6 Wed 17:00 CHE 89
Growth-control of the ordered double-perovskite stucture in $(Pr_{0.5}Ba_{0.5})CoO_{3-\delta}$ thin films — •Felix Gunkel[1], Clemens Hausner[2], David N. Müller[2], Lei Jin[2,3], Chunlin Jia[2,3], Daniel Bick[1], Theo Schneller[1], Ilia Valov[2], and Regina Dittmann[2] — [1]Institute of Electronic Materials (IWE2), RWTH Aachen University — [2]Peter Grünberg Institut, Forschungszentrum Jülich GmbH —

[3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Jülich

The complex oxide compound $(Pr_{0.5}Ba_{0.5})CoO_{3-\delta}$ (PBCO) is considered as an efficient catalytic oxide for oxygen evolution half-reaction (OER) taking place during water splitting operation. We discuss structural and electrical properties of epitaxial PBCO thin films serving a model systems for exploring atomistic processes during OER. PBCO thin films are synthesized in a disordered and in an ordered double-perovskite crystal structure by controlling the growth temperature during pulsed laser deposition. The thin films show defined surface morphology and crystal orientation. During the growth process, the transition from disordered to ordered phase can be monitored directly by means of electron diffraction (RHEED). The epitaxial thin films show catalytic activity comparable to their porous counter parts fabricated by chemical routes, making them ideal model templates for systematic studies. The ability to control the ordered double-perovskite phase of PBCO bears the potential to force the formation of structural oxygen vacancies within the lattice with atomic precision and to tailor active sites for OER on the nanoscale.

DS 32.7 Wed 17:15 CHE 89

Influence of annealing on the conductivity and transparency of niobium doped titanium dioxide electrodes prepared by sol-gel and their function in organic solar cells — •Peter Fischer[1], Roland Rösch[2], Shahidul Alam[2], Ulrich Schubert[2], Harald Hoppe[2], and Edda Rädlein[1] — [1]TU Ilmenau, Inst. für Werkstofftechnik, Gustav-Kirchhoff-Str. 6, 98693 Ilmenau, Germany — [2]Friedrich-Schiller-Universität Jena, Center for Energy and Environmental Chemistry Jena, Philosophenweg 7a, 07743 Jena, Germany

In this work the conductivity and transmittance of niobium doped titanium dioxide (TNO) layers produced by sol-gel technique are investigated. The samples were coated by spin-coating. The thickness of the TNO was adjusted with different spin speeds. A pre-baking of the films on a hot plate at 80°C for one hour was performed. Further, the samples were heated in a rapid thermal processing furnace under different gas atmospheres, temperatures and time. The conductivity of the samples was measured using a four-point set-up and the transparency through a UV-VIS spectrophotometer. The best heating procedure was when the sample is annealed in an N2/H2 atmosphere to 1000°C for 10 minutes. In this case, a good sheet resistance of 181 Ω/Sq. was reached, which enables the use of the TNO processed with sol-gel as an electrode in optical devices. Finally, organic solar cells were manufactured using TNO as the electrode.

DS 32.8 Wed 17:30 CHE 89

Characterization of Unipolar Zinc-Tin-Oxide Devices — •Sofie Bitter, Peter Schlupp, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Exp. Physik II, Germany

Amorphous zinc-tin-oxide (ZTO) consists of naturally abundant, non-toxic elements only and can be deposited at room temperature with a tunable electron density between $10^{16}\,\mathrm{cm}^{-3}$ and $10^{19}\,\mathrm{cm}^{-3}$ and a mobility as high as $10\,\mathrm{cm}^2/\mathrm{Vs}$ [1,2]. Therefore, ZTO is a suitable material for low-cost, flexible, transparent transistors and thus low-cost and bendable electronic applications.

We present metal semiconductor field effect transistors (MESFETs) using amorphous ZTO as *n*-type channel. Room temperature long throw magnetron sputtering from a target with a composition of 67% SnO_2 and 33% ZnO was used to deposit the ZTO channel [3]. On/Off ratios of 10^5 are achieved for reactive sputtered Pt gate contacts. The stability of the MESFETs under positive and negative bias stress is investigated. Further, an aging of unipolar devices based on ZTO is reported, which increases the on/off ratio of the devices.

[1] Bitter et al., ACS Comb. Sci., **18**, 4, 2015.
[2] Jayaraj et al., J. Vac. Sci. & Technol. B, **26**, 2, 2008.
[3] Frenzel et al., Physica Status Solidi (a), **212**, 7, 2015.

DS 33: Transport: Topological Semimetals 2 (jointly with MA/TT)

Time: Wednesday 15:00–17:45 Location: HSZ 204

DS 33.1 Wed 15:00 HSZ 204

Topological properties of magnetic semi-metals with non-symmorphic symmetries — •Andreas P. Schnyder — Max Planck Institute of Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart

Topological semi-metals exhibit band crossings near the Fermi energy, which are protected by the non-trivial topological character of the wave functions. In many cases, these topological band degeneracies give rise to exotic surface states and unusual magneto-transport properties. In this talk, I will discuss this physics in the context of *magnetic* semi-metals with non-symmorphic symmetries. In particular, I will show that non-symmorphic symmetries of cubic magnetic space groups lead to protected four-fold degenerate Dirac points and Dirac lines. As a concrete example, I will examine the topological properties of the antiferromagnet $CuBi_2O_4$ in terms of a low-energy tight-binding model, derived from ab-initio DFT calculations. I will discuss the monopole charges and the associated surface states of this system.

DS 33.2 Wed 15:15 HSZ 204

Density wave instabilities and surface state evolution in interacting Weyl semimetals — Manuel Laubach[1], Chrstian Platt[2], Ronny Thomale[3], Titus Neupert[4], and •Stephan Rachel[1] — [1]TU Dresden — [2]Stanford University — [3]University of Würzburg — [4]University of Zürich

We investigate the interplay of many-body and band structure effects of interacting Weyl semimetals (WSM). Attractive and repulsive Hubbard interactions are studied within a model for a time-reversal-breaking WSM with tetragonal symmetry, where we can approach the limit of weakly coupled planes and coupled chains by varying the hopping amplitudes. Using a slab geometry, we employ the variational cluster approach to describe the evolution of WSM Fermi arc surface states as a function of interaction strength. We find spin and charge density wave instabilities which can gap out Weyl nodes. We identify scenarios where the bulk Weyl nodes are gapped while the Fermi arcs still persist, hence realizing a quantum anomalous Hall state.

DS 33.3 Wed 15:30 HSZ 204

Experimental observation of type-II Weyl states in $TaIrTe_4$ — •Erik Haubold[1], Klaus Koepernik[1], Dmitriy Efremov[1], Seunghyun Khim[2], Alexander Fedorov[1,3], Yevhen Kushnirenko[1], Jeroen van den Brink[1,4], Sabine Wurmehl[1,4], Bernd Büchner[1,4], Timur Kim[5], Moritz Hoesch[5], Kazuki Sumida[6], Kazuaki Taguchi[6], Tomoki Yoshikawa[6], Akio Kimura[6], Taichi Okuda[7], and Sergey Borisenko[1] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]MPI CPfS, 01187 Dresden, Germany — [3]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany — [4]Department of Physics, TU Dresden, 01062 Dresden, Germany — [5]Diamond Light Source, Didcot OX11 0DE, United Kingdom — [6]Graduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan — [7]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

Weyl semimetals have raised a lot of interest lately due to their interesting exotic surface states. $TaIrTe_4$, belonging to the recently introduced class of type-II Weyl semimetals, hosts 4 Weyl points. These are well separated in the Brillouin zone and connected by rather long and parralel Fermi Arcs, making the material especially interesting for further research and future applications. In this work we find direct correspondence between theoretical predictions and ARPES results for both bulk and the surface states. Remarkably, these surface states are spin polarized, highlighting the potential for novel applications.

DS 33.4 Wed 15:45 HSZ 204

Magneto-optical infrared studies of the Weyl semimetals TaAs, TaP and NbP — D. Neubauer[1], R. Kemmler[1], W. Li[1], R. Hübner[2], A. Löhle[1], M. Schilling[1], M. Schmidt[3], C. Shekhar[3], C. Felser[3], M. Dressel[1], and •A. V. Pronin[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]FMQ, Universität Stuttgart, Germany — [3]MPI CPfS, Dresden, Germany

We have investigated the infrared response of TaAs, TaP, and NbP in zero magnetic field and in fields of up to 30 T. Additionally, magneto-transport measurements have been conducted on the same samples. In all compounds, we can reliably trace the transitions between different

Landau levels. The transition frequencies demonstrate a square-root field dependence, typical for the linearly dispersed bands. In TaP, we can also see a sizeable shifting of the plasma edge in magnetic field and an interplay between this plasma-edge shift and the Landau-level transitions. We compare the optical spectra of the three compounds, describe the spectra by the recent models for the (magneto)-optical response of Weyl semimetals, and extract such parameters as the Fermi velocities of the carriers in the Weyl bands and the positions of the Fermi levels relative to the Weyl points.

DS 33.5 Wed 16:00 HSZ 204

Emergent Weyl fermion bulk excitations in TaP evidenced from ^{181}Ta quadrupole resonance — H. Yasuoka[1,2], T. Kubo[1,3], Y. Kishimoto[1,3], D. Kasinathan[1], M. Schmidt[1], B. Yan[1], Y. Zhang[4], H. Tou[3], C. Felser[1], A.P. Mackenzie[1,5], and •M. Baenitz[1] — [1]MPI for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Japan — [3]Department of Physics, Graduate school of Science, Kobe University, Kobe, Japan — [4]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [5]SUPA, School of Physics & Astronomy, University of St. Andrews, UK

The monophosphite TaP has a non centrosymmetric structure and sizable spin orbit coupling and belongs the class of Weyl semimetals. A crossing of lineare dispersive ($E \propto k$) topologically protected polarized bands in a single point in reciprocal space defines the Weyl node where the fermion mass vanishes theoretically and a giant orbital hyperfine coupling is expected [1]. ^{181}Ta quadrupole resonance (NQR) resolves three NQR lines associated to the split level transitions for I=7/2 Ta. The spin lattice relaxation was measured for the $\pm 5/2 \leftrightarrow \pm 3/2$ transition. Above 30 K, a pronounced $(1/T_1T) \propto T^2$ is found. We attributed this to the magnetic excitations of Weyl fermions ($N(E) \propto E^2$) with temperature dependent orbital hyperfine coupling in agreement with the prediction from theory [1].

[1] Z. Okvatovity et al., arXiv:1609.3370v1

15 min. break.

DS 33.6 Wed 16:30 HSZ 204

Magnetic Properties of Dirac Fermions in a Family of Anti-perovskites — •Moritz Mandes Hirschmann and Andreas Philipp Schnyder — Max Planck Institute for Solid State Research, Stuttgart, Germany

We study the magnetic properties of the anti-perovskite materials A$_3$EO, where A denotes an alkaline earth metal, while E stands for Pb or Sn. The low-energy electronic properties of this family of anti-perovskites is described by three-dimensional Dirac fermions, which are gapped out by spin-orbit coupling [1-3]. We discuss the magnetic response of this Dirac electron system, considering both orbital and spin Zeeman effects. Interestingly, a strong Zeeman field splits the gapped Dirac cones into ungapped Weyl points, which are protected by a quantized Chern number. The compound Eu$_3$PbO breaks in its ferromagnetic phase intrinsically the time-reversal symmetry by exhibiting a magnetization that corresponds to a large Zeeman splitting at the Europium atoms. Again we observe Weyl points in the band structure. Using a tight-binding description we calculate these Chern numbers and demonstrate that the Weyl points are connected by Fermi arcs in the surface Brillouin zone. Furthermore, we determine the Landau level structure of the gapped Dirac electrons.

[1] T. H. Hsieh, J. Liu, and L. Fu. *Phys. Rev. B*, 90:081112, Aug 2014

[2] J. Nuss, C. Mühle, K. Hayama, V. Abdolazimi, and H. Takagi. *Acta Crystallographica Section B*, 71(3):300-312, Jun 2015.

[3] D. Samal, H. Nakamura, and H. Takagi. *APL Mater.*, 4(7), 2016.

DS 33.7 Wed 16:45 HSZ 204

Emergent Weyl points from Floquet Weyl semimetals in the resonant limit — •Leda Bucciantini[1], Stithadi Roy[1], Sota Kitamura[2], and Takashi Oka[1] — [1]Max Planck Institute for Physics of Complex Systems, Germany — [2]Tokyo University, Japan

We investigate the formation of Weyl points from a Dirac semimetal after shining it with circularly polarized light, focusing on the resonant frequency limit. Within a Floquet formalism, we describe the phase diagram as a function of the intensity and frequency of the laser. A couple of Weyl points split both from the original Dirac point and from the Floquet side bands. Increasing the value of the laser intensity, the Weyl points emerging from the original Dirac point and the side band merge, annihilate and then gap out. We also compute the monopole charge for each of the emergent Weyl points.

DS 33.8 Wed 17:00 HSZ 204

Self-forming superconducting microstructures from Weyl semi-metals — •Maja D. Bachmann[1], Nityan Nair[3], Felix Flicker[3], Roni Ilan[3], Nirmal J. Ghimire[2], Eric D. Bauer[2], Filip Ronning[2], James G. Analytis[3], and Philip J.W. Moll[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Los Alamos National Laboratory, Los Alamos, NM, USA — [3]Department of Physics, University of California Berkeley, CA, USA

The non-trivial topology of the bulk bands in topological semi-metals protects new electronic states at the surface, such as the famous Fermi arc states. If a superconducting gap is induced in these materials, exotic electronic states are expected to appear at the interface such as zero-energy Majorana modes. These novel states provide insights into the topological aspects of electronic matter and are of interest for quantum coherent applications. Here we will present a new route to reliably fabricating superconducting microstructures from the intrinsically non-superconducting Weyl semi-metals NbAs and TaAs under ion irradiation. The large difference in the surface binding energy of Nb/Ta and As leads to a natural enrichment of Nb/Ta at the surface during ion milling, forming a superconducting surface layer (Tc~3.5K). Being formed from the target crystal itself, the ideal contact between the superconductor and the bulk enables an effective gapping of the nodes due to the proximity effect. Simple low energy ion irradiation may thus serve as a powerful tool to fabricate topological quantum devices from mono-arsenides, even on an industrial scale.

DS 33.9 Wed 17:15 HSZ 204

Angle-dependent magnetoresistance in Weyl semimetals with long-range disorder — •Jan Behrends[1] and Jens H Bardarson[1,2] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]Department of Theoretical Physics, KTH Royal Institute of Technology, Stockholm, SE-106 91 Sweden

The chiral anomaly is one of the most intriguing features of Weyl semimetals. It states that left- and right-handed fermions are not conserved individually, while their sum is. One of its experimental consequences is the negative magnetoresistance predicted in Weyl semimetals. Recent experiments show strong indications for such an anomalous conductivity response, while some outstanding issues remain. Most prominently, the anomalous response is much more sharply peaked for parallel magnetic and electric fields than expected from simple theoretical considerations. Here, we investigate scattering in Weyl semimetals in presence of magnetic fields for a correlated disorder potential. We find a decrease of the internode relaxation time when the magnetic field is tilted away from the separation of the Weyl nodes. Since the internode relaxation time is proportional to the anomaly-related conductivity, this feature may explain the narrow current plume seen experimentally.

DS 33.10 Wed 17:30 HSZ 204

Surface states in holographic Weyl semimetals — •Markus Heinrich, Amadeo Jimenez-Alba, Sebastian Möckel, and Martin Ammon — Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena

Weyl semimetals (WSMs) are a class of gapless topological materials with low-energy excitations behaving as Weyl fermions. Their most prominent feature are topologically protected surface states, so-called Fermi arcs, which were recently tied to an effective axial magnetic field arising at a surface due to lattice deformations. As in the chiral magnetic effect, this field gives rise to an anomalous current at finite chemical potential which is localised at the surface. We performed its subtle computation in the strong coupling limit by using a holographic model. We found a non-trivial unversality of the current, allowing us to interpret it in a simple Fermi arc-like picture. In the end, I will discuss the limits of this universality.

DS 34: Organic Thin Films II

Time: Wednesday 15:00–17:00 Location: CHE 91

DS 34.1 Wed 15:00 CHE 91

Crystallinity and Degradability of Nano- and Microscaled Biopolymer Thin Films — Preetam Anbukarasu[1], Dominic Sauvageau[1], and •Anastasia Elias[1,2] — [1]Chemical and Materials Engineering, University of Alberta, Edmonton, Canada — [2]Leibniz-Institut für Polymerforschung Dresden e. V.

Enzymatically-degradable polymer thin films are attractive for biomedical, packaging, micro-electronic and agricultural applications. The stability and degradability of these materials are known to depend on both the parameters under which they are processed, and on the environmental conditions under which degradation occurs. Processing conditions are especially relevant for semi-crystalline polymers, since the degree of crystallinity of a material is an important determinant of its degradability.

In this work, we examine the effect of nano-scale dimensional constraint on the crystallinity and enzymatic degradability of polyhydroxybutyrate (PHB), a biopolymer. The physical properties of solution-cast PHB films of varying thicknesses were examined by atomic force microscopy (AFM, lamella orientation & surface profile) and x-ray diffraction (XRD, crystallinity & crystal anisotropy). The enzymatic degradability was tested using a diffraction grating-based optical sensor. We found that as the thickness of the samples was reduced from 5 um to less than 100 nm, the crystallinity of the films decreased, while the rate of degradation increased. However, below 100 nm, surprisingly slow degradation rates were observed. This occurs due to the fact that these films are amorphous, inhibiting the binding of the enzymes.

DS 34.2 Wed 15:15 CHE 91

Determination of the molecular orientation in absorptive organic thin films — •Christian Hänisch, Simone Lenk, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics

The overall efficiency of organic light-emitting diodes (OLEDs) is mainly limited by the high refractive index of the organic layers causing a trapping of large portions of the initially emitted light. Using emitter molecules with transition dipole moments parallel to the interface planes of an OLED reduces this loss channel and hence, increases the outcoupling efficiency of the device. The orientation of the molecules' transition dipole moments can be determined by angular resolved photoluminescence spectroscopy.

We investigate the impact of the organic layer's absorption on the determined orientation value by evaluating the emission spectra of single organic layers with thicknesses up to 150 nm. Numerically, these emission layers are represented by a set of radiating electrical dipoles which are homogeneously distributed over the whole layer. To represent the absorption of the excitation light, the single dipoles are weighted by an exponential function according to the Beer-Lambert law.

Using this method, we can show that the orientation parameter of the red phosphorescent emitter Ir(MDQ)$_2$(acac) doped into NPB is stable over a time range of several months at temperatures between room temperature and 80°C which is only 5% below the glass transition temperature of NPB.

DS 34.3 Wed 15:30 CHE 91

Interface-Controlled DNTT Thin Films: Growth, Morphology, and Temporal Evolution — •Andrea Karthäuser[1], Tobias Breuer[1], Hagen Klemm[2], Francesca Genuzio[2], Gina Peschel[2], Alexander Fuhrich[2], Thomas Schmidt[2], and Gregor Witte[1] — [1]FB Physik, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Abt. Chemische Physik, FHI der MPG, 14195 Berlin, Germany

The high charge carrier mobility and chemical stability of dinaphthothienothiophene (DNTT) render this new organic semiconductor (OSC) especially interesting for organic field effect transistors (OFETs) [1, 2]. Despite such device advances, the structure and morphology of DNTT thin films are so far rather unexplored. On the prototypical substrates $\mathrm{SiO_2}$ and graphene we prove a substrate-mediated control of the molecular orientation by means of NEXAFS and XRD measurements. Furthermore, by using atomic force microscopy (AFM) and photoelectron emission microscopy (PEEM) we analyzed the morphology of DNTT films with variable thicknesses and find a temporal dewetting of these films. This pronounced island formation leads to a breakup of the film which is most efficient for thin films of a few monolayers. Finally we have extend this study also to device relevant substrates by analyzing DNTT films that were grown on SAM treated dielectrics. Again a district dewetting is found, which is expected to affect the long-term performance of DNTT devices and appears surprising in view of the reported long term stability of DNTT-OFETs [2].

[1] Yamamoto, T.; J. Am. Chem. Soc. (2007), 129,224. [2] Zschieschag, U.; Org. Electron. (2013), 14, 1516.

DS 34.4 Wed 15:45 CHE 91

Direct photo alignment and optical patterning: Controlling molecular thin film growth on the meso-scale — •Linus Pithan[1,3], Paul Beyer[1], Laura Bogula[1], Anton Zykov[1], Peter Schäfer[1], Jonathan Rawle[2], Chris Nicklin[2], Andreas Opitz[1], and Stefan Kowarik[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Berlin, Germany — [2]Diamond Light Source, Didcot, UK — [3]ESRF, Grenoble, France

A novel strategy for direct photoalignment of molecular materials using optothermal re-orientation is introduced. We show that it is possible to fabricate anisotropic and photolithographically patterned organic molecular thin films based on light-directed molecular self-assembly (LDSA).[1]

Growing tetracene thin films via LDSA on amorphous silica, we employ 532 nm laser illumination, which matches the lower Davydov absorption band, to induce preferential orientations of molecular crystal grains. Based on grazing incidence X-ray diffraction (GIXD) as well as optical spectroscopy we determine a threshold laser power for azimuthal alignment. The patterning and polarized light emission that is possible with LDSA is important for applications such as polarized organic light emitting diodes or photonic metasurfaces.

[1] L. Pithan et. al. Adv. Mater. doi:10.1002/adma.201604382

DS 34.5 Wed 16:00 CHE 91

Modern *in situ* real-time X-ray scattering and nucleation theory for an enhanced understanding of molecular self-assembly — •Anton Zykov[1], Sebastian Bommel[1,2], Yves Garmshausen[3], Linus Pithan[1,4], Paul Beyer[1], Gonzalo Santoro[5], Stefan Hecht[3], Jürgen P. Rabe[1], and Stefan Kowarik[1] — [1]Inst. f. Physik, Humboldt-Universität zu Berlin — [2]DESY, Hamburg — [3]Inst. f. Chemie, Humboldt-Universität zu Berlin — [4]ESRF, Grenoble, France — [5]Inst. de Ciencia de Materiales de Madrid, CSIC, Spain

Quantifying nanoscale processes that drive the self-assembly of organic molecules into functional thin films is the prerequisite to understand and steer structure formation. In a study on the growth of PTCDI-C_8 we unravel a remarkable layer-dependent molecular diffusion behaviour from an innovative simultatineous *in situ* acquisition of X-ray reflectivity growth oscillations and diffusively scattered X-rays and the application of state-of-the-art nucleation theory. This allows us to determine nucleation energies, critical cluster sizes and attempt frequencies.[1] These quantities can be strongly influenced when applying chemical tuning to well-known molecules. We showcase this on the example of the growth of 6P and 6PF2. As a result of the fluorination we achieve a significant film smoothening as desired for applications, where an efficient in-plane charge carrier transport is of importance.

[1]A. Zykov *et al.*, J. Chem. Phys. 146, 052803 (2017)

DS 34.6 Wed 16:15 CHE 91

Modeling of singlet fission in weakly-interacting acene molecules — Sharareh Izadnia[1], David W. Schönleber[2], •Alexander Eisfeld[2], Alexander Ruf[1], Aaron C. LaForge[1], and Frank Stienkemeier[1] — [1]Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden

Singlet fission, a process in which a singlet excited state is converted into two triplet states, is a means to circumvent the Shockley-Queisser limit for energy conversion in solar cells. In a recent experiment, singlet fission was observed in a disordered system where organic chromophores are distributed on the surface of a rare gas cluster. Here we give details on the theoretical modeling of singled fission in this system. Our kinematic model explicitly takes into account the details of the geometrical arrangement of the system as well as the time-dependent populations of the relevant states of each molecule. Using this model, which goes beyond usual mean-field treatment, we study the trends obtained by singlet fission, exciton-exciton annihilation, and singlet hopping on the experimental observables. Our simulations support the conclusion of the experimental observation that SF is present even at weakly interacting conditions.

DS 34.7 Wed 16:30 CHE 91

Ultra-robust thin film devices from metal-terpyridine wires — •Florian von Wrochem[1], Maria Anita Rampi[2], and Wolfgang Wenzel[3] — [1]Materials Science Laboratory, Stuttgart — [2]Dipartimento di Chimica, Universita' di Ferrara — [3]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany

Considerable efforts have been undertaken within the past decades to shift organic-based thin-film devices from basic research to the application level. A major hurdle is given by the thermal deposition of the metal electrodes, which remained elusive due to the damage and the electrical shorts experienced by the fragile molecular layers. Here, we show that large area molecular junctions of outstanding electronic properties and robustness can be realized using densely packed molecular wires consisting of FeII-terpyridine complex oligomers, despite a conventional fabrication process involving top electrode evaporation directly on the molecular layer. Surprisingly, these oligomer-based devices are stable for over 2 years under regular current-voltage cycling, withstanding a wide range of temperatures (150-360 K) and applied voltages (3 V). Electrical studies in conjunction with ab-initio calculations reveal that charge transport (i) occurs via electron (hopping) conduction and is limited by the charge injection through a Shottky barrier (0.72 eV), following Richardson-Schottky injection.

DS 34.8 Wed 16:45 CHE 91

Superradiance from two dimensional brick-wall aggregates of dye molecules: the role of size and shape for the temperature dependence — •Alexander Eisfeld[1], Christian Marquardt[2], and Moritz Sokolowski[2] — [1]MPI-PKS — [2]Uni Bonn

Aggregates of interacting molecules can exhibit electronically excited states which are coherently delocalized over many molecules. This can lead to a strong enhancement of the fluorescence decay rate which is referred to as superradiance (SR). To date, the temperature dependence of SR is described by a $1/T$ law. Using an epitaxial dye layer and a Frenkel-exciton based model we provide both experimental and theoretical evidence that significant deviations from the $1/T$ behaviour can occur for brickwall-type aggregates of finite size leading even to a maximum of the SR at finite temperature. This is due to the presence of low energy excitations of weak or zero transition strength.

DS 35: 2D Materials Beyond Graphene IV (jointly with O)

Time: Wednesday 15:00–17:45 Location: WIL A317

Invited Talk DS 35.1 Wed 15:00 WIL A317

Carbon Nanomembranes (CNM) : 2D Materials Beyond Graphene — •Armin Gölzhäuser — Universität Bielefeld, Physik Supramolekularer Systeme und Oberflächen, Universitätsstr. 25, 33615 Bielefeld

Carbon Nanomembranes (CNMs) are thin (~1nm), synthetic two-dimensional (2D) layers or sheets with tailored physical, chemical or biological function [1]. Their fabrication scheme utilizes a sequence of molecular monolayer assembly on a solid surface and radiation induced cross-linking in two dimensions. The cross-linked 2D-layer is then released from the surface, forming a self-supporting nanomembrane with properties that are determined by properties of the monolayer. Depending on the desired applications, CNMs can be engineered with a controlled thickness, elasticity and surface functionalization. Helium ion microscopy, spectroscopic methods and functional tests are applied to investigate the structure and composition as well as permeation properties. Helium Ion Lithography is used the fabrication of well-defined nanopores [2] and perforated CNMs are tested as ballistic membranes for the separation of gases and liquids.

[1] A. Turchanin and A. Gölzhäuser: Carbon Nanomembranes, Adv. Mater. 28, 6075 (2016).

[2] D. Emmrich, A. Beyer, A. Nadzeyka, S. Bauerdick, J. C. Meyer, J. Kotakoski and A. Gölzhäuser: Nanopore fabrication and characterization by helium ion microscopy, Applied Physics Letters 108, 16310 (2016).

DS 35.2 Wed 15:30 WIL A317

A hybrid MoS2 material for nanopore sensing: interface and asymmetry — Ganesh Sivaraman[1], Fabio A.L. de Souza[2], Rodrigo G. Amorim[3,4], Wanderla L. Scopel[2], Ralph H. Scheicher[3], and •Maria Fyta[1] — [1]Institute for Computational Physics, Stuttgart University — [2]Departamento de Fisica, Universidade Federal do Espirito Santo, Brazil — [3]Department of Physics and Astronomy, Materials Theory, Uppsala University, Sweden — [4]Departamento de Física, Universidade Federal Fluminense, Brazil

An important class of 2D nanomaterials beyond graphene is the family of transition metal dichalcogenides (TMDs) such as molybdenum disulfide (MoS2). In MoS2 a semiconducting (2H) and a metallic (1T) phase can co-exist. We investigate the electronic and transport properties of a hybrid MoS2 monolayer composed by a 1T strip embedded in the 2H MoS2 phase. Using density functional theory based calculations with the non-equilibrium Greens functions (NEGF) approach, we study in detail the structural and electronic properties of hybrid MoS2 and its interface. A clear anisotropy in the electronic and transmission properties of the hybrid material was found and linked to the microstructure of its interfaces. We also show the relevance of such a material to sensing DNA with MoS2 nanopores. In order to understand the formation of this nanopore, a single point-defect analysis is performed also assessing the stability of the hybrid system and the different pore terminations. The current modulation around a nanopore when placing DNA in the pore manifests the strong potential of hybrid MoS2 in next generation biosensing devices.

DS 35.3 Wed 15:45 WIL A317

Semiconductor to Metal Transition in WS_2/Ag(111) — •Charlotte E. Sanders[1], Maciej Dendzik[1], Albert Bruix[1], Matteo Michiardi[2], Arlette S. Ngankeu[1], Marco Bianchi[1], Bjørk Hammer[1], Jill A. Miwa[1], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, Denmark — [2]Department of Physics and Astronomy, University of British Columbia, Canada

Substrate effects play an important role in determining electronic structure in two-dimensional materials (2DMATs). A common effect of a metallic substrate on a semiconducting 2DMAT is renormalization of the band gap, induced by metallic screening, as recently observed in MoS_2/Au(111) [1]. Here we report a substrate effect that goes beyond band gap change due to screening. For WS_2/Ag(111), hybridization between electronic states of Ag and WS_2 leads to a non-zero density of states at the Fermi level (FL), and thus to a transition of WS_2 from a direct band gap semiconductor to a metal. This is evidenced by the asymmetric lineshape observed in core-level photoemission spectra. It is associated particularly with the emergence of states at the FL near the Q point of WS_2, as can be seen in measurements by angle-resolved photoemission spectroscopy (ARPES). Meanwhile, ARPES and time-resolved ARPES confirm that the WS_2 conduction band minimum at K remains well defined and stays above the FL. Electronic structure calculations based on density functional theory shed further light on the reasons for these strong changes in band structure. [1] Phys. Rev. B 93, 165422 (2016)

DS 35.4 Wed 16:00 WIL A317

A many-body view on the not-so-passive role of the substrate: trions and screening in transition metal dichalcogenides — •Matthias Drüppel[1], Thorsten Deilmann[2], Peter Krüger[1], and Michael Rohlfing[1] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Center for Atomic-Scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The strongly enhanced Coulomb interaction due to reduced dimensionality has established transition metal dichalcogenides (TMDC) as promising candidates for next-generation opto-electronic devices. However, in almost all experiments and applications, the monolayer is deposited on a substrate for mechanical stability or - in bulk/few layer materials - interacts with neighboring layers. In this talk we show that the surrounding of the monolayer does *not* play a passive role. In contrast, it distinctly modifies the TMDC excitations.

We subsequently apply DFT → GW → Bethe-Salpeter equation (BSE) to access the optical properties. Our results show how additional charge carriers, that are often induced by substrates, lead to trion formation that might dominate optical spectra. We take our *ab-initio* approach and directly compare trion and exciton spectra, finding that trions split into inter- and intra-valley trions. Additionally, a drastically enhanced screening by a substrate renormalizes both the exciton and trion binding energies and the fundamental band gap. In bilayer and bulk materials, excitons can be excited with electron and hole located on different layers, forming inter-layer excitons.

DS 35.5 Wed 16:15 WIL A317

Simple Screened Hydrogen Model of Excitons in Two-Dimensional Materials — •Thomas Olsen, Simone Latini, Filip Rasmussen, and Kristian Thygesen — Technical University of Denmark

We present a generalized hydrogen model for the binding energies (E) and radii of excitons in two-dimensional (2D) materials that sheds light on the fundamental differences between excitons in two and three dimensions. In contrast to the well-known hydrogen model of three-dimensional (3D) excitons, the description of 2D excitons is complicated by the fact that the screening cannot be assumed to be local. We show that one can consistently define an effective 2D dielectric constant by averaging the screening over the extend of the exciton. For an ideal 2D semiconductor this leads to a simple expression for E that only depends on the excitonic mass and the 2D polarizability α. The model is shown to produce accurate results for 51 transition metal dichalcogenides. Remarkably, over a wide range of polarizabilities the binding energy becomes independent of the mass and we obtain $E = 3/4\pi\alpha$), which explains the recently observed linear scaling of exciton binding energies with band gap. It is also shown that the model accurately reproduces the non-hydrogenic Rydberg series in WS2 and can account for screening from the environment.

DS 35.6 Wed 16:30 WIL A317

Investigation of hexagonal boron-nitride (hBN) on SiC — •Markus Franke[1,2], François C. Bocquet[1,2], Janina Felter[1,2], and Christian Kumpf[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology, 52425 Jülich, Germany

Among 2D materials, hexagonal boron-nitride (hBN) seems to be a promising candidate for a new substrate material to achieve a highly ordered layer of free-standing graphene. It forms a flat hexagonal lattice structure with a lattice constant similar to that of graphene, but (in contrast to graphene) has a wide band gap ($> 5\,\mathrm{eV}$) and is therefore insulating. It should be free of charge traps and dangling bonds and its flat surface should prevent overlying 2D materials from corrugating.

Here, we report on the growth of hBN layers on the wide band gap semiconductor silicon carbide (SiC) by annealing SiC wafers in a borazine ($B_3N_3H_6$) atmosphere. The properties of this system are investigated by XPS, ARPES and HREELS.

DS 35.7 Wed 16:45 WIL A317

Plasmonic Superconductivity in Layered Materials — Malte Rösner[1,2], Roelof G. Groenewald[1], Gunnar Schönhoff[2], Jan Berges[2], Stephan Haas[1], and •Tim O. Wehling[2] — [1]Department of Physics and Astronomy, University of Southern California, USA — [2]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Germany

Due to a lack of screening in two dimensions the Coulomb interaction is generally enhanced and consequently plays a major role to understand many-body effects within layered materials. In the field of superconductivity it is usually introduced as an approximate, static, and adjustable parameter μ^* which describes only effectively the Coulomb repulsion which is therefore responsible for reduced transition temperatures.

Here, we overcome this inadequate handling and present an ab initio based material-realistic Coulomb description for doped single layers of MoS_2 which captures simultaneously material-intrinsic, substrate, and dynamical screening processes. Using this model we can reliably describe the resulting plasmonic excitations including both, their coupling to the electrons and their dependence on the environmental screening and doping level. Utilizing Eliashberg theory we show that the low-energy plasmonic modes originating from the dynamically screened Coulomb *repulsion* can actually lead to an effective Coulomb *attraction* and thus to an enhanced transition temperature (T_c). Furthermore, we find an optimal ratio between the substrate screening and the electron doping which maximizes T_c of the induced plasmonic superconducting state.

DS 35.8 Wed 17:00 WIL A317

MoS2 film conductivity change on periodically poled LiNbO3 substrate determined by nano-FTIR spectroscopy — •Piotr Patoka[1], Georg Ulrich[1], Peter Hermann[2], Bernd Kästner[2], Ariana Nguyen[3], Arne Hoehl[2], Ludwig Bartels[3], Peter Dowben[4], Gerhard Ulm[2], and Eckart Rühl[1] — [1]Physikalische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, Berlin, 10587, Berlin, Germany — [3]Dept. of Chemistry, Univ. of California Riverside, Riverside, CA 92521, USA — [4]Dept. of Physics and Astronomy, Univ. of Nebraska, Lincoln, Lincoln, NE 68588-0299 USA

Coupling of ultra-broadband synchrotron radiation from the Metrology Light Source (MLS) to a scattering-type scanning near-field optical microscope (s-SNOM) allows for contactless conductivity evaluation in the mid-infrared regime. The system is based on an atomic force microscope, such that the optical signal can be directly correlated with topographic information. Using this method, we investigated the influence of a ferroelectric substrate (LiNbO3) enhanced by its surface phonon on thin films of MoS2. Recent electric transport measurements suggest changes in the carrier density due to substrate polarization.[1] The present findings obtained from s-SNOM studies offer a complimentary way of contactless investigations of conductivity changes.[2]

[1] Nguyen, A. et al., Nano Lett. 15, 3364-3369 (2015).
[2] Hermann, P. et al., Opt. Express 21, 2913-2919 (2013).

DS 35.9 Wed 17:15 WIL A317

Band gap transition in few-layer ReS$_2$ investigated by photoemission k-space microscopy — •Mathias Gehlmann[1], Lukasz Plucinski[1], Slavomír Nemšák[1], Irene Aguilera[2], Gustav Bihlmayer[2], Pika Gospodarič[1], Markus Eschbach[1], Ewa Młyńczak[1], Giovanni Zamborlini[1], Vitaliy Feyer[1], Florian Kronast[3], Philipp Nagler[4], Tobias Korn[4], Christian Schüller[4], Stefan Blügel[2], and Claus Michael Schneider[1] — [1]PGI-6, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — [2]PGI-1/IAS-1, Forschungszentrum Jülich GmbH and JARA, D-52425 Jülich, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, D-12489 Berlin, Germany — [4]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

ReS_2 is a promising candidate for novel electronic and sensor applications. The low crystal symmetry of this van der Waals compound leads to highly anisotropic optical and vibrational behavior. However, the details of the electronic band structure of this fascinating material are still largely unexplored. We present a momentum resolved study of the electronic structure of monolayer, bilayer, and bulk ReS_2. Using photoemission k-space microscopy in combination with density functional theory calculations we demonstrate a significant 3D delocalization of the valence electrons in bulk ReS_2. Furthermore, we directly observe the evolution of the valence band dispersion in our photoemission experiments as a function of the number of layers, revealing a varying character of the band gap.

DS 35.10 Wed 17:30 WIL A317

Structural Analysis of h-BN on Cu(111) — •Martin Schwarz[1], Manuela Garnica[1], Jacob Ducke[1], Peter Deimel[1], David Duncan[2], Ari Seitsonen[3], Francesco Allegretti[1], Johannes Barth[1], and Willi Auwärter[1] — [1]Physik Department, Technische Universität München, James Franck Str. 1, 85748 Garching, Germany — [2]Diamond Light Source, Didcot, Oxfordshire, OX11 0DE, United Kingdom — [3]Département de Chimie, École Normale Supérieure, 24 rue Lhomond, F-75005 Paris, France

Atomically thin boron nitride (h-BN) layers on metallic supports represent promising platforms for the adsorption of atoms, clusters, and molecular nanostructures [1-2]. Specifically, STM studies revealed an electronic corrugation of h-BN/Cu(111), guiding the self-assembly of molecules and their energy level alignment. A comprehensive characterization of the h-BN/Cu(111) interface including the spacing between the h-BN sheet and its support - elusive to STM measurements - is crucial to rationalize the interactions within these systems. To this end, we employed complementary techniques including scanning tunneling microscopy (STM), high resolution atomic force microscopy

(AFM), low energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), X-ray standing wave (XSW) and density functional theory (DFT). Thus, our multi-method study yields a complete, quantitative structure determination of the sp2 bonded BN layer on Cu(111).

[1] Joshi, Sushobhan, et al. NL 12.11 (2012): 5821-5828
[2] Urgel, J. I. et al. JACS 137.7 (2015): 2420-2423

DS 36: Postersession I

Time: Wednesday 17:00–19:00 Location: P2-EG

DS 36.1 Wed 17:00 P2-EG

Interaction of oxygen with plasma-deposited Si:N:H primer coatings — •Lisa Wurlitzer[1], Sebastian Dahle[2], and Wolfgang Maus-Friedrichs[1,2] — [1]Clausthal Centre of Material Technology, 38678 Clausthal-Zellerfeld, Germany — [2]Insitute for Energy Research and Physical Technology

The coatings are applied in a two-step process which is carried out through dielectric barrier discharge (DBD) plasma treatments. The DBD plasma is used in the first processing step along with a gaseous mixture of silane and nitrogen to deposit the primer film. In the second processing step, the primer film is converted into a silicon oxide coating. Previous measurements show that this conversion yields stoichiometric silicon dioxide when employing a DBD plasma treatment in air or pure oxygen, while an exposure to air at atmospheric pressures without DBD plasma leads to a partial conversion of the film. This high reactivity against oxygen is now investigated by exposure to small vapor pressures of oxygen in an ultra-high vacuum chamber, again without a DBD plasma treatment. Photoelectron spectroscopy is employed to study the interaction of oxygen with the Si:N:H primer coating.

DS 36.2 Wed 17:00 P2-EG

Flexible, robust and conformal SERS active substrates for rapid trace detection of pesticides — •Samir Kumar and J P Singh — Department of Physics, Indian Institute of Technology Delhi

Silicon wafers and glass slides are two of the most common substrates used for the growth of SERS active layers. However, these substrates are rigid and brittle and hence, these static substrates severely limit the application of plasmonic nanostructures. The metal nanostructures deposited by using conventional techniques such as physical vapor deposition suffers from a low adhesion strength of Ag or Au on to silicon or glass substrates. Here, we demonstrate a simple and facile method for fabricating highly adhesive large area AgNRs arrays embedded in the PDMS film SERS-active, flexible and robust substrate for conformal and rapid extraction and detection of trace molecules. The AgNRs arrays were grown over Si(100) substrates by thermal evaporation of silver powder using glancing angle deposition (GLAD) technique. The AgNRs arrays were embedded in low index PDMS to achieve enhanced portability and mechanical stability. The embedded AgNRs layers show good adhesion onto the PDMS surface. The in situ SERS measurements on these flexible substrates under mechanical tensile strain conditions showed that flexible SERS substrates can withstand a tensile strain (ϵ) value as high as 30% without losing SERS performance. Through strongly enhanced Raman signals on the AgNRs embedded SERS substrate, pesticide thiram was effectively detected on apple peels at concentrations as low as 2.4×10^{-9} g/cm^2.

DS 36.3 Wed 17:00 P2-EG

Zig-zag silver nanorods with high density hotspots for surface enhanced Raman scattering — •Samir Kumar and J P Singh — Department of Physics, Indian Institute of Technology Delhi

In recent years, silver nanorod (AgNR) arrays fabricated by GLAD have attracted significant attention due to their high surface enhanced Raman spectroscopy (SERS) performance. For SERS, the major enhancement mechanism is due to the enhancement of localized electric field generated by metallic nanostructures. The SERS performance significantly depends upon the number of hotspots. On folding a nanorod into zig-zag structure can generate corners or bends and hence it enhances the SERS performance. Among the different types of hotspots nanogaps can tremendously enhance the SERS intensity. In this work, we investigated that the SERS intensity increases with number of hotspots. For this, different arms silver zig-zag nanostructures have been fabricated. Their SERS spectra revealed that the SERS performance can be improved on increasing the number of arms. Further, the role of nanogaps in silver zig-zag nanostructures has been studied. It is observed that the SERS intensity from nanogap zig-zag silver nanorods array is higher than from silver zig-zag nanostructures i.e. nanogaps contributed more in SERS enhancement. The SERS signals was investigated by using Raman probe molecule trans-1,2-bis(4-pyridyl)ethane (BPE). Our observations showed that the Ag zig-zag plasmonic structures with nanogaps between their arms produced extremely high SERS signal. This can be explained due to the plasmon coupling interaction between the Ag nanorods.

DS 36.4 Wed 17:00 P2-EG

Influence of 5-Ammoniumvaleric Acide Iodide on the Stability of Methylammonium Lead Halide Perovskite Films Grown on Zinc Oxide — •Georg Dewald[1,2], Martina Stumpp[1,2], Raffael Ruess[1,2], and Derck Schlettwein[1,2] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Justus-Liebig-University Giessen, Laboratory for Materials Science

As an alternative to TiO_2 in perovskite photovoltaics ZnO deserves closer attention as it possesses a higher conductivity. Further, ZnO can be prepared at low temperatures via electrochemical deposition. However, preparing $CH_3NH_3PbI_3$ directly on top of ZnO, leads to rapid degradation. Such stability problems could be addressed by adding 5-ammoniumvaleric acide iodide (AVAI) to $CH_3NH_3PbI_3$. AVA ions can form hydrogen bonds between the PbI_6 octahedrons of the perovskite and, therefore, influence the resulting morphology and electrical properties. Bond formation across the perovskite/ZnO interface is expected to stabilize it by hindering the deprotonation by the basic zinc oxide surface. In this study, $CH_3NH_3PbI_3$ and $(AVA)_x(CH_3NH_3)_{1-x}PbI_3$ films were prepared via spin-coating on ZnO, which was electrodeposited on micro-structured gold electrode arrays on SiO_2/Si wafers. The current-voltage curves of Au/ZnO/perovskite/ZnO/Au were measured during the annealing process at 100 °C by sweeping the voltage from -2 to +2 V in nitrogen atmosphere. SEM imaging was used to examine the influence of AVAI on the morphology of the perovskite films. The SEM images and I-V characteristics of films with and without 5-AVAI will be discussed.

DS 36.5 Wed 17:00 P2-EG

Electrochemical Deposition of Porous Nickel Oxide Films as Electrodes in Electrochromic Devices and Solar Cells — •Simon P. Schneider[1,2], Christian Lupo[1,2], and Derck Schlettwein[1,2] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Justus-Liebig-University Giessen, Laboratory for Materials Science

Nickel oxyhydroxide films were deposited onto transparent conductive oxide substrates via electrochemical deposition in an aqueous bath containing nickel sulfate and ammonia. The deposition was carried out using cyclic voltammetry in a three-electrode setup, where a Ag/AgCl-electrode was used as reference and a platinum sheet as counter electrode. After deposition, the films were treated at different temperatures to obtain porous nickel oxide. Furthermore, the concentrations and ratios of nickel sulfate and ammonia in the solution were adjusted to optimize the deposition. The film morphology was investigated using scanning electron microscopy revealing homogenously porous film surfaces and a high reproducibility. Different annealing temperatures and bath concentrations did not affect size and shape of the pores. However, the annealing temperature seems to have an influence on the oxidation state of nickel and thus on the optical properties of the films.

DS 36.6 Wed 17:00 P2-EG

Proof of the existence of Sn_3O_4 through Raman spectroscopy: a combined theoretical and experimental study — •Christian Heiliger[1], Bianca Eifert[1], Marcel Giar[1], Martin Becker[2], Christian T. Reindl[2], Lilan Zheng[3], Angelika Polity[2], Yunbin He[3], and Peter J. Klar[2] — [1]Institute of Theoretical Physics, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]I. Institute of Physics, Justus-Liebig-University, Heinrich-

Buff-Ring 16, 35392 Giessen, Germany — [3]Faculty of Materials Science and Engineering, Hubei University, Wuhan 430062, China

The existence of an intermediate phase within the tin oxide system was first reported in 1882. However, its stoichiometry and its crystal structure have been dubious and heavily debated ever since, despite a multitude of structural investigations. Here we show that a combined Raman spectroscopic investigation based on *ab initio* methods and experiments offers an alternative to diffraction studies, which are not conclusive for this material system. It allows us to unambigiuously identify the intermediate phase as Sn_3O_4 and to rule out the other likely candidate, Sn_2O_3. We assign the one-phonon Raman signals of Sn_3O_4 to the mode symmetries of the corresponding point group C_{2h} and confirm the space group as $P2_1/c$ with 14 atoms per unit cell.

DS 36.7 Wed 17:00 P2-EG

BFO based memristor as artificial synapse in machine learning circuits — •Mahdi Kiani[1], Nan Nu[1], Christian Mayr[2], Danio Bürger[1], Iluna Skrupa[1,3], Stefan Shultz[4], Oliver Schmidt[1,5], and Heidemarie Schmidt[1,4] — [1]Materials systems for nanoelectronics, chemnitz university of technology, chemnitz, germany — [2]Highly-parallel vlsi systems and neuro-microelectronics, technische universität dresden, dresden, germany — [3]Helmholtz-zentrum dresden-rossendorf, institute of ion beam Physics and materials research,dresden, germany — [4]Fraunhofer-Institut für Elektronische Nanosysteme, Abteilung Back-End of Line, Technologie, Chemnitz, Germany — [5]Institute for Integrative Nanosciences, IFW Dresden, Dresden, Germany

Neuromorphic engineering takes advantage of artificial neurons and artificial synapses to mimic the most complicated human attribute, learning. BiFeO3 memristor as artificial synapse and newly designed electronic circuit as artificial neuron are used to implement associative, supervised, unsupervised, and deep learning. Spike-timing dependent plasticity (STDP) with a single pairing of one presynaptic voltage spike and one postsynaptic voltage spike with different time delays for Long-term potentiation (LTP) which determine learning status and Long-term depression (LTD) where forgetting occurs and also number cycle dependent plasticity (NCDP) for both student and teacher artificial synapses are demonstrated

DS 36.8 Wed 17:00 P2-EG

An element specific investigation of the disorder induced phase transition in $Fe_{60}Al_{40}$ thin films driven by ion irradiation — •Benedikt Eggert[1], Enrico La Torre[1], Alevtina Smekhova[1,2], Thomas Szyjka[1], Rantej Bali[3], Katharina Ollefs[1,4], Soma Salamon[1], Fabrice Wilhelm[4], Rudra Banerjee[6], Andrei Rogalev[4], Eugen Weschke[5], Jürgen Lindner[3], Biplab Sanyal[6], Carolin Schmitz-Antoniak[2], and Heiko Wende[1] — [1]University of Duisburg-Essen and CENIDE, Duisburg — [2]FZ Jülich (PGI-6), Berlin — [3]HZDR, Dresden — [4]ESRF, ID12, Grenoble — [5]HZB (BESSY II), Berlin — [6]Uppsala University, Uppsala

Chemically ordered $Fe_{60}Al_{40}$ in the B2 structure shows weak ferromagnetism, while the disordered phase with the A2 structure exhibits a ferromagnetic state. Correspondingly the transition leads to an increase of the effective number of Fe-Fe nearest neighbors and of the lattice constant [1]. This phase transition can be driven by ion irradiation. In this work we investigate $Fe_{60}Al_{40}$ thin films before and after 10 and 20 keV Ne^+ irradiation by means of X-ray magnetic circular dichroism (XMCD) at the Fe $L_{2,3}$- and K-edge to analyze the microscopic magnetic structure. For a comparison magnetometry was used concerning the depth-profile of the induced magnetism [2,3]. These results are correlated to the modified structural properties.

[1] J. Fassbender et al. Phys. Rev. B 2008, 77, 174430
[2] R. Bali et al. Nano Lett. 2014, 14 (2), pp 435-441
[3] N. Tahir et al. Phys. Rev. B 2015, 92, 144429

DS 36.9 Wed 17:00 P2-EG

Spectroscopic Ellipsometry as a Method for Structural Investigation of Spinel Ferrite Thin Films — •Vitaly Zviagin[1], Yogesh Kumar[1], Paula Huth[2], Israel Lorite[1], Annette Setzer[1], Daniel Spemann[3], Karsten Fleischer[4], Jan Meijer[1], Reinhard Denecke[2], Pablo Esquinazi[1], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany — [2]Universtät Leipzig, Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Linnéstr. 2, Germany — [3]Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, Germany — [4]School of Physics, Trinity College Dublin, Dublin 2, Ireland

$ZnFe_2O_4$ and composite $Zn_xFe_{3-x}O_4$ thin films were deposited at different conditions on $SrTiO_3$ (100) and MgO (100) substrates by pulsed laser deposition. Features in the diagonal elements of the dielectric tensor, obtained by spectroscopic ellipsometry, hint to the presence of Fe^{2+} and Fe^{3+} cations located within the lattice by assignment of electronic transitions. While the increase of Fe^{2+} cation concentration on octahedral lattice sites corresponds to the increase in conductivity, measured by Hall effect, the increase of Fe^{3+} cation concentration on tetrahedral lattice sites corresponds to the increase in ferrimagnetic response of the spinel thin films, measured by SQUID.[1] In agreement with complimentary methods such as XPS and XAS, the presence of the mentioned cations corresponds to disorder and inversion of the lattice structure, also induced by annealing or irradiation with Si ions.

[1] V. Zviagin et al., Appl. Phys. Lett. **108**, 13 (2016)

DS 36.10 Wed 17:00 P2-EG

Bipolar heterodiodes comprising β-gallium oxide — •Peter Schlupp, Daniel Splith, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für experimentelle Physik II, Germany

The large bandgap of 4.9 eV makes β-gallium oxide interesting for many applications e. g. for power electronics or if alloyed with indium oxide for visible- and solar-blind UV photodetectors [1]. In order to fabricate thin film transistors a gate contact is needed. A reasonable option are highly rectifying contacts which can also be used to perform space charge region based spectroscopy. Beside using Schottky diodes [2] these contacts can be realized by using bipolar heterodiodes.

We present β-gallium oxide bipolar heterodiodes grown on sapphire substrates by pulsed laser deposition (PLD). The *p*-type layers are realized by nickel oxide and amorphous zinc cobalt oxide fabricated by PLD at room-temperature. Best diodes exhibit rectification ratios of more than eight orders of magnitude and ideality factors of about 1.5. Temperature dependent current voltage measurements from 90 K to 300 K will be dicussed as well as space charge region based spectroscopy.

References

[1] Zhang et al., Appl. Phys. Lett. **108**, 123503 (2016)
[2] Splith et al., Phys. Status Solidi A **211**, 40 (2014)

DS 36.11 Wed 17:00 P2-EG

Temperature dependent investigation on Pt Schottky contacts on PLD grown In_2O_3 thin films — •Steffen Lanzinger, Daniel Splith, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Germany

Indium oxide is a material which, in its highly tin doped form, is already widely used for applications as a transparent conducting oxide. However, in recent years also interest in the semiconducting properties of In_2O_3 arose. First rectifying contacts on In_2O_3 thin films were realized by von Wenckstern et al. [1,2], utilizing reactively sputtered platinum or the p-type semiconductors zinc cobalt oxide or nickel oxide. Utilizing these rectifying contacts, the investigation of electronic defect states using space charge region based measurements was possible [3].

In this contribution we investigated the electrical properties of reactively sputtered platinum Schottky diodes on PLD grown undoped and Mg-doped In_2O_3 on c-plane sapphire by means of current voltage measurements and temperature dependent current voltage measurements between $T = 85$K and $T = 330$K. Additionally, the Schottky contacts were used to investigate the electronic defect states of the In_2O_3 thin films using thermal admittance spectroscopy.

[1] H. von Wenckstern *et al.*, APL Mat., 2, 4: 046104 (2014)
[2] H. von Wenckstern *et al.*, Adv. Electron. Mater., 1, 4 (2015)
[3] F. Schmidt *et al.*, Phys. Status Solidi B, 252, 10: 2304-2308 (2015)

DS 36.12 Wed 17:00 P2-EG

Synthesis of Carbon Nanowalls from a single source metalorganic precursor — •Nicolas Wöhrl, André Giese, and Volker Buck — Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

In this work the deposition of carbon nanowalls (CNWs) by an inductively-coupled-plasma-assisted chemical vapor deposition process (ICP-PECVD) is investigated. The CNWs are electrically conducting and show a large specific surface area, which is a key characteristic to make them applicable for sensors, catalysts or energy storage systems.

Here, CNWs are deposited from the single source metalorganic precursor aluminum-acetylacetonate. This precursor in combination with the ICP-PECVD is relatively unknown in literature. Silicon, stainless steel, nickel and copper can be used as substrate materials without any pretreatment. The deposited CNWs are characterized by SEM, Raman spectroscopy and AES. The combination of Bias-voltage, substrate temperature, and substrate material revealed a strong influence on the morphology of the nano-graphitic CNWs, strongly influencing the surface area. With regard to these results, a first growth model for the deposition of CNWs by ICP-PECVD using aluminum-acetylacetonate is proposed that takes the surface diffusion into account.

DS 36.13 Wed 17:00 P2-EG

Epitaxial growth of GeTe Phase Change Alloy on Si(111) Substrate by Pulsed Laser Deposition — •Isom Hilmi[1], Andriy Lotnyk[1], Jürgen W. Gerlach[1], Philipp Schumacher[1], and Bernd Rauschenbach[1,2] — [1]Leibniz-Institut für Oberflächenmodifizierung e.V., 04318, Leipzig, Germany — [2]Universität Leipzig, Institut für Experimentelle Physik II, 04103, Leipzig, Germany

GeTe phase change thin films have been grown on highly lattice-mismatched Si(111) substrates by means of pulsed laser deposition technique. Depending on the substrate temperature, the films grew in amorphous, oriented polycrystalline and single crystalline structures, consecutively, between RT and 300°C, as revealed by reflection high-energy electron diffraction (RHEED), x-ray diffraction and transmission electron microscopy (TEM). The narrow epitaxial window of GeTe on Si(111) is observed around 230°C. The crystalline thin films grow mainly in a distorted rock-salt structure, with the out-of-plane and in-plane epitaxial relationships were determined to be GeTe[111]//Si[111] and GeTe[11-2]//Si[11-2], respectively. The RHEED and atomic force microscopy measurements revealed that the film grew according to Stranski-Krastanov mode. The TEM measurements showed the presence of overlapping twins and the out of plane rotated grains in the thin films.

DS 36.14 Wed 17:00 P2-EG

Pulsed laser deposition of epitaxial Sb2Te3 thin films on Si(111) — •Isom Hilmi[1], Andriy Lotnyk[1], Jürgen W. Gerlach[1], Philipp Schumacher[1], and Bernd Rauschenbach[1,2] — [1]Leibniz-Institut für Oberflächenmodifizierung e.V., 04318, Leipzig, Germany — [2]Universität Leipzig, Institut für Experimentelle Physik II, 04103, Leipzig, Germany

An attempt to deposit a single crystalline chalcogenide phase change materials is of interests to improve the material performance for an application in non-volatile memory. In this report, the fabrication of high-quality Sb2Te3 by pulsed laser deposition is presented. The thin films were epitaxially grown on Si(111) substartes. The epitaxial growth was achieved at elevated substrate temperature ranging from 130° to 260°C. The films were grown in layer-by-layer mode. X-ray diffraction and transmission electron microscopy reveal that the films possess trigonal Sb2Te3 structure containing twin domains. The thin film growth starts with Sb/Te passivation layer. This results open up the feasibility to fabricate thin multilayer structure of chalcogenide phase change materials.

DS 36.15 Wed 17:00 P2-EG

Ruddlesden-Popper interface in correlated manganite heterostructures induces magnetic decoupling and dead layer reduction — Alexandr Belenchuk[1], Oleg Shapoval[1], Vladimir Roddatis[2], •Vitaly Bruchmann-Bamberg[3], Konrad Samwer[3], and Vasily Moshnyaga[3] — [1]IIEN, Academy of Sciences of Moldova, str. Academiei 3/3, MD-2028 Kishinev, Republic of Moldova — [2]Institut für Materialphysik, Georg-August-Universität-Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [3]I. Physikalisches Institut, Georg-August-Universität-Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We report on the interface engineering in correlated manganite heterostructures using embedded stacks of atomic layers that form the Ruddlesden-Popper structure. A room temperature magnetic decoupling was achieved through insertion of (SrO)$_2$–TiO$_2$–(SrO)$_2$ sequence of atomic layers at the interface between ferromagnetic metallic La$_{0.7}$Sr$_{0.3}$MnO$_3$ and (La$_{0.7}$Sr$_{0.3}$)(Mn$_{0.9}$Ru$_{0.1}$)O$_3$ films. Moreover, the narrowing of interfacial dead layer in ultrathin La$_{0.7}$Sr$_{0.3}$MnO$_3$ films was demonstrated by deposition of a single (SrO)$_2$ rock-salt layer at the interface with SrTiO$_3$ (100) substrate.

The obtained results are discussed basing on the symmetry breaking and disconnection of the MnO$_6$ octahedra network at the interface that may lead to the improved performance of all-oxide magnetic tunnel junctions. We suggest that octahedral decoupling realized by formation of Ruddlesden-Popper interfaces is an effective structural mechanism to control functionalities of correlated perovskite heterostructures.

DS 36.16 Wed 17:00 P2-EG

Electrical properties of CVD molybdenum disulfide — •wajid awan[1], tommy schönherr[1], antony george[2], andrey turchanin[2], stefan facsko[1], and artur erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Fredrich-Schiller-Universität Jena, Germany

Two dimensional materials are attractive for the use in next-generation nanoelectronic devices as compared to one dimensional material because it is relatively easy to fabricate complex structures from them. Recently the layered 2D semiconducting Transition metal dichalcogenides came into the picture and got a place in a wide range of novel applications as well as in basic research. Strikingly, MoS_2 receives significant attention since it undergoes transition from indirect bandgap (bulk form) to a direct bandgap (1.8eV) semiconductor due to the 2D confinement. The bandgap is an essential property for tunable 2-D nanodevices. We performed electrical transport measurements at room temperature for CVD grown MoS_2 on SiO_2/Si substrate. Standard Electron beam lithography (EBL) was used to pattern Gold (Au) metal contacts on MoS_2 flakes. For the purpose of sample characterization, we performed the Atomic Force Microscopy (AFM) and Raman Spectroscopy techniques, respectively, which confirm that the thickness of the CVD grown MoS_2 triangular flakes corresponds to single layers. Low temperature characterization of the electrical properties of the layers elucidates the exact mechanisms of charge transport in the 2d-layers. This knowledge will be used to modify the electrical properties in a controlled way, for example by ion irradiation.

DS 36.17 Wed 17:00 P2-EG

Direct observation of the M2 phase with its Mott transition in a VO$_2$ film — Hoon Kim[1,2], Tetiana Slusar[3], •Dirk Wulferding[1,4], Ilkyu Yang[1], Jin-Cheol Cho[3], Minkyung Lee[1,5], Hee Cheul Choi[1,5], Yoon Hee Jeong[2], Hyun-Tak Kim[3], and Jeehoon Kim[1,2] — [1]CALDES, Institute for Basic Science, Pohang, Korea — [2]Dept. of Phys., POSTECH, Pohang, Korea — [3]ETRI, Daejeon, Korea — [4]IPKM und LENA, TU-BS, Braunschweig, Germany — [5]Dept. of Chem., POSTECH, Pohang, Korea

In VO$_2$, the explicit origin of the insulator-to-metal transition is still disputable between Peierls and Mott insulators. Along with the controversy, its second monoclinic (M2) phase has received considerable attention due to the presence of electron correlation in undimerized vanadium ions. However, the origin of the M2 phase is still obscure. We study a granular VO$_2$ film using conductive atomic force microscopy and Raman scattering. Upon the structural transition from monoclinic to rutile, we observe directly an intermediate state showing the coexistence of monoclinic M1 and M2 phases. The conductivity near the grain boundary in this regime is six times larger than that of the grain core, producing a donut-like landscape. Our results reveal an intragrain percolation process, indicating that VO$_2$ with the M2 phase is a Mott insulator. [H. Kim, et al., arXiv:1611.09508 (2016).]

DS 36.18 Wed 17:00 P2-EG

Performance characterization of a custom quadrupole setup for creation of an energy and mass selective hyperthermal ion beam — •Michael Mensing[1], Philipp Schumacher[1], Jürgen W. Gerlach[1], Stephan Rauschenbach[2], and Bernd Rauschenbach[1,3] — [1]Leibniz Institute of Surface Modification, Leipzig, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Faculty of Physics and Earth Sciences, Leipzig University, Leipzig, Germany

To explore the influence of the ion kinetic energy and ion species, i.e. molecular or atomic nitrogen ions, on the growth and the resulting properties of ultrathin nitride films an existing ion-beam assisted molecular beam epitaxy (IBA-MBE) setup is equipped with a radio-frequency quadrupole ion optical setup. Prerequisite to such investigations is a thorough characterization of the properties of the generated ion beam. In this contribution (i) the performance of the mass separation is quantified. (ii) The distribution of the ion energy and its scaling within the hyperthermal energy range (20 eV - 200 eV) is discussed. As the present setup utilizes a constricted glow-discharge plasma source, the controlled extraction of the ions from the plasma determines the ion kinetic energy of the resulting ion beam. (iii) The ion beam shape is determined and (iv) achievable ion beam currents are presented. Furthermore, the influence of space charge effects in individual segments of the setup is evaluated and clarified by ion trajectory simulations using the SIMION computer code. In conclusion, the mass and energy selected ion beam fulfills the requirements for nanofilm growth studies.

DS 36.19 Wed 17:00 P2-EG

Influence of processing conditions on the properties of kesterite thin films from solution-deposition — •Vincent Steininger, Mohamed Sayed, and Levent Gütay — Laboratory for Chalcogenide Photovoltaics, Department of Energy and Semiconductor Research, Institute of Physics, University of Oldenburg, D-26111 Oldenburg, Germany

Kesterite semiconductor compounds are being considered as attractive alternative absorbers for thin film solar cells. Various chemical solution deposition techniques have been widely employed for the fabrication of kesterite thin films including spin coating and doctor blading. Doctor blading technique offers a lot of advantages for the processing of thin films due to its simplicity, cost effectiveness and its application for large area deposition.

The precursor processing conditions such as blading parameters and selenization parameters play a critical role and have significant impact on the properties of the kesterite thin films and hence the device performance. In this study we have deposited Cu_2ZnSnS_4 (CZTS) precursors by doctor blading technique under ambient air followed by an annealing step in selenium atmosphere to obtain $Cu_2ZnSn(S,Se)_4$ (CZTSSe) thin films.

The influence of different processing conditions on the properties of the prepared thin films was investigated using SEM, XRD and Raman spectroscopy.

CZTSSe thin film solar cells were fabricated and the resulting efficiencies are discussed in context of the varied parameters.

DS 36.20 Wed 17:00 P2-EG

Modeling of current voltage characteristics of Schottky contacts on Ga_2O_3 and In_2O_3 — •Daniel Splith, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

We present a model for the calculation of current voltage characteristics of Schottky contacts (SCs) taking into account barrier height inhomogeneities and variations of the net doping density in growth direction determining the spatial dependence of band bending. For each barrier height the band diagram was calculated using the finite element method. Subsequently, thermionic and thermionic field emission (TE and TFE) currents were calculated using the transfer matrix method. Additionally, charging currents were taken into account.

The model was used to calculate the IV characteristics of SCs on β-Ga_2O_3 and In_2O_3, utilizing the barrier parameters determined from temperature dependent IV measurements. Using a homogeneous doping profile for the β-Ga_2O_3, the modeled and measured temperature dependent characteristics are in good agreement. The modeled data shows that in the reverse direction, charging and TFE currents are dominant. For SCs on In_2O_3 the influence of the thickness of a Mg-doped layer on top of a nominally undoped thin film was investigated. Assuming a step-like doping profile and using the barrier parameters of the contact with the thickest Mg-doped layer, the modeled characteristics show a good agreement to the measured data for different layer thicknesses. The TFE current, while dominant for thin Mg-doped layers, is reduced with increasing layer thickness.

DS 36.21 Wed 17:00 P2-EG

Pulsed Radiofrequency sputtering of gallium oxide — •Philipp Schurig[1], Angelika Polity[1], Peter Klar[1], and Martin Eickhoff[2] — [1]1. Physikalisches Institut, AG Funktionelle Dünnschichten, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Universität Bremen, Institut für Festkörperphysik, Festkörpermaterialien, Otto-Hahn Allee 1, 28359 Bremen

The interest in transparent semiconductor materials is still at a high level due to possible applications in the field of (opto-)electronics, for example as photoresistors/-diodes and solar cells. One transparent oxide with a band gap of around 4.9 eV is the oxide of gallium, with its thermodynamically most stable phase β-gallium oxide. One critical parameter during deposition is the growth temperature which is relatively high with 650°C for β-gallium oxide. For industrial applications it is desirable to lower this value. Recent studies [Nak14] have shown that pulsed sputter deposition allows an increase of the coupled rf power and at the same time a decrease of the growth temperature without severe structural degradation of the material. This approach was adopted to the deposition of gallium oxide and the influence of parameters like pulse frequency or duty cycle time on the layer characteristics was examined. Nevertheless, post growth annealing was still necessary and performed at temperatures of 1000 °C in oxidizing atmosphere. UV-Vis-NIR, XRD, EDX and SEM measurements were performed after deposition. [Nak14] E. Nakamura et al.: Dramatic reduction in process temperature of InGaN-based light-emitting diodes by pulsed sputtering growth technique; (2014) Doi: 10.1063/1.4864283

DS 36.22 Wed 17:00 P2-EG

Synthesis of 2D lead-free hybrid perovskites (CnH2n+1NH3BX4; B = Mn, Cu; X = Cl, Br, I) and characterization — •Irina Anusca, Adela Bronja, Martina Pantaler, Christian Fettkenhauer, and Doru C. Lupascu — Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitätsstraße 15, 45141 Essen, Germany

Organic-inorganic lead halide perovskites have a high content of toxic lead which may eventually hamper their commercialization [1]. 2D perovskites (CnH2n+1NH3BX4; B = Mn, Cu; X = Cl, Br, I) can be alternative classes of lead free perovskite for optoelectronic application. We prepare different series of Cu and Mn perovskites by mixing of different CnH2n+1 organic ammonium cation (alkyl and aromatic) and X halide ion and we studied the optical properties in such systems. Properties were analyzed using x-ray diffraction und UV-VIS spectroscopy.

[1] Daniele Cortecchia, Herlina Arianita Dewi et al., Inorganic Chemistry, 2016, 55(3) pp. 1044-1052.

DS 36.23 Wed 17:00 P2-EG

Investigation of the structural and electrical properties of PLD grown gallium oxide thin films on quartz glass — •Laurenz Thyen, Daniel Splith, Stefan Müller, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Germany

For high power electronics, β-gallium oxide (Ga_2O_3) is of great interest due to its bandgap of 4.5 to 4.9 eV[1] at room temperature. As an alternative to homoepitaxy, being still costly nowadays, and heteroepitaxy on crystalline substrates, we investigated the structural, optical and electrical properties of SiO_2-doped β-gallium oxide thin films on quartz glass substrates. In that process, Ga_2O_3 thin films were fabricated by pulsed laser deposition at different temperatures and oxygen pressures. Additionally, the influence of an undoped Ga_2O_3 buffer layer was investigated in order to optimize the properties of the thin films on quartz glas. X-ray diffraction measurements yield that the thin films are amorphous up to a growth temperature of 400°C. At higher temperatures polycrystaline growth was observed. The roughness of the thin films which were directly grown on glass substrate is comparable to that of thin films grown on c-plane sapphire substrate. For the investigation of the electrical properties, PtO_x-Schottky contacts were fabricated on the Ga_2O_3 thin films by sputtering. From current-voltage characteristics, ideality factors of 1.2, effective barrier heights up to 1.35 eV and rectification ratios of 10^7 were determined. [1] T. Matsumoto *et al.*, Jpn. J. Appl. Phys. 13, 1578 (1974).

DS 36.24 Wed 17:00 P2-EG

Bismuth and antimony-based lead free double perovskites — •Martina Pantaler, Irina Anusca, Christian Fettkenhauer, and Doru C. Lupascu — Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg Essen, Universitätsstraße 15 45141 Essen

Bismuth- or antimony-based lead-free double perovskites as Cs2AgBiBr6 have been considered as alternatives to the emerging lead-based perovskites for solar cell applications. Until now, the class of compounds, Cs2AgBiBr6 and Cs2AgBiCl6 have been synthesized, which crystallize in 3D crystal structure, where the rock-salt arrangement of B and C cations is energetically favored, primarily because of the large charge difference between monovalent and trivalent C cations. These Pb-free double perovskites have been reported to have promising PV properties, including long carrier recombination lifetime,good stability against air and moisture, and low carrier effective masses. In our work, we report the different synthesis paths (solid state synthesis, solution state synthesis and hydrothermal synthesis) including single crystals synthesis of a halide double perovskite, A2BCX6 (A=Cs+, Rb+, MA+, B=Ag+, Cu+, C=Sb3+, Bi3+, X=Cl-, Br-, I-). We explore different properties and possibility to be used in PV. Film deposition was performed using spin coating and vapor deposition. References [1] Zewen Xiao et al., ChemSusChem 2016, 9, 2628-2633

DS 36.25 Wed 17:00 P2-EG

Surface-enhanced Raman spectroscopy (SERS) on $La_{0.7}Ca_{0.3}MnO_3$: Indication for a Jahn-Teller dominated surface structure — •Sebastian Merten, Bernd Damschke, Konrad Samwer, and Vasily Moshnyaga — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

Raman spectroscopy is a powerful tool to study different degrees of freedom at the same time. However, for thin films its use is limited by the normally strong background of the substrate. SERS allows one to overcome this limitation and opens new insights into the structural properties of ultrathin films and surfaces due to the small penetration depths of less than 5 nm. Here we report SERS measurements on thin TiO_2 and $La_{0.7}Ca_{0.7}MnO_3$ films grown by metalorganic aerosol deposition (MAD). As model system we used 20nm thick TiO_2 on a Si(100) substrate and a gold nano-layer on top of it, both grown by MAD. Only Si background is seen in the Raman spectrum of bare TiO_2. After deposition of the Au-layer, a strongly enhanced E_g-mode at 143 cm^{-1} of the anatase TiO_2 phase was observed. LCMO/MgO(100) and LCMO/$LaAlO_3$(001) films show a strong enhancement of the Jahn-Teller modes compared with normal Raman spectroscopy. This suggests the presence of cooperative Jahn-Teller effect at the film surface due to symmetry-breaking-induced electron-lattice reconstruction. Financial support from DFG via SFB 1073 (TP B01 and B04) is acknowledged.

DS 36.26 Wed 17:00 P2-EG

Effect of Bi-content and Gd-doping on the multiferroic properties of $BaTiO_3$-$BiFeO_3$ superlattices — •Stefan Hohenberger[1], Michael Lorenz[1], Vera Lazenka[2], and Marius Grundmann[1] — [1]Institut für Experimentelle Physik II, Universität Leipzig, D-04103 Leipzig, Germany — [2]Instituut voor Kern- en Stralingsfysica, KU Leuven, B-3001 Leuven, Belgium

Epitaxial superlattices consisting of $BaTiO_3$-$BiFeO_3$ double layers show vastly improved magnetoelectric (ME) voltage coefficients α_{ME} of up to 49 V cm^{-1} Oe^{-1} [1], compared with single-phase $BiFeO_3$ films. The microscopic origins of this enhanced ME coupling, however, are currently not fully understood. A series of films were prepared by pulsed laser deposition on $SrTiO_3$ substrates using $BiFeO_3$ targets with overstochiometric Bi-content ($Bi_{1.1}FeO_3$), as well as targets doped with Gd ($Bi_{1-x}Gd_xFeO_3$). These modifications have shown to increase the ferromagnetic and ferroelectric properties in single phase $BiFeO_3$ films.

The samples were studied with a vibrating sample magnetometer in a magnetocryostat at 10 K and 300 K. Ferroelectric polarization hysteresis measurements were carried out with a thin film analyzer. Furthermore, piezo-force microscopy was carried out. The results show the impact of chemical composition and rare earth doping on the multiferroic performance of oxide superlattices.

[1] M. Lorenz, V. Lazenka, P. Schwinkendorf, M. J. Van Bael, A. Vantomme, K. Temst, M. Grundmann, T. Höche, Adv. Mater. Interfaces **3**, 11 (2016).

DS 36.27 Wed 17:00 P2-EG

Epitaxial growth of NiO on GaN(0001) by molecular beam epitaxy and its photocatalytic application — •Melanie Budde, Carsten Tschammer, Jumpei Kamimura, and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

Nickel oxide is a transparent and semiconducting p-type oxide, which is interesting for various applications. For example, it works as a cocatalyst which allows for higher stability and efficiency of GaN photocatalysts for hydrogen generation. Furthermore, it can be used in normally off GaN-based heterojunction field-effect transistors as a gate dielectric to reduce the distance between source and drain. Therefore, well-defined and smooth NiO layers on GaN are required. Here NiO was grown by plasma-assisted molecular beam epitaxy on GaN templates. The topography and layer quality for different growth parameters was investigated using in-situ reflecticion high-energy electron diffraction as well as ex-situ x-ray diffraction and atomic force microscopy. The epitaxial relationship between substrate and layer was defined and rationalized by the concept of domain matching epitaxy. The impact of NiO layers on the stability of the photocatalytic application was tested.

DS 36.28 Wed 17:00 P2-EG

Thermal Conductivity of Thin Films Determined via IR thermography — •Natalie Galfe[1], Anton Greppmair[1], Benedikt Stoib[1], Nitin Saxena[2], Caroline Gerstberger[1], Peter Müller-Buschbaum[2], Martin Stutzmann[1], and Martin S. Brandt[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching — [2]Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Strasse 1, 85748 Garching

In fields such as microelectronics and thermoelectrics, heat management becomes increasingly important. However, with the continuous miniaturization of the corresponding devices, established methods for the determination of the thermal conductance face severe challenges. Here, we demonstrate a simple and quick method for the measurement of the in-plane thermal conductance of thin films via steady-state infrared thermography. The films are suspended above a hole in an opaque substrate and homogeneously heated by a visible light source. The temperature distribution of the thin films is captured via IR microscopy and fitted to the analytical expression obtained for the specific hole geometry used in order to obtain the in-plane thermal conductivity. For thin films of PEDOT:PSS post-treated with ethylene glycol and of polyimide we find conductivities of 1.0 W/mK and 0.4 W/mK at room temperature, respectively. Furthermore, we are able to demonstrate the influence of varying the electrical conductance of the PEDOT:PSS films on the resulting thermal conductance. All results are in very good agreement with literature values.

DS 36.29 Wed 17:00 P2-EG

Thermoelectric Characterization of Organic Thin Films — •Kiana Baumgaertner[1], Alexander Steeger[1], Florian Huewe[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

Conducting organic thin films have recently been proposed as innovative thermoelectric materials to recover waste heat at low cost[1]. To characterize their thermoelectric figure of merit zT it is necessary to determine the materials' electrical and thermal conductivity as well as their Seebeck coefficient. In this study, we developed an experimental setup to consistently measure this set of parameters on a single thin film sample for temperatures ranging from 4 K to 300 K. The thermal conductivity is characterized based on the 3ω-method by periodic Joule heating of a metal strip deposited atop the film. This metal strip acts as a heater creating a temperature gradient across the sample for measurement of the Seebeck voltage between two separate contacts. Optimizing the measurement geometry by performing finite-element simulations on thin films of thicknesses below $d = 1\,\mu\mathrm{m}$ and thermal conductivities of $\kappa \leq 1\,\mathrm{W/(mK)}$, the functionality of this setup has been verified on oxide as well as polymeric thin film samples. First results on the thermoelectric performance of functionalized organic layers will be presented that highlight the potential of this material class. [1] O. Bubnova et al., Nat. Mater. 2011, 10, 429.

DS 36.30 Wed 17:00 P2-EG

Resistive switching dynamics in BiFeO3 — •Nan Du[1], Niveditha Manjunath[1], Yuan Li[1], Tiangui You[1], Danilo Buerger[1], Ilona Skorupa[1,2], Damian Walczyk[3], Christian Walczyk[3], Thomas Schroeder[3], Stephan Menzel[4], Eike Linn[5], Rainer Waser[4,5], Oliver G. Schmidt[1,6], and Heidemarie Schmidt[1] — [1]Faculty of Electrical and Information Engineering, TU Chemnitz — [2]Institute of Ion Beam Physics and Materials Research, HZDR — [3]Leibniz-Institut für innovative Mikroelektronik, IHP — [4]Peter Grünberg Institut, Forschungszentrum Jülich — [5]Institut für Werkstoffe der Elektrotechnik, RWTH Aachen — [6]Institute for Integrative Nanosciences, IFW Dresden

Experimental and model impedance and dynamic switching experiments for the study of hopping transport of electron charges and positively charged oxygen vacancies in memristive BiFeO3 switches with substitutional Ti donors close to the bottom electrode are reported. The drift velocity of oxygen vacancies in the electric field of the writing pulse determines the dynamics of resistive switching. The modelled activation energy for trapping and release of oxygen vacancies at the bottom electrode reflects the local enhancement of the electrostatic potential profile at the bottom electrode due to the Ti donors. The data analysis of the experimental electrostatic potential profile will be useful for a quantitative comparison between experimental and future principles computational design of memristive oxide switches with substitutional dopants for trapping and releasing oxygen vacancies.

DS 36.31 Wed 17:00 P2-EG

Morphological and structural studies of perovskite layers deposited on various substrates — Mohammad I. Hossain, Mohammed I. Helal, and •Abdelhak Belaidi — Qatar Environment & Energy Research Institute (QEERI), Hamad Bin Khalifa University (HBKU), Qatar Foundation, P.O. Box 5825 Doha, Qatar

Perovskite, (CH3NH3PbI3), is an organic-inorganic material that has showed vast potential as an absorber in the photovoltaic (PV) research due to its suitable electronic, optical, and structural properties. Morphological studies of such layers are beneficial for PV applications due to the variation in grain size which affects directly the charge transport. In this work, we have prepared perovskite (CH3NH3PbI3) layers using one step solution process in air on various substrates, like FTO and TiO2, with various concentration ratios of PbI2/ CH3NH3I from 0.3 to 1.1. The deposited layers were then characterized after post-annealing treatment in air at 100oC using XRD, SEM, and UV-Vis. The crystallographic structure of the layers deposited using such solution process depends on the ratio of PbI2/CH3NH3I. XRD results confirm that for the ratio 1.1 both perovskite and PbI2 phases exist, however for ratios 0.8, 0.7, and 0.6 only the perovskite phase exists. Interestingly, SEM images show that the morphology of the deposited films with ratios 1.1 and 0.8 are fibrous shape, whereas, for the other ratios the shape disappears. UV-Vis results confirm the bandgap of perovskite layers laying around 1.63 eV. Hence, the study of the variation of PbI2/CH3NH3I ratio is promising to design perovskite solar cells with the optimum morphological properties.

DS 36.32 Wed 17:00 P2-EG

Effect of a moderating etching front in reactive ion beam figuring of optical aluminium surfaces — •Jens Bauer, Frank Frost, and Thomas Arnold — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, D-04318 Leipzig, Germany

Shape-adapted mirror optics are highly interesting for short-wavelength applications. Ion beam figuring is an established method in high-end optical surface manufacturing. But the direct machining of optical Al surfaces failed up to now, since the surface roughness increases drastically as a result of structural, crystallographic and chemical matrix irregularities. Our contribution focuses RIBE figuring of RSA Al6061 and Al905 with O_2 and N_2 containing process gas. In contrast to the classical RIBE scheme, no volatile process products are generated, but the machined surface is determinately chemically modified. A very stable and non-hazardous etch mechanism is obtained. The etch behaviour is analysed by WLI, AFM, and TOF-SIMS. Supplemented by Monte Carlo simulations a phenomenological model is presented. In particular, due to the impact of the energetic reactive ions a homogeneous and temporally stable surface oxide or nidride layer is formed. This layer results from a quasi-stationary equilibrium between ion implantation and sputter erosion. The surface layer acts as an etching front moderating the inhomogeneous structural conditions of the aluminium bulk material. Thus, the surface roughness is preserved almost in its initial state. Deterministic narrow ion beam operation via a dwell-time approach is now qualified for ultra-precision figure error correction of high-quality Al mirror optics.

DS 36.33 Wed 17:00 P2-EG

Microstructure of pulsed-laser deposited Ge-Sb-Te phase-change thin films on surface-reconstructed silicon substrates — •Ulrich Ross, Andriy Lotnyk, Isom Hilmi, and Bernd Rauschenbach — Leibniz Institut für Oberflächenmodifizierung e.V. Permoserstr. 15 D-04318 Leipzig

The stable layered phases of Ge-Sb-Te based phase-change thin films are of technological interest for a number of novel properties, most prominently the crystalline resistance switching behaviour in stacked superlayers. In order to provide such thin films for structure and property investigations, precise control and understanding of the crystalline thin film growth behaviour is required.

Thin films of the prototypical phase-change material Ge_2-Sb_2-Te_5 were grown by pulsed laser deposition onto (111) oriented silicon substrates. The Si(111) 7x7 surface reconstruction was achieved by thermal treatment before natural cooldown to the final deposition temperature. The growth process was observed by in-situ RHEED measurements, and the resulting crystalline quality evaluated by SEM and XRD. Cross-sectional specimens were investigated by aberration-corrected STEM using analytic techniques as well as atomic-resolution imaging and image simulation. The results reveal a highly characteristic surface-passivated Van-der-Waals interface structure for the epitaxial growth regime, while the crystalline lattice structure is dominated by stoichiometric stacking disorder. At intermediate deposition temperatures, the domain-epitaxy growth results in stressed in-plane rotation domains and twin formation.

DS 36.34 Wed 17:00 P2-EG

Noble gas ion-induced pattern formation on indium oxide thin films — •Hans Hofsäss, Omar Bobes, and Ronja Langendorf — Fakultät für Physik, Universität Göttingen, Göttingen, Germany

Formation of self-organized surface patterns by noble gas ion irradiation has been studied in the past. Ripple pattern formation on oxides was mainly investigated for fused silica [1], sapphire [2] and also Indium-Tin-oxide (ITO) [3]. Whereas silica and sapphire exhibits the expected behavior regarding ripple formation, ripple formation on ITO was investigated only for grazing incidence, where parallel ripple were observed. It was conclude that crystallinity plays a crucial role for pattern formation on ITO [3]. We studied the pattern formation on ITO for 1 keV Ar and Xe ion irradiation and a broad range on ion incidence angles. We find flat surfaces except for grazing ion incidence where perpendicular ripples similar to [2] are observed. Results for ion irradiation at lower ion energy will be presented. We compare the existing data for silica, sapphire and ITO with predictions from linear theories, where we use curvature coefficients determined from Monte Carlo simulations. The simulation results are in good quantitative agreement with the experiments done with silica and sapphire but not for ITO.

[1] A. Keller et al., J. Phys.: Condens Matter 21 (2009) 495305
[2] H. Zhou et al., Phys. Rev. B 78 (2008) 165404
[3] T. Škereň et al., Thin Solid Films 589 (2015) 315

DS 36.35 Wed 17:00 P2-EG

Comparison of pattern formation of Si and Si_3N_4 by N^+ and $N_2{}^+$ ion irradiation — •Hans Hofsäss, Omar Bobes, and Lukas Janos Richter — Fakultät für Physik, Universität Göttingen, Göttingen, Germany

Recently Bradley and Hofsäss introduced ion implantation as an additional effect contributing to pattern formation. Ion implantation should contribute to surface instability an pattern formation at larger ion incidence angles, typically above 45-50°. To demonstrate the the effect of ion implantation, we compare N^+ and $N_2{}^+$ ion irradiation of Si and silicon nitride substrates. Silicon itride cannot accommodate N beyond the given stoichiometry and implanted N must diffuse out. The stoichiometry of the films remains unchanged irradiation with N and additional N incorporation can be neglected. On the other hand, N will be incorporated into Si and an amorphous SiN_x layer will form. Here, implanted N should contribute to pattern formation. We irradiated Si and silicon nitride samples with ions in the energy regime few keV up to 10 keV and ion incidence angles between 60° and 75°. We find no pattern formation on Si_3N_4 for all investigated irradiation parameters. In contrast, N irradiation of Si leads to pronounced ripple patterns. The behavior can be understood from a comparison with simulation results based on the crater function formalism and Monte Carlo simulations of the ion solid interaction. We find strong support that pattern formation on N ion irradiated Si is mainly determined by N ion implantation.

DS 36.36 Wed 17:00 P2-EG

An explanation for the unusual pattern formation behavior on Ge — •Hans Hofsäss, Omar Bobes, and Kun Zhang — Fakultät für Physik, Universität Göttingen, Göttingen, Germany

Pattern formation on Germanium surfaces due to ion irradiation has been extensively studied experimentally [1,2,3]. Common to these experiments is that the onset of parallel ripple patterns occurs at an unusual large critical angle of incidence of about 60° and only for heavier ions such as Kr and Xe. For Ar and Ne no pattern formation was found for all angles of incidence [1]. This behavior cannot be understood on the basis of the Bradley-Harper and the Carter-Vishnyakov model.

We have carried out experiments, which confirm the above mentioned experimental results. Monte Carlo simulations using the SDTrimSP program were performed to calculate the curvature coefficients using the crater function formalism. We take into account incorporation of noble gas ions and density reduction due to swelling and void formation. We find that pattern formation on Ge surfaces should indeed be absent for keV Ne and Ar ion irradiation and is suppressed for keV Kr and even Xe ions, except for large angles of incidence.

[1] M. Teichmann, J. Lorbeer, B. Ziberi, F. Frost, and B. Rauschenbach, New. J. Phys. 15 (2013) 103029.

[2] J. C. Perkinson, C. S. Madi, and M. J. Aziz, J. Vac. Sci. Technol. A 31 (2013) 021405.

[3] E. Anzenberg, J. C. Perkinson, C. S. Madi, M. J. Aziz, and K. F. Ludwig, Phys. Rev. B 86 (2012) 245412.

DS 36.37 Wed 17:00 P2-EG

Neon ion beam induced surface pattern formation on Si — •Hans Hofsäss, Kun Zhang, and Omar Bobes — Fakultät für Physik, Universität Göttingen, Göttingen, Germany

The development of self-organized surface patterns on Si due to noble gas ion irradiation has been studied extensively in the past. However, in nearly all experiments to date, no pattern formation on Si was observed for ion irradiation with Ne ions [1]. One exception is an experiment carried out by Carter et al. in 1995 where parallel ripple patterns with about 1.1 μm wave length are observed for 20 keV Ne ions incident on Si at an angle of 45° [2].

We present experimental data on pattern formation for Ne ion irradiation of Si with different ion energies and incidence angles larger than 45°. Using the crater function formalism and Monte Carlo simulations we calculate curvature coefficients of linear continuum models of pattern formation. Our simulations show that pattern formation is strongly suppressed for most ion energies. However, at very low energies $<$ 500 eV and also for energies above 20 keV parallel ripples can be expected. The role of incorporation of noble gas ions and a reduced density due to possible void formation is discussed.

[1] F. Frost, B. Ziberi, A. Schindler, B. Rauschenbach, Appl. Phys. A 91 (2008) 551.

[2] G. Carter, V. Vishnyakov, Yu. V. Martynenko, and M. J. Nobes, J. Appl. Phys. 78 (1995) 3559.

DS 36.38 Wed 17:00 P2-EG

Carbon ion beam induced surface pattern formation on amorphous carbon — •Hans Hofsäss, Omar Bobes, and Kun Zhang — Fakultät für Physik, Universität Göttingen, Göttingen, Germany

Using a mass selected carbon ion beam provided by our ion beam deposition system, we are able to perform irradiations of substrates with carbon ions at defined energies between about 100 eV and 60 keV and for variable ion incidence angle. We investigate the formation of ripple patterns on a-C films on Si. The hydrogen-free a-C films with thickness of 270 nm were grown on Si wafers by vacuum arc deposition and had a sp^3 bond fraction of about 60 percent. The special interest in carbon ion irradiation has several reasons:

(i) Unlike noble gas ion irradiation, carbon ions are incorporated into the a-C film as self atoms. Therefore we can study the effect of ion implantation on pattern formation without the complication of compound formation.

(ii) The sputter yield of carbon is rather low, in particular for the case of carbon ion irradiation. We therefore have a system where mass redistribution should be the dominant mechanism for pattern formation.

(iii) Carbon is even lighter than Ne and the comparison between C and Ne ion irradiation should provide further insight into the pattern formation mechanisms.

In this contribution we compare recent experimental results with Monte Carlo simulations using the SDTrimSP program.

DS 36.39 Wed 17:00 P2-EG

Combinatorial approach to structural and electrical properties of (In,Ga)$_2$O$_3$ thin films grown by pulsed laser deposition — •R. Hölldobler, H. von Wenckstern, D. Splith, J. Lenzner, H. Hochmuth, M. Lorenz, and M. Grundmann — Universität Leipzig, Fakultät für Physikund Geowissenschaften, Institut für Experimentelle Physik II,Linnéstr. 5, 04103, Leipzig, Germany

Combinatorial approaches in solid state science have been used more and more in recent years for an efficient exploration of novel materials. One approach is the growth of thin films with lateral composition gradient(s) and their spatially resolved characterization. We present the growth of (In,Ga)$_2$O$_3$ thin films by pulsed laser deposition (PLD) using a single but segmented PLD target [1]. The samples are deposited at various growth temperatures and oxygen pressures. Spatially resolved investigations of the chemical composition, structural and electrical properties are presented show an interplay between growth temperature, oxygen pressure and desorption of gallium sub-oxides as previously reported for molecular beam epitaxy [2]. Our results allow growth of alloyed thin film with tailored properties for specific application such as rectifiers or photodetectors.

[1] H. von Wenckstern, Z. Zhang, F. Schmidt, J. Lenzner, H. Hochmuth, and M. Grundmann, CrystEngComm **15**, 10020 (2013).

[2] P. Vogt and O. Bierwagen, Appl. Phys. Lett. **109**, 062103 (2016).

DS 36.40 Wed 17:00 P2-EG

Investigation of oxygen-degraded organometallic halide perovskite via photoluminescence and photothermal deflection spectroscopies — •Alexandra Bausch[1,2], Paul Fassl[1,2], Qing Sun[1,2], David Becker-Koch[1,2], Paul E. Hopkinson[1,2], and Yana Vaynzof[1,2] — [1]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [2]Centre for Advanced Materials, Heidelberg University, Germany

In recent years organo-metallic perovskite solar cells have been enthusiastically investigated due to their high power conversion efficiencies, low production costs and simple device fabrication. While the performance and electronic properties of perovskite photovoltaic devices are extensively researched, their environmental stability remains a major challenge to their potential integration into industrial application and is far less investigated. In order to develop a deeper understanding of the degradation processes taking place in perovskite solar cells when exposed to oxygen and light, we study the optical properties of degraded methylammonium lead iodide using photoluminescence and photothermal deflection spectroscopies. For this purpose, perovskite films fabricated using different methods are exposed to simulated sunlight under precisely controlled levels of oxygen in a dry environment. Longtime photoluminescence measurements reveal the effect of oxygen induced degradation on the efficiency of emission from the perovskite layers. Furthermore, photothermal deflection spectroscopy allows careful evaluation of the absorption edge of the perovskite layers, which enables the calculation of the Urbach energy.

DS 36.41 Wed 17:00 P2-EG

In Situ Stress Analysis In Ion-Implanted GaAs — •Paul Kutza, Emanuel Schmidt, Sascha Creutzburg, and Elke Wendler — Institut für Festkörperphysik, Friedrich-Schiller-Universität, Jena, Germany

Stress and damage formation in GaAs ion-implanted at room temperature are investigated. 1 MeV Si-ions are implanted with fluences up to 5E15 cm^{-2}. Various ion fluxes between 3E10 cm^{-2}s^{-1} and 5E11 cm^{-2}s^{-1} were applied. The stress evolution during the implantation is investigated in situ by measuring the radius of curvature of a GaAs cantilever via the position of a HeNe laser beam reflected by the bent surface of the GaAs sample. A strong dependence of damage formation on the chosen ion flux is observed. While ion fluxes up to 2.3E11 cm^{-2}s^{-1} feature a steady increase of stress up to saturation, rates above 3E11 cm^{-2}s^{-1} exhibit a stress maximum at a certain fluence followed by a significant stress decrease until a lower saturation value is reached. Ex Situ Rutherford Backscattering Spectroscopy in channeling mode (RBS/C) measurements reveal that only samples showing the latter stress evolution have developed an amorphous layer. When only point defects or extended defects are formed, stress relaxation does not occur. The fluence dependences are modeled, combining the damage concentration determined by RBS/C and the stress evolution. Additionally, effects of a low temperature implantation and a sudden shutdown of the Si-ion beam are investigated.

DS 36.42 Wed 17:00 P2-EG

Thermal Conductivity in Kesterite Crystals — •Martin Handwerg[1,2], Rüdiger Mitdank[1], Laura-Elisa Valle-Rios[2,3], Susan Schorr[2,3], and Saskia F. Fischer[1] — [1]Novel Materials, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany — [3]Free University Berlin, Institute of Geological Sciences, 14195 Berlin, Germany

The kesterite materials Copper-Zinc-Tin-Sulfide and -Selenide are of huge interest for future solar cell applications due to the ideal band gap and high absorption rate. Insight in the thermal conductivity of a solar absorption material is important for the thermal management of the cell and therefore for the temperature-dependent efficiency. However, thermal conductivity investigations are rare actually.

Here we used the 3ω-method[1] to investigate the thermal conductivity of CZTSe macro-crystals with different compositions. The crystal thicknesses were in the range of several hundred micrometers. The metal heater lines with a width of 10 μm were deposited on the polished crystal surface. The measured thermal conductivity values are about 3 Wm^{-1}K^{-1}. The measured temperature-dependence of the thermal conductivity allows conclusions concerning the transport process. Phonon-phonon-Umklapp-scattering dominates the thermal conductivity for $T > 180$ K and point-defect-scattering occurs for $T < 180$ K. [1] Handwerg *et al.*, Semicond. Sci. Technol. **30**, 024006 (2015).

DS 36.43 Wed 17:00 P2-EG

Production of fully Au-embedded ^{163}Ho for Neutrino Mass Measurements — •Tom Kieck[1,2], Christoph Düllmann[1], Lisa Gamer[3], Leonard Winkelmann[2], and Klaus Wendt[2] — [1]Institut für Kernchemie, Johannes Gutenberg-Universität Mainz, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [3]Kirchhoff-Institut für Physik, Universität Heidelberg, Germany

The ECHo collaboration aims at measuring the electron neutrino mass by recording the spectrum following electron capture of ^{163}Ho using metallic magnetic calorimeters (MMC). The radioisotope ^{163}Ho has been produced from enriched ^{162}Er in a high flux nuclear reactor and has to be fully embedded into the 250 x 250 μm^2 MMC-absorbers with minimum losses [1].

The application of resonant laser ionization at the RISIKO mass separator guarantees optimum elemental and isotopic selectivity for ultra-pure ^{163}Ho ion implantation with a sub millimeter beam spot [2]. An in-situ deposition of gold using the technique of pulsed laser deposition (PLD) ensures a homogeneous ^{163}Ho/Au layer production as absorber of the MMC. In this way a saturation of the implantation-dose by sputtering effects is prevented and the targeted activity of 10 Bq per detector is achieved.

[1] Hassel et al., J. Low Temp. Phys. 184, 910-921 (2016)

[2] Schneider et al., NIM B 376, 388-392 (2016)

DS 36.44 Wed 17:00 P2-EG

Protective ceramic layers deposited by chemical vapor deposition on complex 3D tools — Gregor Fornalczyk[1], •Sebastian Schipporeit[2,3,4], Frank Mumme[1], Friederike Deuerler[2], and Volker Buck[3,4] — [1]Gemeinnützige KIMW Forschungs-GmbH, Luedenscheid — [2]University of Wuppertal, School of Mechanical Engineering and Safety Engineering, Material Technology, Wuppertal — [3]University Duisburg-Essen, Thin Film Technology Group, Faculty of Physics, Duisburg — [4]CENIDE, Duisburg

Yttrium-doped ZrO_2 coatings are well-known to protect metallic tools and injection molds from wear and corrosion. This material is a highly anti-corrosive and wear resistant ceramic. It is particularly suitable for coating steel substrates, because their thermal expansion coefficient and mechanical properties are similar. We used a mixture of metal acetylacetonates in a 3D conformal aerosol-assisted chemical vapor deposition process. These precursors decompose at low temperatures (<500°C) and, thus, allow the deposition of layers into narrow cracks and holes without corroding or mechanically harming the steel substrates. We deposited films with excellent adhesion and wear properties at a nearly constant coating rate in aspect ratios up to 1:50 in 0.1 mm thin columns.

DS 36.45 Wed 17:00 P2-EG

Neon ion beam induced pattern formation on amorphous carbon surfaces — •Omar Bobes, Hans Hofsäss, and Kun Zhang — II. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

We investigate the ripple pattern formation on amorphous carbon surfaces at room temperature during low energy Ne ion irradiation as a function of ion incidence angle. Monte Carlo simulations of the curvature coefficients applied to the Bradley-Harper and Cater-Vishnyakov models, including the recent extensions by Harrison-Bradley and Hofsäss and taking into account the incorporation of the ions into the film predict that pattern formation on amorphous carbon should be possible for low energy Ne ions from 250 eV up to 5 keV. Moreover, simulations are able to explain the absence of pattern formation in certain cases. Our experimental results are compared with prediction using current linear theoretical models and applying the crater function formalism as well as Monte Carlo simulations to calculate curvature coefficients using SDTrimSP program.

DS 36.46 Wed 17:00 P2-EG

Low temperature transport measurements of metallic nanostructures prepared by area-selective atomic layer deposition on ultrathin platinum templates fabricated with focused electron beam induced deposition — •Peter Gruszka, Giorgia Di Prima, Roland Sachser, and Michael Huth — Goethe Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main

Focused electron beam induced deposition (FEBID) is a serial, bottom-up and direct write approach with superior lateral resolution (< 10 nm) but results in samples with poor material purity. Much effort is put into the investigation of optimal deposition parameters to increase the material yield which in most cases is an impossible task. In contrast, atomic layer deposition(ALD) allows for depositing high purity thin films with sub-monolayer accuracy but lacks lateral control. Mackus, et al.[1] developed a combined technique which uses FEBID to predefine templates for the subsequent area selective ALD process.

We performed the combined FEBID-ALD process using purified platinum FEBID nanostructures as templates utilizing a purification technique developed by Sachser, et al.[2]. Afterwards the purified platinum templates were processed with ALD in our scanning electron microscope while monitoring in-situ the conductance over time. Additionally, our transport measurements in a Helium-3 cryostat showed that with this approach one can achieve high purity thin film nanostructures which behave nearly like platinum bulk samples.

[1] Mackus, et al., J. Appl. Phys 107 (2010), 116102

[2] Sachser, et al., ACS Appl. Mater. Interfaces 6 (2014), 15868 - 15874

DS 36.47 Wed 17:00 P2-EG

On-chip lateral anodic oxidation of titanium — •Daniela Welk, Svenja Herbertz, Thomas Heinzel, Paulus Aleksa, and Mara Zielinski — Solid State Physics Laboratory, Heinrich-Heine-Universität Düsseldorf

We demonstrate that it is possible to generate and increase the width of a TiO_x line in a Ti film by application of a DC voltage. The process has the character of an on-chip anodic oxidation and can be used to generate as well as tune electronic circuit elements on-chip. During oxidation, the TiO_x line changes its width, height, roughness and resistance. This growth of the oxide is studied under different ambient conditions.

DS 36.48 Wed 17:00 P2-EG

Solution-processed bottom-contact metal-oxide thin-film transistors with transparent monolayer graphene electrodes — •Ersoy Subasi[1], Sebastian Meyer[2], Duy-Vu Pham[2], Claudia Bock[1], and Ulrich Kunze[1] — [1]Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, Bochum, Germany — [2]Evonik Resource Efficiency GmbH, Electronic Solutions, Marl, Germany

In this study we demonstrate the suitability of monolayer graphene (MLG) electrodes for solution-processed metal-oxide thin-film transistors (MOTFTs), which are capable of being used in the field of flexible and transparent low-cost electronics.

Solution-processed metal-oxide films are promising candidates to replace amorphous silicon as the active layer used in TFTs, e.g. in display applications, because of there simplicity, low-cost and high performance. Since conventional metal electrodes are not suitable for transparent electronics graphene is a promising material for next-generation transparent electrodes. We successfully prepared solution-processed bottom-contact MOTFTs with MLG electrodes and mobilities comparable to those of amorphous silicon $\mu_{\mathrm{FE,sat}} \approx 1.4$ cm^{2}V^{-1}s^{-1}. Using ultraviolet photoelectron spectroscopy under ambient conditions we determined the work function of the MLG electrodes to 5.0 eV. Since the electron affinity of the metal-oxide amounts approximately 3.7 eV [1] the work function of the MLG electrodes should be reduced (e.g. by doping). We achieved a reduction of the work function via a thin Al-film on top of the MLG electrodes ($\Delta\Phi_{\mathrm{M}} \approx -1.0$ eV).

[1] O. Lang *et al.*, J. Appl. Phys. 86, 5687 (1999).

DS 36.49 Wed 17:00 P2-EG

Temperature dependent absorption measurement at oxide semiconductors — •Jonathan Prexl[1], Karim Imani[3], Matthias Kleine-Boymann[3], Matthias Elm[2], and Sangam Chatterjee[2] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Germany — [2]Institute of Experimental Physics I, Justus-Liebig-University Giessen, Germany — [3]Institue of Physical Chemistry, Justus-Liebig-University Giessen, Germany

Thermochromic oxide-semiconductors are highly interesting for a wide range of applications due to their intriguing optical properties. Quantitative measurements of their thermo-optical properties require stable thermal conditions for the sample in combination with a well-defined ambient gas atmosphere. The heating unit should, furthermore, enable a large number of experimental possibilities like spectrally and spatially resolved transmission or reflections measurements, multiple beam setups etc.

Here, we present an in-house developed, low cost heating unit for stable temperatures up to 800°C. We discuss the technical approach and constructing details to create stable environments and present some exemplary temperature dependent absorption data on CeO2 and (Ce,Zr)O2 samples prepared by pulsed laser deposition.

DS 36.50 Wed 17:00 P2-EG

Raman study of orthorombic Ga_2O_3 — •Daniel Zink, Marcel Weinhold, Max Kracht, Martin Eickhoff, and Peter J. Klar — Justus-Liebig-Universität Gießen, I. Physikalisches Institut, Heinrich-Buff-Ring 16, 35392 Gießen

In the fifties *Roy et al* reported five polymorphs of Ga_2O_3 obtained from solvothermal synthesis. Subsequently many studies of their catalytic properties werer performed. The availability of epitaxial synthesis routes recently gave rise to a new interest in this material system, also in the context of optoelectronic devices. Therefore a comprehensive structural analysis is required. The more so as the different synthesis ways with nanocrystalline mixed phases led to a confused naming of the Ga_2O_3-polymorphs. We will give a brief review of all known Ga_2O_3-structures and present Raman measurements of Sn-doped Ga_2O_3 prepared by plasma assisted MBE.

DS 36.51 Wed 17:00 P2-EG

Sputter Deposition of Nitrogen doped ZnMgO Thin Films — •Hannes Giese, Philipp Schurig, and Angelika Polity — I. Physikalisches Institut, Justus-Liebig-Universität, Giessen, Deutschland

ZnO is an intrinsic n-type semiconductor, which is favourable for the use as a transparent conductive thin film produced by sputter deposition. The addition of MgO results in a ternary system that has a tuneable band gap in dependence on the amount of Mg inside the system. The Mg content also has an influence on the crystal structure of the material. For many years theoretical calculations have shown the possibility of p-type doped ZnMgO for usage as optoelectronic devices made of ZnMgO homojunctions for example. The most promising way is doping the material with nitrogen to create the necessary defect levels above the valence band. The thin films are produced by RF sputter deposition from a self-made ceramic target with a composition of Zn(0,8)Mg(0,2)O with argon and oxygen as sputtering gases. Furthermore, an addition of nitrogen-gas as a reactive gas should lead to defects that provide a p-type doping. The nitrogen gas flow is varied in a wide range to investigate this influence. The changes in crystal quality, optical properties and electric behaviour are characterized by XRD, UV/Vis spectroscopy and Hall-effect measurements.

DS 36.52 Wed 17:00 P2-EG

Structural and optical investigations of Sn-doped $(Ga,Al)_2O_3$ thin films — •Anna Werner, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany

Deep ultraviolet photodiodes find wide use in applications such as flame and oil spill detection or water desinfection. Ga_2O_3 is a suitable detector material and has a large bandgap of 4.5–4.9 eV[1], which band gap can be increased by alloying with Al_2O_3.

We present structural and optical investigations of $(Ga,Al)_2O_3$-thin films grown by pulsed laser deposition on c-plane sapphire using different oxygen pressure p_{O_2} and temperature T_g. Furthermore the thin films were doped with 1% SnO_2 to improve the electric conductivity. We investigated the $(Ga,Al)_2O_3$-thin films with X-ray diffraction (XRD), which shows that the crystal grew along the (−201) direction. Also optical transmission measurements were performed. We find that the cation composition ratio strongly depends on the deposition parameters. For lower (higher) p_{O_2} (T_g) the incorporation of Al is favored due to desorption of gallium sub-oxides during growth[2]. This leads to a change of lattice constant and absorption edge.

[1] T. Matsumoto, M. Aoki, A. Kinoshita, and T. Aono, Jpn. J. Appl. Phys. 13, 1578 (1974)

[2] P. Vogt and O. Bierwagen, APL Mater. 4, 086112 (2016)

DS 36.53 Wed 17:00 P2-EG

Influence of strain on the binding energies of Rydberg excitons in Cu_2O — •Sjard Ole Krüger, Peter Grünwald, Florian Schöne, and Stefan Scheel — Institut für Physik, Universität Rostock, D-18059 Rostock, Germany

In recent years, excitons in Cu_2O have emerged as a promising platform for the study of Rydberg physics [1], showing a strong Rydberg blockade. Experiments examining the collective behaviour of multi-exciton systems often employ effective trapping potentials which can be induced by nonuniform straining of the crystal. One experimental advantage of Rydberg excitons over Rydberg atoms is the feasibility of almost arbitrary trap geometries. Here, we will examine the influence of a uniform strain on the Rydberg exciton resonances in Cu_2O as a preliminary step to the description of Rydberg excitons in such traps. This will be achieved by the inclusion of the strain-induced deformation of the Γ_7^+ valence band [2] in numerical calculations, which include the full valence band nonparabolicity [3].

[1] T. Kazimierczuk *et al.*, Nature **514**, 7522 (2014)

[2] K. Suzuki and J.C. Hensel, Phys. Rev. B **9**, 10 (1974)

[3] F. Schöne *et al.*, Phys. Rev. B. **93**, 075203 (2016)

DS 36.54 Wed 17:00 P2-EG

Synthesis and crystal structure characterization of W5O14 and W18O49 nanowires — •Muhammad Saqib, Maja Remskar, and Janez Jalenc — Institut Jozef Stefan, Condensed matter Physics department, Ljubljana, Slovenia

Compared with other transition metal oxides, tungsten oxides have attracted great attention and have been investigated extensively due to their outstanding electrochromic, optochromic, and gas chromic properties. The individual W5O14 nanowires (NWs) made good ohmic contacts with W and Pt at room temperature and had excellent field-emission properties. Photoelectron spectroscopy revealed the metallic conductivity of the W5O14 NWs, which was confirmed by direct-transport measurements on a double stranded NWs. Here we report on achieving of reduction of tungsten three oxides to different sub- oxides nanowires by adding of elemental tungsten into the growth process. W5O14 and W18O49 nanowires are synthesized by the transport reaction in the presence of nickel as growth promoter and iodine as transport agent. The scanning electron microscope revealed rigid W5O14 and W18O49 NWs. Morphology and current-voltage characteristics of individual W5O14 NWs put on graphite were measured by scanning tunneling microscope operating in ultra-high vacuum. Surface structure of the W5O14 NWs was found affected by tunneling current, particularly on the NWs with weak interaction with the substrate. The work function of the NWs has been determined by Kelvin microscopy in non-contact atomic force microscopy operating in ultra-high vacuum.

DS 37: Focus Session on 2D Materials: Ballistic Quantum Transport in Graphene (jointly with HL, MA, TT)

Ballistic electron waves yielded a plethora of insights already in 2D semiconducting heterostructures. Recent experimental techniques have paved the way to this regime also for graphene. The massless, relativistic, and chiral nature of its charge carriers enriches ballistic transport by qualitatively new physical phenomena, such as ambipolar states near pn-junctions, Klein tunneling, or a zeroth Landau level in a perpendicular magnetic field. This session will review the actual status.

Organisation: Wolfgang Häusler, Universität Augsburg; Reinhold Egger, Universität Düsseldorf; Klaus Richter, Universität Regensburg

Time: Thursday 9:30–13:00 Location: HSZ 03

Invited Talk DS 37.1 Thu 9:30 HSZ 03
Kondo Screening of a Vacancy Magnetic Moment in Graphene — •Eva Y. Andrei — Dept. of Physics, Rutgers University, Piscataway, NJ

Graphene in its pristine form has transformed our understanding of 2D electron systems leading to fundamental discoveries and to the promise of important applications. When the perfect honeycomb lattice of graphene is disrupted by single atom vacancies new phenomena emerge including the buildup of local charge and the appearance of a local moment. Using scanning tunneling microscopy to identify Kondo screening of the vacancy moment by its spectroscopic signature, we demonstrate that the local magnetic moment can be controlled either by doping or through the local curvature. This allows to detect and map the quantum phase transition separating magnetic from nonmagnetic states in this pseudogap system.

Invited Talk DS 37.2 Thu 10:00 HSZ 03
Higher-Than-Ballistic Conduction in Viscous Electron Fluids — •Leonid Levitov — Physics Department, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge MA02139

This talk will argue that in viscous electron flows interactions facilitate transport, allowing conductance to exceed the fundamental Sharvin-Landauer quantum-ballistic limit. The effect is particularly striking for the flow through a viscous point contact, a constriction exhibiting the quantum-mechanical ballistic transport at zero temperature but governed by electron hydrodynamics at elevated temperatures. The crossover between the ballistic and viscous regimes occurs when the mean free path for e-e collisions becomes comparable to the constriction width. Further, we will discuss the negative nonlocal response, a signature effect of viscous transport. This response exhibits an interesting nonmonotonic behavior vs. temperature at the viscous-to-ballistic transition. The response is negative but small in the highly viscous regime at elevated temperatures. The value grows as the temperature is lowered and the system becomes less viscous, reaching the most negative values in the crossover region where the mean free path is comparable to the distance between contacts. Subsequently, it reverses sign at even lower temperatures, becoming positive as the system enters the ballistic regime. This peculiar behavior provides a clear signature of the ballistic-to-viscous transition and enables a direct measurement of the electron-electron collision mean free path.

Invited Talk DS 37.3 Thu 10:30 HSZ 03
Electron Optics in Ballistic Graphene — •Ming-Hao Liu — Department of Physics, National Cheng Kung University

Electrons in clean graphene are known to behave like “charged photons” due to its celebrated energy dispersion linear in momentum, providing an ideal platform for exploring electron optics. Despite the discovery of graphene in 2004, devices of ultraclean samples with micron-scale mean free paths became accessible only recently. Reliable quantum transport simulations in the ballistic limit for understanding and predicting high-quality transport experiments have therefore become increasingly demanded nowadays. In this talk, an overview of our recent progress on simulating a variety of ballistic graphene transport experiments will be given, such as Fabry-Pérot interference, snake states, and gate-defined electron waveguides [1]. Keys to such quantum transport simulations will be briefly introduced [2]. Ongoing works possibly including *pnp* junctions in the presence of 2D Moiré superlattice and Weiss oscillation due to 1D periodic gating will be mentioned at the end of the talk.

[1] P. Rickhaus *et al.*, Nat. Communs. **4**, 2342 (2013); M. Drienovsky *et al.*, Phys. Rev. B **89**, 115421 (2014); A. Varlet *et al.*, Phys. Rev. Lett. **113**, 116601 (2014); P. Rickhaus *et al.*, Nat. Communs. **6**, 6470 (2015); P. Rickhaus *et al.*, Nano Lett. **15**, 5819 (2015).
[2] M.-H. Liu *et al.*, Phys. Rev. Lett. **114**, 036601 (2015).

15 min. break.

Invited Talk DS 37.4 Thu 11:15 HSZ 03
Ballistic Transport in Mesoscopic Graphene Devices — •Christoph Stampfer — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

The recent technological advances in encapsulating graphene by hexagonal boron nitride forming artificial van-der-Waals heterostructures allows the fabrication of graphene devices with high electronic quality. Outstanding charge carrier mobilities and mean free paths with more than 10 micrometer are now accessible making this material stack interesting for studying ballistic transport. By further structuring the graphene-hBN based heterostructures mesoscopic devices can be fabricated on which phase coherent ballistic quantum transport can be studied.

Here, I will present low-temperature magneto-transport measurements on both (i) graphene quantum point contacts and (ii) high mobility graphene rings encapsulated in hexagonal boron nitride. Our experiments allow to extract information on quantized conductance, renormalized Fermi velocities close to the charge neutrality point as well as the co-existence of weak localization, Aharonov-Bohm oscillations and universal conductance fluctuations in graphene rings.

Invited Talk DS 37.5 Thu 11:45 HSZ 03
Interaction-Induced Conductance from Zero Modes in a Magnetic Graphene Waveguide — •Alex Zazunov — Heinrich-Heine-Universität Düsseldorf

We consider a waveguide formed in a clean graphene monolayer by a spatially inhomogeneous magnetic field. The single-particle dispersion relation for this waveguide exhibits a zero-energy Landau-like flat band, while finite-energy bands have dispersion and correspond, in particular, to snake orbits. For zero-mode states, all matrix elements of the current operator vanish, and a finite conductance can only be caused by virtual transitions to finite-energy bands. We show that Coulomb interactions generate such processes. In stark contrast to finite-energy bands, the conductance is not quantized and shows a characteristic dependence on the zero-mode filling. Transport experiments thereby offer a novel and highly sensitive probe of electron-electron interactions in clean graphene samples.

DS 37.6 Thu 12:15 HSZ 03
Ballistic thermophoresis on graphene — •Emanuele Panizon[1], Roberto Guerra[1,2], and Erio Tosatti[1,2,3] — [1]SISSA, Trieste, Italy — [2]CNR-IOM Democritos, Trieste, Italy — [3]ICTP, Trieste, Italy

The textbook thermophoretic force acting on a diffusing body in a fluid is proportional to the local temperature gradient. This is not the case for a diffusing physisorbed body on a submicron sized 2D suspended layer. A Non-Equilibrium Molecular Dynamics study of a test nanosystem - a gold nanocluster adsorbed on a single graphene sheet of length L clamped between two temperatures ΔT apart - reveals a phoretic force that is parallel to, but essentially independent of, the gradient magnitude $\Delta T/L$ up to a substantial L of $150nm$.

This is argued to represent ballistic thermophoresis, where the force is provided by the flux of massively excited flexural phonons, whose flow is in turn known to be ballistic and distance-independent up to relatively long scattering lengths before the eventual onset of the more standard diffusive regime. The surprising thrust and real momentum provided by the flexural modes are analysed and understood in terms of the large mass non/uniformity involved with these modes. The ensuing surf-riding of adsorbates on the vibrating 2D hard sheet, and the resulting gradient independent thermophoretic force, are not unlikely to possess practical applications.

DS 37.7 Thu 12:30 HSZ 03

Quantum time mirrors in two-band systems with and without broken time-reversal symmetry — •Phillipp Reck[1], Cosimo Gorini[1], Arseni Goussev[2], Viktor Krueckl[1], Mathias Fink[3], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Department of Mathematics, Physics and Electrical Engineering, Northumbria University, Newcastle Upon Tyne, UK — [3]Institut Langevin, ESPCI, CNRS, PSL Research University, Paris

Both metaphysical and practical considerations intrigued generations of scientists to devise and implement time-inversion protocols – in particular the Hahn echo [1], different forms of “time mirrors” for classical waves (see e.g. [2]), and recently an instantaneous time mirror for water waves [3]. With our proposal for an instantaneous Quantum Time Mirror [4], we showed the possibility to extend the family of time reversal protocols to *continuous quantum* systems, more precisely to wave packets in Dirac-cone systems, by changing the propagation direction with a short, time-dependent pulse.

In this talk, we discuss the effect on the Quantum Time Mirror of both, a static, out-of-plane magnetic field, which breaks time-reversal symmetry, and band structures other than the Dirac cone, e.g. the valence and conduction bands in direct gap semi-conductors.

[1] E. L. Hahn, Spin echoes. Phys. Rev.. 80, 580 (1950)
[2]M. Fink, IEEE Trans. Ultrason. Ferroelectr. Freq. Control, 39, 555, (1992)
[3]V. Bacot, et al., Nat. Phys. 12, 972–977 (2016)
[4]P. Reck, et al., arXiv:1603.07503 (2016)

DS 37.8 Thu 12:45 HSZ 03

Current flow paths in deformed graphene and carbon nanotubes — Erik Kleinherbers, •Nikodem Szpak, and Ralf Schützhold — Faculty of Physics, University of Duisburg-Essen, Germany

Due to imminent applications in nanoelectronics it is of high interest to understand the precise conductance properties of deformed graphene and bent carbon nanotubes. Since low-energy electronic excitations behave like massless Dirac fermions the current flow can be approximated semiclassically and used as a guide in the design of conducting nanoelectronic elements and nanosenors. Taking into account the curvature effects as well as an emerging inhomogeneous pseudo-magnetic field we calculate the current flow paths theoretically and compare them with numerical simulations of the full electronic transport.

DS 38: Focussed Session: Memristive Devices for Neuronal Systems I

Today’s computer science is characterized by a time of upheaval. The extremely successful down scaling of CMOS devices and circuit integration during the last decades will soon face physical limits. The predictable fade away of Moore-law, puts advance device structures paired with conceptual new non-Boolean architectures, such as cellular automata, quantum computer or neuromorphic circuits, more and more into the spot light of research and industry. In this respect the symposium will focus on novel opportunities of memristive devices in the field of bio-inspired computing. This symposium aims to overview of the interdisciplinary, covering interfacial physics, and electronic properties and the theory of memristive devices up to the complex architecture in biological nerve systems. This symposium aims to provide an overview of the status quo of memristive devices in neural systems by some of the leading experts in the field. Moreover, all speakers will discuss and work out the most promising and most exciting future directions, such as cognitive computing and memristive brain chips.

Organizers: Hermann Kohlstedt (CAU Kiel), Ronald Tetzlaff (TU Dresden), and Thomas Mikolajick (TU Dresden)

Time: Thursday 9:30–13:15 Location: CHE 89

Topical Talk DS 38.1 Thu 9:30 CHE 89

Memristive devices for neuromorphic systems — •Martin Ziegler — Nanoelektronik, Technische Fakultät der Christian-Albrechts-Universität zu Kiel, Germany

Biological nerve systems of vertebrates and invertebrates outperform today’s most powerful digital computers when it comes to pattern recognition, cognitive functionality or autonomous interaction with a steadily changing and noisy environment. Memristive devices offer attractive features to mimic biological functions of nerve systems in an elegant and efficient way. The talk provides an overview of recent developments in memristive devices and neuromorphic circuits based on memristive systems. In particular, it is shown how neural functionality can be emulate with memristive devices and how memory and learning processes can be replicate with electronic circuits based-on memristive devices.

Financial support by the German Research Foundation through FOR 2093 is gratefully acknowledged.

Topical Talk DS 38.2 Thu 10:00 CHE 89

Learning in Silico: neuromorphic models of long-term plasticity — •Elisabetta Chicca — Bielefeld University, Bielefeld, Germany

Synaptic plasticity empowers biological nervous systems with the ability to learn from experience and adjust to environmental changes. Such abilities are a must for artificial autonomous systems and therefore researchers have been devoting significant efforts to the understanding and modelling of plasticity mechanisms. In particular, the field of neuromorphic engineering focuses on the development of full-custom hybrid analog/digital electronic systems for the implementation of models of biological computation and learning in hardware. In this talk, I will give a short historical overview of the most important plasticity circuits developed following the approach originally proposed by Carver Mead in the late eighties. Afterwards, I will present recent advancements in this field.

DS 38.3 Thu 10:30 CHE 89

Emulation of neural synchrony with memristive devices — •Marina Ignatov, Martin Ziegler, Mirko Hansen, and Hermann Kohlstedt — AG Nanoelektronik, Christian-Albrechts-Universität zu Kiel, Germany

Conscious and perception are without doubt one of the most fascinating functionalities of the human brain and results from massive parallel computing in a huge self-organizing dynamical neural network. Neural synchrony is an elegant concept which tries to explain the underlying computing scheme by using dynamical network behaviours. In this talk we show that memristive devices allow a new degree of freedom to the concept of neural synchrony: a local memory which supports a transient connectivity. By using a 4-inch full device technology electrochemical metallization (ECM) cells with the layer sequence Ag/TiO_{2-x}/Al are fabricated. Those devices are used to couple self-sustained van der Pol oscillators in an electronic circuit. As a result an autonomous frequency adaptation and phase locking is observed. The underlying circuit and device requirements and their impact to neuromorphic computing are discussed in this talk.

Financial support by the German Research Foundation through FOR 2093 is gratefully acknowledged.

[1] M. Ignatov et al., Appl. Phys. Lett. 108(8), 084105 (2016)

DS 38.4 Thu 10:45 CHE 89

Quantitative spectroscopic analysis of memristive thin films — •Julian Strobel[1], Mirko Hansen[2], Krishna Kanth Neelisetty[3], Venkata Sai Kiran Chakravadhanula[3], Hermann Kohlstedt[2], and Lorenz Kienle[1] — [1]Institut für Materialwissenschaft, Technische Fakultät der CAU Kiel, Kaiserstr. 2, 24143 Kiel — [2]Institut für Elektrotechnik, Technische Fakultät der CAU Kiel, Kaiserstr. 2, 24143 Kiel — [3]Institut für Nanotechnologie, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

Memristive NbOx/AlOx tunnel barriers have been analyzed by electron energy-loss spectroscopy to the effect of gaining information on the electronic structure. Slight oxidation of the bottom electrode, likely occurring during fabrication of the overlying oxide layers, is observed but is expected to have little to no effect on the I-V characteristics. The AlOx layer was found to exhibit states within the bandgap caused by oxygen vacancies. A model for quantification of the oxygen vacancies is presented and discussed with respect to expected accuracy.

DS 38.5 Thu 11:00 CHE 89

MemFlash: Memristive operation of MOSFETs with external capacitances — •Henning Winterfeld[1], Nico Himmel[1], Martin Ziegler[1], Henning Hanssen[2], Detlef Friedrich[2], Wolfgang Benecke[2], and Hermann Kohlstedt[1] — [1]Nanoelektronik, Technische Fakultät, Christian-Albrechts Universität zu Kiel, Germany — [2]Fraunhofer-Institut für Siliziumtechnologie (ISIT), Itzehoe, Germany

Memristive devices have the potential to act as key elements in neuromorphic circuits. However, system integration has turned out to be difficult, as it requires a wafer level fabrication technology. Therefore, MemFlash cells are an interesting alternative to state-of-the-art memristive devices. MemFlash cells are single floating gate transistors operating in a memristive operation mode. In this talk it will be shown that MOSFETs can act as MemFlash cells by using an external capacitor. Fabricated devices vary in channel length and width with tunneling windows between 4 μm^2 and 100 μm^2. Furthermore, tunnel barrier thicknesses between 3 nm up to 10 nm were realized. The elevation of charges through the tunneling window onto the floating gate via Fowler-Nordheim tunneling allows hysteresis measurements. Measurements show on-off resistance values of about 40 kOhm and 4.2 GOhm, respectively. The electrical characteristics of those devices will be presented, while based on this data, possible advantages and disadvantages of the MemFlash device with respect to conventional memristive devices will be discussed.

Financial support by the German Research Foundation through FOR 2093 is gratefully acknowledged.

15 min. break.

Topical Talk DS 38.6 Thu 11:30 CHE 89

Design and CMOS Co-Integration of ReRAM Devices and Crossbar Arrays for Neuromorphic Applications — •Yusuf Leblebici — Swiss Federal Institute of Technology (EPFL), Lausanne, Switzerland

Resistive RAM (ReRAM) elements based on transition-metal oxide layers are rapidly becoming viable options for nonvolatile information storage and for neuromorphic operations, allowing easy integration with conventional CMOS technologies. In this talk, we will review the ongoing research at EPFL on the realization of various ReRAM elements based on TiOx, TaOx, WOx and HfOx layers tailored for low voltage operation, as well as the design and co-integration of the CMOS peripheral circuitry for the read/write operations. In particular, the chip embedding platform enabling post-processing of diced samples for fabrication of memristive elements will be discussed, and examples will be provided for potential neuromorphic functions such as spike-timing-dependent-plasticity (STDP) and back-propagation implemented on cross-bar arrays.

Topical Talk DS 38.7 Thu 12:00 CHE 89

Neuromorphic Memristive Systems — •Bernabe Linares-Barranco — Instituto de Microelectronica de Sevilla IMSE-CNM (CSIC), Av. Americo Vespucio s/n, 41092 Sevilla, Spain

Nanoscale memristors promise to be fabricated over CMOS substrates with densities of over 4x10^{12} elements per cm^2 (which corresponds to a 50nm pitch). This would provide an overwhelming memory density very tightly coupled to CMOS computing elements. There are many fields where this disruptive advantage can be exploited. One of them is neuromorphic computing and learning systems. In this talk we present some ideas on how to exploit this technological possibility for implementing hybrid memristive-CMOS systems. We will start by introducing event-driven spiking neural systems, how they can learn through Spike-Timing-Dependent-Plasticity (STDP), and how this can be exploited with combined memristor-CMOS chips. Recent state-of-the-art results will be shown.

DS 38.8 Thu 12:30 CHE 89

Gate-tunable, normally-on to normally-off memristance transition in patterned LaAlO3/SrTiO3 interfaces — Patrick Maier, •Fabian Hartmann, Judith Gabel, Maximilian Frank, Silke Kuhn, Philipp Scheiderer, Berengar Leikert, Michael Sing, Lukas Worschech, Ralph Claessen, and Sven Höfling — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, D-97074 Würzburg

The state- and time-dependent resistance of memristors enables the emulation of synaptic functionalities, and hence memristor-based artificial synapses may be implemented in novel, brain inspired computing architectures. We report reversible and irreversible control of memristive switching in patterned LaAlO3/SrTiO3 interfaces via gate voltages and annealing, respectively. The inherent memory functionality (memristance) can be switched on and off with back gate voltages of a few volts. Irreversible control of the memristive switching is demonstrated by annealing the device at 300 °C in nitrogen atmosphere, during which oxygen vacancies are created in the SrTiO3 substrate. These vacancies release mobile electrons that screen the electric field of the back gate. Tuning the amount of mobile electrons with the annealing time allows switching on and off the memristance at zero gate voltage leading to normally-on and normally-off memristors, respectively. The presented irreversible and reversible control of memristive characteristics may allow to compensate fabrication variabilities of memristors.

DS 38.9 Thu 12:45 CHE 89

Thin carbon nanotube (CNT) film networks and their memristive behaviors in cooperation with noble metal clusters — •Victor Kaidas, Alexander Vahl, Sandra Hansen, Fabian Schütt, Jürgen Carstensen, Sören Kaps, Franz Faupel, and Rainer Adelung — Institut für Materialwissenschaften der Christian Albrechts Universität, Kiel, Deutschland

Memristic devices have gained lot of attention since their discovery leading to many different fabrication ways. The first ones were based on the movement of oxygen vacancies or other charge carriers (e.g. Ag ions) in metal oxides induced by an applied field and a resulting drift in the respective matrix. As a consequence different matrix materials were investigated like polymers, biomaterials and carbon nanotubes (CNTs) in regards of their memristive effect in various systems, which is the main focus here as well. Our approach is based on a previous study in which semiconducting high aspect ratio materials in the micrometer regime and different hybridized carbon species were brought together and successfully checked for their memristive characteristics. Here we present a thin CNT film and the formation of a conducting network between two Au electrodes. To obtain the film different ways of applying the CNTs were used like spin, drop or spray coating until a sufficient network was achieved. By adding noble metal clusters into the network it is now possible to induce memristive effects by letting the corresponding ions move. Our long term goal is fabricating structures even with a higher range of interconnection with the outlook to obtain 3D memristive structures using this approach.

DS 38.10 Thu 13:00 CHE 89

Ion dynamics in double barrier memristive devices — •Sven Dirkmann[1], Mirko Hansen[2], Martin Ziegler[2], Enver Solan[3], Karlheinz Ochs[3], Hermann Kohlstedt[2], and Thomas Mussenbrock[4] — [1]Ruhr-Universität Bochum, Lehrstuhl für Theoretische Elektrotechnik, 44780 Bochum — [2]Christian-Albrechts-Universität zu Kiel, Nanoelektronik, 24143 Kiel — [3]Ruhr-Universität Bochum, Lehrstuhl für Digitale Kommunikationssysteme, 44780 Bochum — [4]Brandenburgische Technische Universität Cottbus-Senfenberg, Theoretische Elektrotechnik, 03046 Cottbus

In this work we analyze the role of ion transport for the dynamic behavior of a double barrier quantum mechanical memristive device using a consistent simulation model.[1,2] The device consists of an ultra-thin NbxOy solid state electrolyte sandwiched between an Al2O3 tunnel barrier and a Schottky-barrier at the NbxOy/Au interface. Many interesting features, as an intrinsic current compliance, a relatively long retention time and no need for an initialization step, make this device technologically interesting, particularly for applications in neuromorphic systems. The electron transport is mimicked by a lumped element circuit model consistently coupled with a 3D kinetic Monte Carlo model, describing the ion transport. The simulation results prove that the ionic motion within the NbxOy layer is the key factor for the resistive switching behavior.This work is funded by the DFG in the frame of Research Unit FOR2093 ”Memristive Devices for Neural Systems”.

[1] M. Hansen et al., Scientific Reports 5, 13753 (2015)

[2] S. Dirkmann et al., Scientific Reports 6, 35686 (2016)

DS 39: Thin Film Applications

Time: Thursday 9:30–13:15 Location: CHE 91

DS 39.1 Thu 9:30 CHE 91

Transport properties of nanostructured graphene — •Victor Aristov[1,2,3], Olga Molodtsova[1,4], Sergey Babenkov[1], Han-Chun Wu[5], Alexander Chaika[2], Dmitry Marchenko[6], Andrei Varykhalov[6], Alexei Zakharov[7], Yuran Niu[7], Alexei Preobrajenski[7], Denis Vyalikh[8], Barry Murphy[9], Sergey Krasnikov[9], and Igor Shvets[9] — [1]DESY, Hamburg, Germany — [2]ISSP RAS, Chernogolovka, Russia — [3]TU Bergakademie, Freiberg, Germany — [4]ITMO, Saint Petersburg, Russia — [5]BIT, Beijing, China — [6]BESSY, Berlin, Germany — [7]Max-lab, Lund, Sweden — [8]TU Dresden, Germany — [9]Trinity College, Dublin, Ireland

Trilayer graphene reveals unique electronic properties appealing for fundamental science and electronic technologies. We propose a simple method to open a charge transport gap and achieve a high on-off current ratio in Bernal-stacked trilayer graphene synthesized on vicinal SiC(001). Low-temperature measurements show that self-aligned, periodic nanodomain boundaries induce a huge charge transport gap of more than 1.3 eV at 10 K and 0.4 eV at 100 K. Our studies indicate the feasibility of creating electronic nanostructures using graphene on cubic-SiC/Si wafers.This work was supported by the RAS, RFBR grants No 17-02-01139 and No 17-02-01291.

DS 39.2 Thu 9:45 CHE 91

Co-doping of VO$_2$ with W and Sr for intelligent glazing — •Florian Kuhl, Angelika Polity, and Peter J. Klar — I. Physikalisches Institut, Justus Liebig University, Heinrich-Buff-Ring 16, DE-35392 Giessen, Germany

Vanadiumdioxide is a thermochromic material that undergoes a semiconductor-to-metal transition (SMT) at about 68 °C due to a phase change from monoclinic to rutile phase. At this transition the transmittance and reflectivity in the near infrared is decreased, thus it is an interesting material for intelligent window coatings for controling the temperature in buildings passively. But due to its transition temperature and optical properties, VO$_2$ thin films are not used for window coatings. Literature reports that the doping with tungsten will decrease the transition temperature and the doping with alkaline earth metals like Sr will enhance the optical properties.

We present our results on thin films that are co-doped with W and Sr in the rf sputtering process. With this method we can use both effects. On the one hand the transition temperature is reduced and on the other hand the optical properties can be improved so that the thin films show comparable properties to comercially available electrochromic window glazings. Furthermore we produced multi layer systems with anti reflective coatings to obtain coatings with enhanced properties for the use as intelligent glazings.

DS 39.3 Thu 10:00 CHE 91

SrZrO Interlayer — •Corinna Müller, Patrick Salg, Aldin Radetinac, Philipp Komissinskyi, and Lambert Alff — Technische Universität Darmstadt, Germany

We present SZO thin film utilized as a oxygen diffusion barrier grown by PLD. SZO is grown between BST and SMO in an all-oxide varactor to inhibit the oxidation of SMO. In the past STO has been used for this purpose but the performance was not optimized yet. SZO is very promising because of its very low oxygen diffusion constant in the range of $10^{-12} cm^2 s^{-1}$ compared to STO with $10^{-4} cm^2 s^{-1}$ [1],[2]. This work shows that SZO grows on top of SMO with very low oxygen partial pressure. Growth studies are performed with different parameters like laser fluence and substrate temperature. It could be shown that SZO is very invariant to these parameters. The problem of SZO is the big lattice constant compared to the substrate. Reciprocal space maps show that the resulting films relax instead of growing strained. To optimize this behaviour a mixture of STO and SZO is grown. The performance as an oxygen diffusion barrier is investigated with in-situ XPS studies. For that the SMO is capped with SZO and annealed under oxygen atmosphere.

[1] C. Nivot et al., "Oxygen diffusion in SrZrO3", Solid State Ionics, vol. 180, no. 17-19, pp. 1040-1044, 2009.

[2] T. Bieger et al., "Kinetics of oxygen incorporation in SrTiO3 (fe-doped): An optical investigation", Sensors and Actuators B: Chemical, vol. 7, no. 1-3, pp. 763-768, 1992.

DS 39.4 Thu 10:15 CHE 91

Sensor applications of indium tin oxide nano-columns formed by glancing angle deposition — •Kenneth Harris[1,2], Abebaw Jemere[1], Donghai Lin[1], Nora Chan[3], Véronique Balland[4], and Benoît Limoges[4] — [1]National Research Council Canada, National Institute for Nanotechnology, Edmonton, Canada — [2]Leibniz Institute of Polymer Research, Dresden, Germany — [3]Defense Research and Development Canada, Suffield, Canada — [4]Université Paris Diderot 7, Molecular Electrochemistry Laboratory, Paris, France

The glancing angle deposition (GLAD) technique can be used to fabricate nano-columnar structures with precisely-controlled shapes (including cylinders, helices, zig-zags and others) and in a wide variety of materials (including metals, oxides, ceramics and small-molecule organics). In this presentation, I will describe glancing angle deposition of the transparent conductor indium tin oxide (ITO), discussing deposition conditions and post-treatments to control electrical conductivity and transparency to visible light. Sensing applications of these GLAD-ITO structures will then be presented. Due to their large and accessible surface area, GLAD-formed structures can adsorb (or interact with) large quantities of analytes. With ITO-based sensors, both light transparency and electrical conductivity are also built into the materials system, allowing electrical and optical phenomena to be actively monitored during exposure to analytes of interest. Data from two representative GLAD-ITO sensing platforms will be presented: sensors for detection of bacterial surface proteins, and spectro-electrochemistry electrodes to observe the evolution of chemical redox reactions.

DS 39.5 Thu 10:30 CHE 91

Optical Investigation of Structural Disorder in Normal Spinel Ferrites in Relation to Magnetic Properties — •Vitaly Zviagin[1], Yogesh Kumar[1], Paula Huth[2], Israel Lorite[1], Annette Setzer[1], Daniel Spemann[3], Jan Meijer[1], Reinhard Denecke[2], Pablo Esquinazi[1], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany — [2]Universität Leipzig, Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Linnéstr. 2, Germany — [3]Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, Germany

We present an optical investigation of structural disorder in spinel ferrites grown at different temperatures and pressures on MgO (100) and SrTiO$_3$ (100) substrates by pulsed laser deposition. Optical transitions in the diagonal elements of the dielectric tensor, obtained by spectroscopic ellipsometry, were identified and related to the presence of Fe^{2+} and Fe^{3+} cations located at different lattice sites corresponding to disorder and inversion of the normal crystal structure. Procedures such as annealing and irradiation with Si ions were applied to induce disorder and to alter the crystal structure of the investigated thin films. A direct correlation between the overall magnetic response, measured by SQUID, and the presence of Fe^{3+} on the tetrahedral lattice sites has been found and can be explained by the ferrimagnetic order of the crystal due to the dominating nature of the oxygen mediated coupling between the tetrahedral and octahedral lattice sites.

DS 39.6 Thu 10:45 CHE 91

Nanostructured Freestanding Silicon Nitride Membranes for Field Electron Emission Based Detectors in Mass Spectrometry — •Stefanie Haugg, Chris Thomason, Christian Henkel, Robert Zierold, and Robert H. Blick — Institute of Nanostructure and Solid State Physics, Universität Hamburg, Hamburg, Germany

Freestanding nanomembranes can potentially be utilized in the detector unit of commercial time-of-flight (TOF) mass spectrometers because of their (i) quasi-dynamic mode of vibration or (ii) phonon-assisted field electron emission properties.[1]

Herein, rod-shaped nanostructures on freestanding silicon nitride membranes have been processed via a top-down approach using gold nanodots as hard mask for subsequent reactive ion etching. We show that geometrically enhanced field electron emission can be observed—in a emitter-grid-anode test setup connected to a transimpedance amplifier—on such nanostructured membranes compared to their planar counterparts.

Moreover, we employ microchannel plates for signal amplification of field electron emission from our nanostructured membranes. This configuration offers the possibility to combine sample characterization with TOF mass spectrometry measurements without changing the setup.

[1] Park, J.& Blick, R. H. A silicon nanomembrane detector for matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) of large proteins. Sensors 13 (2013)

DS 39.7 Thu 11:00 CHE 91

Nanoscale picosecond acoustic spectrometry of phononic superlattices — •Dennis Meyer[1], Henning Ulrichs[1], Florian Döring[2], and Hans-Ulrich Krebs[2] — [1]I. Physikalisches Institut, Universität Göttingen, Germany — [2]Institut für Materialphysik, Universität Göttingen, Germany

We show how the characteristics of acoustic resonances in metallic nano-cavities can be tailored by tuning the interplay with an underlying phononic crystal. For this purpose we exploit ultrafast optical excitation, which enables us to address a resonant surface mode with frequency around 180 GHz in a wedge-shaped tungsten thin film, grown on a MgO/ZrO$_2$ phononic crystal. The lifetime of the surface mode was found to vary between 60 and 250 ps, depending on the position on the wedge. Vice versa, one can also regard our results as a demonstration of a nanoscale acoustic spectrometry principle for investigation of the elastic wave band structure of a superlattice: a strong response of the surface layer only appears for frequencies inside an acoustic mini-band gap. By spatially moving the laser across the wedge, the first mini-band gap was mapped out. These results are in good agreement to a theoretical model of the system. In addition to these findings, we see an unexpected increase in frequency in the experimental data, when crossing the lower band-gap edge from above. We acknowledge financial support by the DFG within the CRC 1073 'Atomic scale control of energy conversion'.

15 min. break.

DS 39.8 Thu 11:30 CHE 91

Minimizing thermal conductivity in laser deposited multilayers — •Döring Florian and Krebs Hans-Urlich — Institut für Materialphysik, Universität Göttingen

Minimizing thermal conductivity is essential for modern applications in the field of thermal barrier coatings, thermoelectrics, cryogenics and space-applications. The reduction of thermal conductivity can be achieved by an increase of phonon scattering and phonon localization as well as by a reduction of phonon mean free path and velocity. These effects happen typically in materials with a high amount of interfaces and result in a thermal boundary resistance. Thus, the goals in order to minimize the thermal conductivity are on the one hand to maximize the interface density and on the other hand to maximize the thermal boundary resistance at each interface, which gives a high overall thermal resistance and thereby a low thermal conductivity. Those goals can be achieved by combining materials with a high acoustic mismatch in nanoscale multilayers. A prominent method for this purpose is pulsed laser deposition, which is a very versatile thin film method, allowing combining materials with very different properties such as metals, oxides and polymers and thus fabricating materials with a high density of interfaces between dissimilar materials that show a high thermal resistance. In this contribution, multilayers of W/polycarbonate and W/ZrO2 as well as measurements on their thermal conductivity, showing very low values, are presented. While the first material combination excels by a very high acoustic mismatch, the second material combination is outstanding in terms of thermal stability.

DS 39.9 Thu 11:45 CHE 91

Ion-beam-induced magnetic and structural phase transformation of fcc Fe thin films on different substrates — •Jonas Gloss[1], Michal Horký[1,2], Bernhard Ruch[1], Viola Křižáková[2], Lukáš Flajšman[2,3], Michael Schmid[1], Michal Urbánek[2,3], and Peter Varga[1,3] — [1]Inst. of Appl. Phys., TU Wien, AT — [2]Inst. of Phys. Engineering, Brno University of Technology (BUT), CZ — [3]Central European Inst. of Tech. BUT, CZ

It has been shown that 5-10 ML thick Fe films on Cu(100) have an fcc structure and are nonmagnetic at room temperature [1]. Ion beam irradiation of the fcc films causes a structural transformation from fcc to bcc as well as a magnetic transformation from nonmagnetic to ferromagnetic. To remove the 10-ML thickness limit of fcc Fe we alloyed it with 22% of Nickel to form the metastable fcc Fe [2]. To make use of the metastable films for magnonic crystals, we replaced the Cu(100) with two new alternative substrates H-Si(100) and C(100), which are also more suitable for applications and optical analysis. The first substitute is hydrogen terminated Si(100) with a Cu buffer layer. The as-grown Fe$_{78}$Ni$_{22}$ is corrugated, but metastable. The second successfully adapted substrate is undoped diamond C(001), on which metastable Fe$_{78}$Ni$_{22}$ films can be grown in 4-ML steps followed by post annealing.

[1] A.Biedermann, R.Tscheließnig, M.Schmid and P.Varga, Phys. Rev. Lett. **87** (2001) 086103

[2] J. Gloss, S. Shah Zaman, J. Jonner, Z. Novotny, M. Schmid, P. Varga, M. Urbánek, Appl. Phys. Lett. **103** (2013) 262405

DS 39.10 Thu 12:00 CHE 91

A Novel Approach to Monitor Surface Driven Photocatalysis Reactions at Titania-Organic Dye Interfaces — •Cenk Aktas, Muhammad Zubair Ghori, Mohammed Emami, Alexander Wahl, Oleksandr Polonskyi, Thomas Strunskus, and Franz Faupel — Institute for Materials Science, Chair for Multicomponent Materials, Faculty of Engineering, Christian-Albrechts-University of Kiel, Kaiserstraße 2, D-24143 Kiel, Germany

Titania is one of semi-conductor oxides which has been extensively studied in the past due to its high photocatalytic activity. On the other hand there is still a lack of knowledge in understanding mechanism of titania photocatalysis. Basically the degradation of an organic dye is monitored by time in terms of its optical absorption to analyse the photocatalytic activity. Most of these analyses are carried out in wet environment and there is relatively less study on characterisation of photocatalytic activity in gas or solid phase. While former gives an indirect measure, later may provide details of the surface reactions taking place directly at the titania-organic layer interface. This work covers a novel analytic approach to investigate details of the photocatalytic reaction at the titania surface using a dry test medium (organic dye in the form of a thin film). A comparative study between the wet and dry analysis approaches is also provided to understand the overall mechanism involved in the photocatalysis.

DS 39.11 Thu 12:15 CHE 91

The Effect of Surface Modification by Atomic Layer Deposition on the Field Emission Characteristic of Free-Standing Diamond Nanomembranes for Mass Spectrometry — •Christian Henkel, Chris Thomason, Stefanie Haugg, Robert Zierold, and Robert H. Blick — Institute of Nanostructure and Solid State Physics, Universität Hamburg, Hamburg, Germany

For mass spectrometry of large proteins, a nanomembrane based detector can be used for high-resolution measurements in the range > 100 kDa. Its efficiency is heavily influenced by the eletromechanical properties of the membrane in the detector unit.

As an improvement, zinc oxide is deposited on the surface of suspended diamond nanomembranes by means of atomic layer deposition. Electron field emission is measured as a function of the applied electric field for different cycle numbers in a home-made test setup at room temperature. The field emission characteristic is found to be highly dependent on the surface modification by ALD, possibly due to a change of the intrinsic electrical properties of the emitting material. Specifically, we found a decrease in work function as well as turn-on field of field emission for film thicknesses less than 1 nm, while thicker films lead to a huge increase of both.

Hereby, we prove that chemical surface modification by means of ultra-thin ALD coatings might lead to enhanced field emission properties of nanomembranes.

DS 39.12 Thu 12:30 CHE 91

A hybrid molecular beam epitaxy based growth method for large-area synthesis of stacked hexagonal boron nitride/graphene heterostructures — •Siamak Nakhaie[1], Joseph M. Wofford[1], Thilo Krause[1], Xianjie Liu[2], Manfred Ramsteiner[1], Michael Hanke[1], Henning Riechert[1], and J. Marcelo J. Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]Department of Physics, Chemistry and Biology, Linköping University, SE-58183 Linköping, Sweden

Devices based on the graphene/hexagonal boron nitride (h-BN) materials system offer a host of potential advantages, including high speed, extremely low power consumption, and various novel functionalities. As a result, the large-area synthesis of this material has been extensively researched over the past few years using various crystal growth techniques. In this contribution, we introduce a method for the production of h-BN/graphene heterostructures which allows both materials to form on the surface of the Ni substrate. We exploit the finite solubility of C in Ni by first saturating the metal film, then depositing a few-layer thick h-BN film from elemental B and N on the exposed Ni surface, and finally ramping the sample temperature down to controllably precipitate the C and form graphene at the interface between the h-BN and Ni. The resulting heterostructures are studied using various characterization techniques, such as UV and visible Raman spectroscopy, x-ray photoelectron spectroscopy and synchrotron-based grazing incidence spectroscopy to learn about their structural properties and quality.

DS 39.13 Thu 12:45 CHE 91

Phase transforming magnetocaloric Heuslers for multiferroic devices — •Yi-Cheng Chen[1,2], Parul Devi[1], Benedikt Ernst[1], Roshnee Sahoo[1], Ying-Hao Chu[2], Sanjay Singh[1], Gerhard Fecher[1], and Claudia Felser[1] — [1]MPI- CPfS, Dresden, Germany — [2]National Chiao Tung University, Hsinchu, Taiwan

Ni-Mn based magnetocaloric Heusler alloys show large resistance change at their magneto-structural (austenite-martesnite) phase transition. The martensite transition in these alloys is very much sensitive to the external pressure or strain and phase fraction of martensite can be easily tuned via strain. Therefore, a large resistance change can be realized in a magnetocaloric Heusler/Piezo heterostructure via the strain control of a ferroelectric substrate. We prepared the $Ni_2Mn_{1-x}In_x$ Heusler thin film on PMN-PT substrate using DC-magnetron sputtering and studied them using x-ray diffraction, EDX and magnetization measurements. The x-ray diffraction reveals a coexistence of austenite and modulated martensite phase at room temperature. The magnetization measurements show martensite transition over a broad temperature range as evident by the observed thermal hysteresis. Our future perspective is to obtain sharp austenite-martensite transition and to apply strain with electric field on this heterostructure film, which induces a change in the phase fraction and hence resistance that can be used as multiferroic devices .

DS 39.14 Thu 13:00 CHE 91

Growth and characterization of NbSe2 on Al2O3 (0001) using molecular beam epitaxy — •Avanindra Kumar Pandeya, Kai Chang, Amilcar bedoya Pinto, Ilya Kostanovskiy, and Stuart Parkin — Max Planck Institute of Microstructure Physics

The most common way to produce transition metal dichalcogenide (TMDC) thin films is via mechanical exfoliation, a method which is not well-suited to fabricate heterostructures with coherent interfaces or large-area thin film applications. Moreover, spintronic effects such as spin transfer torque are extremely sensitive to the quality of the heterointerface. Our approach is to use molecular beam epitaxy (MBE) to grow in-situ TMDC heterostructures and assess the layer and interface quality using in-situ characterization (RHEED, LEED, XPS and STM). Employing a two-step growth scheme, we achieved high-quality, single-crystalline NbSe2 layers on Al2O3 (0001) substrates. A superconducting transition was observed below 4K and is found to be driven by the carrier density in the metallic layers. The achievement of epitaxial, high-quality TMDC layers with high spin-orbit coupling opens up good prospects to realize an efficient spin transfer in TMDC/ferromagnet bilayers.

DS 40: Focussed Session: Memristive Devices for Neuronal Systems II

Today's computer science is characterized by a time of upheaval. The extremely successful down scaling of CMOS devices and circuit integration during the last decades will soon face physical limits. The predictable fade away of Moore-law, puts advance device structures paired with conceptual new non-Boolean architectures, such as cellular automata, quantum computer or neuromorphic circuits, more and more into the spot light of research and industry. In this respect the symposium will focus on novel opportunities of memristive devices in the field of bio-inspired computing. This symposium aims to overview of the interdisciplinary, covering interfacial physics, and electronic properties and the theory of memristive devices up to the complex architecture in biological nerve systems. This symposium aims to provide an overview of the status quo of memristive devices in neural systems by some of the leading experts in the field. Moreover, all speakers will discuss and work out the most promising and most exciting future directions, such as cognitive computing and memristive brain chips.

Organizers: Hermann Kohlstedt (CAU Kiel), Ronald Tetzlaff (TU Dresden), and Thomas Mikolajick (TU Dresden)

Time: Thursday 15:00–16:45 Location: CHE 89

Topical Talk DS 40.1 Thu 15:00 CHE 89

Brain-inspired neurocomputing with memristive synapses — •Daniele Ielmini — Dipartimento di Elettronica, Informazione e Bioingegneria, Politecnico di Milano, Italy

As Moore's law of CMOS downscaling slows down, research on alternative computing devices and architectures receives an increasing interest. Among these, memcomputing and neurocomputing combine a relatively simple concept (e.g., analog/digital circuits, CMOS compatible materials, room operation operation) with attractive functionalities, such as reconfigurability, ultra-low power operation, and brain-like computing capabilities including learning and inference. Merging memcomputing and neurocomputing may result in novel conceptual schemes with high energy efficiency, high speed, excellent scalability, and brain-like computing capabilities.

This talk will show recent advances on neuro-computing using memristive synapses made of resistive switching memory (RRAM) devices. Hybrid CMOS/memristive synapses capable of spike-timing dependent plasticity (STDP) and spike-rate dependent plasticity (SRDP) will be experimentally demonstrated. Pattern learning will be demonstrated by a feedforward neural network with up to 4x4 input images, 2 post-synaptic firing neurons, handling both static and dynamic moving images. The prospects of such new achievements for brain-inspired computing will be discussed.

Topical Talk DS 40.2 Thu 15:30 CHE 89

Exploring evolutionary biology and neuromorphic computing with quantum materials — •Shriram Ramanathan — Purdue University, USA

I will introduce frontier problems in evolutionary biology, their dynamics and intimate connection to neuromorphic information processing in my presentation. I will particularly emphasize the promise of adaptive quantum materials, such as strongly correlated oxide semiconductors and contrast their physics with filamentary switches and chalcogenides. The following problems will be considered: (1) structural symmetry breaking and electronic transitions driven by external stimuli in correlated electron systems, (2) the use of electrolyte membranes to create soft interfaces for neural computing circuits and (3) disorder and extreme carrier doping to create emergent phases whose volatility can be controlled by design. Connections to artificial intelligence and synergies with circuits research that is typically materials agnostic will be highlighted.

DS 40.3 Thu 16:00 CHE 89

Implementation of memristive devices in a crossbar-based pattern recognition scheme — •Mirko Hansen, Martin Ziegler, Finn Zahari, and Hermann Kohlstedt — AG Nanoelektronik, Christian-Albrechts-Universität zu Kiel, Germany

While several neuron-based learning concepts like Hebbian learning or spike-timing-dependent-plasticity have been successfully shown using single devices, their realization of whole systems using memristive devices remains challenging. Due to the progress in the field and the increase of devices per circuit, additional problems in terms of reliability and requirements in device quality arise.

We will present simulation results for a pattern recognition scheme using the MNIST benchmark dataset[1]. Parameters for these simulations were extracted from automated pulse measurements on niobium-oxide based double barrier memristive devices (Nb/Al-AlO_x/Nb_xO_y/Au)[2]. These devices show analog switching behavior, a high resistance and a strong I-V-nonlinearity, making them good candidates for the presented pattern recognition system. Aside from general pattern recognition performance, the impact of imperfect devices for the recognition rate will be shown. This includes the whole range of fabrication problems from shorted devices to devices with a high variability in switching, over to non-switching high resistance devices. Financial support by the German Research Foundation through FOR 2093 is gratefully acknowledged.

[1] F. Zahari et al., AIMS Materials Science 2: 203-216 (2015)

[2] M. Hansen et al., Scientific Reports, vol. 5, p. 13753 (2015)

DS 40.4 Thu 16:15 CHE 89

A Concentrated Model of the Double Barrier Memristive Device for LTSpice Simulations — •Enver Solan[1], Sven Dirkmann[2], Martin Ziegler[3], Mirko Hansen[3], Hermann Kohlstedt[3], Thomas Mussenbrock[4], and Karlheinz Ochs[1] — [1]Ruhr-Universität Bochum, Lehrstuhl für Digitale Kommunikationssysteme, 44780 Bochum — [2]Ruhr-Universität Bochum, Lehrstuhl für Theoretische Elektrotechnik, 44780 Bochum — [3]Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel, 24143 Kiel — [4]Brandenburgische Technische Universität Cottbus-Senftenberg, Fachgebiet Theoretische Elektrotechnik, 03046 Cottbus

The double barrier memristive device is a technical implementation of a memristive system. It consists of an ultra-thin memristive layer sandwiched between a tunnel barrier and a Schottky-like contact. In principle, it is a nonlinear resistor with memory, whereby the resistance depends on energetic states at the interfacial barriers. This leads to a continuous resistance range, which is desired for neuromorphic applications. To understand the underlying physical and chemical phenomena, a distributed model of the device, using a kinetic Monte-Carlo simulation, has been implemented. Such simulations are very time-consuming and therefore not suitable for real-time implementations, e.g. for emulation purposes. Starting from the distributed model a concentrated model of the device with physically meaningful parameters has been developed. It can be used for reproducible analyses and emulation purposes. The concentrated model was verified by comparisons with Monte-Carlo simulations as well as with measurements.

DS 40.5 Thu 16:30 CHE 89

An FPGA Implementation of a Memristive System Based on Wave Digital Principles — •Enver Solan[1], Benedikt Janssen[2], Karlheinz Ochs[1], and Michael Hübner[2] — [1]Ruhr-Universität Bochum, Lehrstuhl für Digitale Kommunikationssysteme, 44780 Bochum — [2]Ruhr-Universität Bochum, Lehrstuhl für Eingebettete Systeme der Informationstechnik, 44780 Bochum

The massively parallel structure of neuromorphic circuits leads to efficient computations of complex problems. Depending on the learning process, the interconnections between neurons are differently weighted. This functionality can be modeled by memristive devices * nonlinear resistors with memory.

These devices in nanotechnology contain always parameter spread, which makes reproducible analyses hard. Additionally, some neuromorphic applications may need a desired but not realizable memristive functionality. Simulation models can be used, but they are very time-consuming and even less suited for hardware emulation purposes. Due to these issues, hardware emulators of memristive systems are needed.

Our approach pursues an FPGA implementation of memristive systems based on wave digital principles. This leads to a generic memristive emulator by maintaining the passivity of the analog device.

DS 41: Layer Properties: Electrical, Optical, and Mechanical Properties II

Time: Thursday 15:00–16:45 Location: CHE 91

DS 41.1 Thu 15:00 CHE 91

Magnetoconductivity in ZnMnO thin films with anisotropic, highly conductive surface layers modelled by the Thouless diffusion length and valley degeneracy factor. — •Sahitya V. Vegesna[1], Danilo Bürger[1], Rajkumar Patra[1], Barbara Abendroth[2], Ilona Skorupa[1,3], Oliver G. Schmidt[1,4], and Heidemarie Schmidt[1] — [1]Material Systems for Nanoelectronics, Technische Universität Chemnitz, 09126 Chemnitz, Germany — [2]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Straße 23, 09596 Freiberg, Germany — [3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [4]Institute for Integrative Nanosciences, IFW Dresden, Dresden 01069, Germany.

Magnetoresistance (MR) of n-type ZnMnO thin films with Mn 5 at% on sapphire have been studied in in-plane and out-of-plane magnetic fields up to 6 T in the temperature range from 5 K to 300 K. Superimposed positive and negative MR model for ZnCoO thin films [1], has been extended in order to include a valley degeneracy factor which accounts for the formation of electronic levels close to the Fermi level of n-ZnMnO due to substitutional Mn ions and their effect on the negative MR in ZnMnO. MR has been modeled with s-d exchange of 0.2 eV and Mn electron spin (5/2) for single layer transport in two dimensions and for single layer transport in three dimensions and for two layer parallel transport in two and three dimensions. Modeled Thouless diffusion length is proportional to $T^{-0.5}$ [2]. [1]Q. Xu et al., Phys. Rev. B 76, (2007).[2]T. Andrearczyk et al., Phys. Rev. B 72, (2005).

DS 41.2 Thu 15:15 CHE 91

ZrO_2 as a high-k dielectric matrix for electrical applications - formation of embedded Ge nanocrystals and a Ta-stabilized orthorhombic phase — •David Lehninger[1], Julia Wünsche[1], Frank Schneider[1], Volker Klemm[2], Mykhaylo Motylenko[2], David Rafaja[2], and Johannes Heitmann[1] — [1]Institut für Angewandte Physik, TU Bergakademie Freiberg, D-09596 Freiberg — [2]Institut für Werkstoffwissenschaft, TU Bergakademie Freiberg, D-09596 Freiberg

Germanium nanocrystals (nc) embedded in dielectric matrices are discussed as absorbers for third generation solar cells, as sensitizers for rare earth elements, and as charge trapping layer for nonvolatile memories. Here, the formation of Ge nc in a $TaZrO_x$ matrix was studied. Single $GeTaZrO_x$ and $TaZrO_x$ layers as well as superlattices consisting of alternating $GeTaZrO_x$- and $TaZrO_x$-layers with different compositions were sputtered. Crystallization of Ge and $TaZrO_x$ was characterized by transmission electron microscopy, Raman scattering, and X-ray diffraction. It has been found that Ge nc with spherical shape and well-defined size embedded in amorphous $TaZrO_x$ can be formed. The superior properties of single layers of such Ge nc for charge trapping applications were already shown [1]. At elevated annealing temperatures the amorphous $TaZrO_x$ matrix crystallizes in a non-centrosymmetric orthorhombic phase. This makes this material system attractive for fully CMOS compatible ferroelectric applications. [1] D. Lehninger, P. Seidel, M. Geyer, F. Schneider, V. Klemm, D. Rafaja, J. von Borany, J. Heitmann, *Appl. Phys. Lett.* **106**, 023116 (2015)

DS 41.3 Thu 15:30 CHE 91

Controlling the Conductivity of Ti_3C_2 MXenes by Inductively Coupled Oxygen and Hydrogen Plasma Treatment and Humidity — •Florian M. Römer[1], Ulf Wiedwald[1], Tanja Strusch[1], Joseph Halim[2], Elisa Mayerberger[2], Michel W. Barsoum[2], and Michael Farle[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Department of Materials Engineering, LeBow Engineering Center 27-445, Drexel University, Philadelphia, PA 19104-2875, United States of America

Herein we report on the conductivity of plasma and humidty treated Ti_3C_2 MXene thin films of 13 nm thickness. The latter were produced by spincoating a colloidal solution, which was made by LiF/HCl etching of Ti_3AlC_2 powders. We exposed the films to oxygen and hydrogen plasma, measured the resistivity and investigated them by X-Ray photoelectron spectroscopy. We found that the metallic resistivities can be switched reproducibly by plasma treatment between $5.6\mu\Omega$m (oxidized state) and $4.6\mu\Omega$m (reduced state).

By removing the relative humidity from 80% down to ultra high vacuum conditions, we decreased the resistance from 6340Ω to 243Ω – a 26 fold reduction. This makes MXenes a possible candidate as high precision nano sized humidity and gas sensors.

DS 41.4 Thu 15:45 CHE 91

Competing order in the fermionic Hubbard model on the hexagonal graphene lattice — •Dominik Smith[1], Lorenz von Smekal[1], Pavel Buividovich[2], and Maksim Ulybyshev[2] — [1]Justus-Liebig-Universität, Gießen, Deutschland — [2]Universität Regensburg, Regensburg, Deutschland

We study the phase diagram of the fermionic Hubbard model on the hexagonal lattice in the space of on-site and nearest neighbor couplings with Hybrid-Monte-Carlo simulations. With pure on-site repulsion this allows to determine the critical coupling strength for spin-density wave formation with the standard approach of introducing a small mass term, explicitly breaking the sublattice symmetry. The analogous mass term for charge-density wave formation above a critical nearest-neighbor repulsion, on the other hand, would introduce a fermion sign problem. The competition between the two and the phase diagram in the space of the two coouplings can however be studied in simulations without explicit sublattice symmetry breaking. Our results compare qualitatively well with the Hartree-Fock phase diagram.

DS 41.5 Thu 16:00 CHE 91

Hybrid Monte-Carlo simulations at the van Hove singularity in mono-layer graphene — •Michael Körner, Dominik Smith, and Lorenz von Smekal — Institut für Theoretische Physik, Justus-Liebig-Universität Gießen

We use Hybrid Monte-Carlo (HMC) simulations to investigate the influence of long range electron-electron interactions on the electronic band structure of single layer graphene. Here we are particularly interested in the region where the fermi surface crosses the van Hove singularity, and where a topological electronic transition called a neck-disrupting Lifshitz transition occurs. We simulate with HMC a partially screened Coulomb potential and, due to the fermion sign problem, a spin-dependent chemical potential to study the influence of long range interactions on this topological transition in finite volumes and at non-vanishing temperatures. Our goal is to determine how interactions change the character of the topological transition and if there is a set of parameters for which a real phase transition in the thermodynamic sense can occur.

DS 41.6 Thu 16:15 CHE 91

The Phase Diagram of the hexagonal Hubbard Model with Dyson-Schwinger Equations — •Katja Kleeberg and Lorenz von Smekal — Institut für Theoretische Physik, Justus-Liebig Universität Gießen

We study the semimetal-insulator transition on the hexagonal lattice within the framework of Dyson-Schwinger equations. The coupled Dyson-Schwinger equations are formulated for the two competing phases, either realized by a charge-density wave formation or a spin-density wave formation. We investigate the critical behaviour for zero temperature within an extended Hubbard model with on-site and nearest-neighbour interaction. The critical coupling strengths are determined for an unscreened interaction (i.e. in Hartree-Fock approximation) and with static Lindhard screening included. The resulting phase diagrams for the fermionic Hubbard model are compared. The Dyson-Schwinger euqations are solved numerically by fixed-point iteration on GPU's for very large lattices which gives access to the study of the associated magnetic and finite-size scaling behaviour.

DS 41.7 Thu 16:30 CHE 91

Laser spectroscopic in-situ temperature measurements on surfaces — •Eugen Speiser and Norbert Esser — Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V, Department Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany

Laser spectroscopic methods for investigations of surface optical properties often require high incident excitation power (in MW/cm^2 range) leading to considerable heating effects which distort the measurements results. In many cases the heat transfer from the surface is hindered by interface effects or unfavorable substrate characteristics (e.g. low heat conductivity). A precise sample temperature determination becomes an issue, since conventional methods are not able to deliver a local temperature within the laser spot. An evaluation of Stokes to anti-Stokes ratios in Raman spectroscopy is a well-established in-situ method for local temperature measurements. However its imitation regarding a low signal to noise ratio and necessity for instrument corrections makes it often unfeasible. We propose a new vibrational spectroscopy based method for in-situ temperature determination on surfaces minimizing these drawbacks by exploiting the low energy Stokes and anti- Stokes range in Raman spectra. As an example temperature measurements on (4×1) metallic In nanowires on Si(111) in the range between 50 K and 450 K will be shown.

DS 42: Metallic Nanowires on Semiconductor Surfaces (jointly with O)

Time: Thursday 15:00–17:45 Location: WIL C107

DS 42.1 Thu 15:00 WIL C107

Femtosecond electronic response of photo-excited in situ grown Indium wires — •Mariana Chavez-Cervantes[1], Sven Aeschlimann[1], Hubertus Bromberger[1], Razvan Krause[1], Andrea Cavalleri[1,2], and Isabella Gierz[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, United Kingdom

Strong electronic correlations in one-dimensional wires lead to a metal-to-insulator transition at low temperatures. The low-temperature insulating phase is characterized by a complex order parameter with amplitude (size of the band gap) and phase. Photo-doping with femtosecond laser pulses excites carriers across the band gap and leads to an instantaneous reduction of the amplitude of the order parameter followed by amplitude and possibly phase oscillations. We have grown one-dimensional indium wires in situ on a Si(111) substrate and characterized them with low-energy electron diffraction (LEED) and angle-resolved photoemission spectroscopy (ARPES). At room temperature the system exhibits three one-dimensional metallic bands that undergo a complex metal-to-insulator transition at T=110K. We excited the indium wires with intense femtosecond pulses at 1.5eV and probed the response of the electronic structure with time-resolved ARPES at extreme ultraviolet wavelengths. We analyze the dynamics of the complex order parameter and the energy-dependence of the photo-excited population life time.

DS 42.2 Thu 15:15 WIL C107

Ginzburg-Landau-Langevin theory for the phase transition in In/Si(111) — •Yasemin Ergün and Eric Jeckelmann — Appelstraße 2, 30167 Hannover

We investigate thermal fluctuations and collective excitations in quasi-one-dimensional charge-density-wave systems using the Ginzburg-Landau (GL) theory. Starting from a microscopic Su-Schrieffer-Heeger-like model for In/Si(111), we generalized the GL theory for grand canonical Peierls transitions. The equilibrium properties and the non-equilibrium dynamics are simulated using the Langevin approach.

We calculated the phonon spectrum for the Landau-Langevin theory. We discuss our theoretical results in relation to doping and spectroscopy experiments for In/Si(111). Extending this approach for local fluctuations within a two-dimensional Ginzburg-Landau-Langevin is computationally expensive. We developed a frequency filter for smoothing fluctuations included in the linear response spectrum by finite simulation size and time. Support from the DFG through the Research Unit FOR 1700 is gratefully acknowledged.

DS 42.3 Thu 15:30 WIL C107

Pinning of topological solitons at extrinsic defects in a quasi one-dimensional charge density wave — •Samad Razzaq[1], Stefan Wippermann[1], Taehwan Kim[2], and Hanwoong Yeom[2] — [1]Max Planck Inst fuer Eisenforschung GmbH — [2]IBS Center for Artificial Low Dimensional Electronic Systems , University of Pohang

Quasi one-dimensional (1D) electronic systems are known to exhibit exotic physical phenomena, such as, e.g., Jahn Teller distortions, charge density wave (CDW) formation and non-Fermi liquid behavior. Solitonic excitations of the charge density wave ordered ground state and associated topological edge states in atomic wires are presently the focus of increasing attention. We carried out a combined ab initio and scanning tunneling microscopy (STM) study of solitonic and non-solitonic phase defects in the In/Si(111) atomic wire array. While free solitons move too fast to be imaged directly in STM, they can become trapped at extrinsic defects within the wire. We discuss the detailed atomistic structure of the responsible extrinsic defects and trapped solitons. Our study highlights the key role of coupled theory-experimental investigations in order to understand also the elusive fast moving solitons. S. W. gratefully acknowledges financial support from the German Research Foundation (DFG), grant No. FOR1700.

DS 42.4 Thu 15:45 WIL C107

Ultrafast Peierls Transition in In/Si(111) Nanowires Probed by trARPES — •C. W. Nicholson[1], A. Lücke[2], M. Puppin[1], L. Rettig[1], R. Ernstorfer[1], W. Gero Schmidt[2], and M. Wolf[1] — [1]Fritz-Haber-Institut, Berlin — [2]Universität Paderborn

Quasi-1D metals on semiconducting substrates, of which In/Si(111) is one of the most interesting and intensively studied systems, promise not only novel 1D physics, but also control over electronic properties and dimensionality. In/Si(111) undergoes a structural transition from a (4x1) to an (8x2) unit cell at around 120 K, concomitant with a metal-to-insulator transition. A recent combined DFT and Raman study [1] points strongly to a Peierls-like scenario, whereby a combination of shear and rotary distortions leads to the opening of band gaps at specific points in the band structure.

Here we investigate the momentum resolved changes of the electronic structure during the ultrafast photoinduced Peierls transition using high-harmonic-driven trARPES with 50 fs time resolution. Starting from the (8x2) phase, we track the evolution of states both above and below the Fermi level following pulsed excitation and observe the transition from (8x2) to (4x1) phases on a 500 fs time scale. By comparison to complementary DFT calculations we analyse the contributions from the expected shear and rotary distortions to the transient electronic band structure. The observation of coherent phonon oscillations at 2.4 THz provides further insights into the many-body interactions in the system.

[1] E. Jeckelmann et al. Phys. Rev. B, 93, 241407(R) (2016)

DS 42.5 Thu 16:00 WIL C107

Tuning of 1D Plasmon properties on Si(hhk)-Au by adsorbates — •Zamin Mamiyev, Timo Lichtenstein, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany

Gold-induced atomic wires on Si(hhk) surfaces possess intriguing properties of collective electron excitations which are strongly responsive to the electronic state and also to structural motifs. The modification and control of plasmonic excitations in metallic nanowires are of particular interest due to their fundamental and technological importance. In this work, the effect of O$_2$ and H$_2$ adsorption on the plasmons in arrays of single [Si(557)-Au] and double chains of gold [Si(553)-Au] have been examined by Electron Energy Loss Spectroscopy with high resolution both in energy and momentum. Theoretical results show that oxygen and hydrogen atoms bind preferably not to the Au chains directly, but to adjacent Si-honeycomb chains (Si-HC) and Si-adatom rows (The latter exist only in Si(557)-Au). The Si-HC turns out to be mostly responsible for the plasmonic changes. While atomic H reduces the plasmon frequency on Si(553)-Au, as predicted theoretically, adsorbed oxygen leaves it unchanged, whereas a frequency increase is found to be induced by oxygen in Si(557)-Au, indicating an enhanced electron density in the partially filled surface band(s). Comparing the oxygen results on Si(553)-Au and Si(557)-Au, both the structural motifs (double vs. single chain), as well as electronic distribution across the terraces play a role. These effects still need further detailed consideration in order to separate them clearly.

DS 42.6 Thu 16:15 WIL C107

Analysis of the electronic and atomic structure of Pb/Si(557) by polarization dependent two-photon photoemission — •Abdul Samad Syed[1], Vesna Miksic-Trontl[1], Manuel Ligges[1], Ping Zhou[1], Herbert Pfnür[2], Christoph Tegenkamp[2], and Uwe Bovensiepen[1] — [1]Universität Duisburg-Essen, Fakultät für Physik und Zentrum für Nanointegration (Cenide), 47048 Duisburg — [2]Leibniz-Universität Hannover, Institut für Festkörperphysik, Appelstrasse 2, 30167 Hannover

The local structure of atomic wires Pb/Si(557) is determined (i) by the macroscopic quasi one dimensional symmetry imposed by the vicinal cut substrate and (ii) local arrangement of Pb atoms on the Si terraces. We analyze the electronic structure by angle-resolved two-photon photoemission (2PPE) as a function of light polarization and find a dichroism in the 2PPE intensity for opposite electron momenta along the terraces k_x and $-k_x$. Considering earlier work [1] on Pb/Si(111) which concluded on the coexistence of the H3 and T4 symmetry in the $\sqrt{3}\times\sqrt{3}$ reconstruction, the observed polarization dependent dichroism suggests a combination of three and six fold symmetry of the Pb arrangement on Si(557) in agreement with a compressed structure along the Si terrace.

Funding by the DFG through FOR 1700 is gratefully acknowledged.

[1] A. Baumann, E. Speiser, S. Chandola, J. Räthel, P. Kratzer, S. Sakong, C. Tegenkamp, N. Esser (2016).

DS 42.7 Thu 16:30 WIL C107

Spin correlations in the Si(553)-Au nanowire system — •Bernd Hafke[1], Tim Frigge[1], Tobias Witte[1], Boris Krenzer[1], Julian Aulbach[2], Ralph Claessen[2], Jörg Schäfer[2], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — [2]Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), 97074 Würzburg

Deposition of 0.5 ML Au on Si(553) at 650 °C results in the formation of Au double-strand chains per Si terrace with a twofold periodicity along the wire. These metallic wires are structurally terminated by Si step edge atoms, which exhibit a three-fold periodicity of half-filled dangling bonds of the Si atoms along the steps. Theory predicts an antiferromagnetic spin ordering of every third Si step edge atom [1]. The long-range interaction of the two-fold and three-fold periodicity is investigated by spot-profile analysis in LEED at a sample temperature of 80 K. The strict two-fold periodicity of the Au atoms is not correlated between adjacent wires as concluded from the streak like intensity in LEED. In contrast, the threefold ordering of the Si spins exhibit a clear ordering perpendicular to the Au wires. A modification of the structure model [2] explains the structural correlation between adjacent Si step edge atoms. The resulting frustrated structure indicates the formation of a 2D spin-liquid in this system [2].

[1] S. C. Erwin and F. J. Himpsel, Nature Commun. **1**, 58 (2010).

[2] B. Hafke, *et al.* PRB **94**, 161403(R) (2016).

DS 42.8 Thu 16:45 WIL C107

The electronic structure of rare earth silicide nanowires on Si(001) — •Stephan Appelfeller, Martin Franz, Hans-Ferdinand Jirschik, and Mario Dähne — Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin

Trivalent rare earths are known to form silicide nanowires on Si(001). Based on the chemical similarity of the rare earths and the similar appearance of the nanowires in scanning tunneling microscopy, it is generally assumed that the nanowires have the same atomic structure for all rare earths. On the other hand, angle resolved photoemission spectroscopy (ARPES) studies of Gd and Dy silicide nanowires disagree with each other in the observed band structure, even though both studies indicate an one-dimensional dispersion [1,2]. Here, we report on ARPES experiments on Y and Tb silicide nanowires. Their electronic structure is quasi-one-dimensional, showing only small oscillations of the Fermi contours. Furthermore, the disagreement in the literature data is resolved by the observation of strong matrix element effects in our data, in which all the bands described in the literature are observed indicating that the nanowires have the same electronic properties and, consequently, also the same atomic structure.

This work was supported by the DFG (FOR1700, project E2). We kindly acknowledge the support of K. Horn and coworkers, C. Papp, and of BESSY II (HZB Berlin), where the photoemission experiments were carried out at the beamline UE56/2 PGM-1.

[1] H. W. Yeom et al., Phys. Rev. Lett. **95**, 205504 (2005).
[2] M. Wanke et al., Phys. Rev. B **83**, 205417 (2011).

DS 42.9 Thu 17:00 WIL C107

Strain induced quasi-one dimensional structure of rare earth silicides on Si substrates — Frederic Timmer[1], Robert Oelke[1], Christof Dues[2], Simone Sanna[2], Wolf Gero Schmidt[2], Martin Franz[3], Stephan Appelfeller[3], Mario Dähne[3], and •Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Germany — [2]Lehrstuhl für Theoretische Physik, Universität Paderborn, Germany — [3]Institut für Festkörperphysik, Technische Universität Berlin, Germany

One dimensional (1D) systems have attracted a lot of attention since their physical properties are distinctively different from structures of higher dimensionality. Recently, a new class of quasi-1D systems based on rare earth silicides has attracted attention. Here, we report on combined studies on quasi-1D structures by scanning tunneling microscopy (STM), spot profile analysis of low-energy electron diffraction (SPA-LEED) and density functional theory (DFT).

Depositing rare earth elements as Dy or Tb at elevated temperature on Si(111), a $2\sqrt{3}\times\sqrt{3}$ superstructure is observed. This structure is attributed to the formation of periodically arranged Si vacancies in different silicide layers. The complex structure of this superstructure with buckled surface layer, $\sqrt{3}\times\sqrt{3}$ superstructure in the first subsurface layer $2\sqrt{3}\times\sqrt{3}$ superstructure in the second subsurface layer can only be analyzed applying the different techniques used here. The anisotropic character of this structure is emphasized by the formation of periodically arranged domain boundaries. The width of the silicide domains formed in two domains is roughly two unit cells.

DS 42.10 Thu 17:15 WIL C107

Infrared Spectroscopy of Charge Carrier Excitation in Metallic Nanowires on the Atomic Scale — Annemarie Pucci and •Fabian Hötzel — Kirchhoff Institute for Physics, Heidelberg University, Germany

Atomic chains, as for example gold superstructures on vicinal silicon surfaces, may show infrared resonances that can be attributed to plasmonic excitations in nanowires of a finite length of the order of 100 nm. The appearance of the resonances clearly indicates the metallic character of the atomic chains. The quantitative analysis of the spectral weight and the resonance position yields the data on the nanowire conductivity and complementary information on the electronic band structure. Conductivity changes upon doping can be directly seen in the infrared spectra. Furthermore, as we have recently found out, the plasmonic resonances are sensitive to the changes of the polarization of the silicon step edges with temperature.

DS 42.11 Thu 17:30 WIL C107

Functionalization of Si(553)-Au surface with hydrogen and small organic molecules — •Julian Plaickner[1], Sandhya Chandola[1], Eugen Speiser[1], Svetlana Suchkova[1], Norbert Esser[1], and Simone Sanna[2] — [1]Schwarzschildstrasse 8, 12489 Berlin — [2]Warburger Str. 100, 33098 Paderborn

Atomic metallic chains deposited on vicinal Si substrates form templates for the growth of hybrid molecule-solid nanostructures. The advantage of these structures is the possibility to vary the substrate geometry and the metallic element. We investigate the adsorption of toluene-3,4-dithiol molecules on hydrogen-passivated Si(553)-Au surfaces as model system/process. Hydrogen is able to drive a reversible metal-insulator transition on the Si(553)-Au surface and is also changing the adsorption geometry of organic molecules, extending the functionalization possibilities of the surface in organic electronics and biosensing.

We are using a set of polarization-sensitive optical techniques, such as Raman Spectroscopy (RS), Reflection Anisotropy Spectroscopy (RAS) and Infrared Spectroscopic Ellipsometry (IRSE). Our approach consists in establishing a direct connection between optical spectra and surface structure via ab-initio calculations. Optical fingerprints allow us to gain information on structural and electronic properties of the system.

The plan for the future is the realization of highly ordered molecular array geometries and the understanding of charge transfer between molecules and atomic wires. This will open possibilities for further functionalization through modification of terminal groups of molecules.

DS 43: Quantum Optics at the Nanoscale: From Fundamental Physics to Quantum Technologies (Joint Session HL, DS, O, and TT, organized by DS)

Time: Thursday 17:00–17:30 Location: CHE 91

DS 43.1 Thu 17:00 CHE 91

Sensing weak radio-frequency radiation by pulsed Autler-Townes spectroscopy — Timo Joas, Andreas M. Waeber, Georg Braunbeck, and •Friedemann Reinhard — TU München, Walter Schottky Institut and Physik-Department

Nano-emitters have shaped a new era of quantum optics, serving as convenient single photon sources, e.g. to launch surface plasmons [1,2] or to build long-distance entanglement [3]. So far, they have mostly been used in the optical (100THz) domain.

Here we employ a nano-emitter and a quantum-optical protocol to detect weak radiation in the radio-frequency (GHz) range. Our scheme is based on Autler-Townes spectroscopy [4]. We extend this technique to a pulsed protocol, which greatly improves spectral resolution, sensitivity and robustness to experimental fluctuations.

We demonstrate our approach on a NV center in diamond, where it might enable various applications. Specifically, we consider radioastronomy, ultrasound detection and spin-phonon coupling.

[1] A.V. Akimov et al., Nature 450, 402 (2007)
[2] R. Kolesov et al., Nature Physics 5, 470 (2009)
[3] B. Hensen et al., Nature 526, 682 (2015)
[4] J.A. Gordon et al., Appl. Phys. Lett. 105, 024104 (2014)

DS 43.2 Thu 17:15 CHE 91

Free-electron quantum optics — •Katharina E. Priebe, Christopher Rathje, Armin Feist, Sergey V. Yalunin, Sascha Schäfer, and Claus Ropers — 4th Physical Institute - Solids and Nanostructures, University of Göttingen, Göttingen, Germany

Besides being a powerful tool for time-resolved measurements of nanoscale dynamics, ultrafast transmission electron microscopy (UTEM) serves as an ideal test bench for quantum optical experiments studying the interaction with free-electron beams. Specifically, inelastic scattering between the electrons and strong optical near-fields [1] allows for a coherent manipulation of the electron quantum state [2]. The optical near-field imprints a sinusoidal phase modulation on the electron wavefunction, which is manifest in a comb of sidebands in the electron kinetic energy distribution. In this contribution, we will demonstrate how multiple near-fields can be employed to coherently control the free-electron momentum superposition states [3,4]. Furthermore, dispersive propagation translates the phase modulation into a density modulation: the electron wavefunction is self-compressed into a train of attosecond bursts. This temporal structuring of free-electron beams may find applications in electron microscopy with attosecond resolution.

[1] B. Barwick *et al.*, Nature, **462**, 902 (2009).
[2] A. Feist *et al.*, Nature, **521**, 200-203 (2015).
[3] K. E. Echternkamp *et al.* Nat. Phys **12**, 1000-1004 (2016).
[4] K. E. Priebe *et al.* In preparation.

DS 44: Postersession II

Time: Thursday 17:00–19:00 Location: P1C

DS 44.1 Thu 17:00 P1C

Fascinating vanadium oxide nanostructured thin films for sensing applications — •Megha Singh, Prabhat Kumar, and Gade B. Reddy — Thin Film Laboratory, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016

Vanadium oxides (V-O) have enticed scientists and researchers due to their various properties offering wide optical band gap, good thermal and chemical stabilities. This makes oxides of vanadium, highly suitable, to be used in wide variety of devices applications including sensing. It is essential for any device to be employed in sensing applications to have high aspect ratio and surface area. We report the synthesis of vanadium oxide nanostructured thin films (NTFs) over wide area (400 mm2) using a novel technique plasma assisted sublimation process (PASP). Vanadium oxide NTFs were synthesized on glass substrates in N2 plasma and N2 gas. SEM micrographs show rod like morphology of microstructures with flake like nanostructures on the surface revealing very high surface area. HRTEM images of film revealed that flake like morphology as was observed in SEM, confirming results obtained on morphological studies. XRD and Raman spectroscopic studies confirm long range order in reduced V2O5 (O/V ratio ~ 2.2) indicating structures are highly crystalline in nature. In absence of plasma, the crystallinity as well as surface morphology deteriorated, thereby indicating important role of plasma in microstructure, nanostructure as well as crystal structure of vanadium oxides NTFs with different stoichiometry. Hence, high surface area nanostructured thin films are obtained for sensing applications.

DS 44.2 Thu 17:00 P1C

Plasma assisted synthesis of core-multishell nanostructured thin films — •Prabhat Kumar, Megha Singh, and Gade B Reddy — Thin Film Laboratory, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016

The ability to modify and tune the properties of core-multishell heterostructures nanoflakes (CMN) enables them to be used in wide range of applications. Firstly, we have carried out the sulfurization of MoO3 nanostructured thin films using H2S/Ar plasma. XRD analysis shows that films after sulfurization have monoclinic MoO2 and hexagonal MoS2 phases. Maximum sulfurization is accomplished at 550°C in 60min. Core-shell was confirmed by the HR-TEM micrographs. XPS analysis shows that in all samples surface was completely sulfurized to form MoS2 with good stoichiometry. From results, it was revealed that the depth of penetration of sulfur species in MoO3, converting it into MoS2 increased with the increase in time and reduction of MoO3 by hydrogen species was much more as compared to sulfur species. Secondly, core-shell heterostructures were treated in O2 plasma for different durations of time. XRD and Raman analysis show that films after oxidation have MoO2, MoS2 along with MoO3. HR-TEM micrographs revealed that nanoflake have acquired CMN. XPS analysis shows that surface consist of Mo oxidation states. The aim of this work is to achieve the appropriate growth conditions to obtain CMNs thin films on different substrates and to control their properties by using various reactive species environment of H2S/Ar and O2 gas plasma.

DS 44.3 Thu 17:00 P1C

Photo absorption of adsorbed azobenzene monolayers: impact of graphene substrate — •Qiang Fu, Caterina Cocchi, Dmitrii Nabok, Andris Gulans, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

To reveal the impact of a graphene substrate on the photo-absorption of azobenzene (AB), we investigate the optical spectra of both isolated and adsorbed AB monolayers within the framework of density-functional theory (DFT) and many-body perturbation theory (MBPT), as implemented in the full-potential all-electron code `exciting` [1]. In spite of weak hybridization, the optical excitations of AB monolayers are remarkably modulated. The excitation energies are affected via two counteracting mechanisms: Substrate polarization reduces the band-gap of the adsorbate, and enhanced dielectric screening weakens the attractive interaction between electrons and holes. The competition of the two effects give rise to a blueshift of peaks from intramolecular excitations and a redshift of peaks from intermolecular ones. Excitations corresponding to intermolecular electron-hole pairs, which are dark in the isolated AB monolayers, are activated by the presence of graphene. Our results demonstrate that the photoswitching property of weakly adsorbed azobenzene undergoes notable changes on a carbon-based substrate.

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

DS 44.4 Thu 17:00 P1C

Tuning excitons by 3D stacking of hexagonal boron nitride layers — •Wahib Aggoune[1,2], Caterina Cocchi[2], Dmitrii Nabok[2], Karim Rezouali[1], Mohamed Akli Belkhir[1], and Claudia Draxl[2] — [1]Laboratoire de Physique Théorique, Faculté des sciences exactes, Université de Bejaia, 06000 Bejaia, Algérie — [2]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

The opto-electronic properties of hexagonal boron-nitride (h-BN) are investigated from first principles, considering the five possible stacking arrangements obtained by translation of the two layers in the unit cell. We find the most stable structure in agreement with experiment [1] and with an earlier first-principles study [2]. All structures exhibit a quasi-particle gap, with values between 4.5 and 6 eV as calculated from the G_0W_0 approach. From the solution of the two-particle Bethe-Salpeter equation an intense excitonic peak is found in the UV region for any stacking arrangement. Depending on the order of the h-BN layers, the lowest-energy excitation can be either bright or dark. We characterize the main optical excitations for all stacking arrangements and discuss them in the context of symmetry-induced selection rules. All calculations are performed using the `exciting` code [3], a full-potential all-electron package implementing the families of linearized augmented planewave methods.

[1] R. S. Pease, Nature (London) **165**, 722 (1950). [2] L. Liu *et al.*, Phys. Rev. B **68**, 104102 (2003). [3] A. Gulans *et al.*, J. Phys. Condens. Matter. **26**, 363202 (2014).

DS 44.5 Thu 17:00 P1C

Diffusion in thin films — •Max Wolff[1], Gunnar Palsson[1], Anton Devishvili[1], Joe Dura[2], and Boris Toperverg[3] — [1]Department for Physics and Astronomy, Uppsala University, Sweden — [2]National Institute for Standards and Technology, Gaithersburg, MD, USA — [3]Ruhr-University Bochum, Bochum, Germany

A surface imposes a singularity to materials, and with decreasing size of objects such as in nano-technology, they can dominate the physical properties. One apparent example of a surface effect is the reduction of the freezing temperature of ice in the surface layers, which allows skiing or skating on ice. Reflectometry is a powerful tool to explore interfaces and surfaces. More recently grazing incidence scattering techniques attracted more and more interest and in particular grazing incidence small angle scattering becomes more widely used to probe the interfacial structure of e.g. polymer systems. In the case of neutrons many studies suffer from limited incident flux. This applies even more for the case of neutron spectroscopy offering unique opportunities to probe dynamics in materials.

In this presentation the opportunities and challenges of gracing incidence neutron spectroscopy will be evaluated. Wave field enhancement in a potential well to access the study of dynamics in thin films and surfaces might be one possibility to overcome the limitations in neutron flux. The method will be discussed on the example of a thin film of vanadium loaded with hydrogen.

DS 44.6 Thu 17:00 P1C

Particular electronic properties of F_{16}CoPc: A decent electron acceptor material — •Florian Rückerl, Daniel Waas, Bernd Büchner, and Martin Knupfer — Leibniz Institute for Solid State and Materials Research Dresden, Institute for Solid State Research, Helmholtzstraße 20, D-01069 Dresden, Germany

Various interfaces with F_{16}CoPc as one of the partners are characterized by a charge transfer across the interface and a concomitant reduction of the Co central atom in these molecules. We summarize recent photoemission spectroscopy results and compare those to the data from equivalent interfaces comprising F_{16}CuPc. In the latter, the Cu center remains unchanged indicating the particular role of Co in F_{16}CoPc as the electron accepting site.

DS 44.7 Thu 17:00 P1C

Surface functionalization of WSe_2 by $F_{16}CoPc$ — •Tom Klaproth, Florian Rückerl, Roman Schuster, Bernd Büchner, and Martin Knupfer — Leibniz Institute for Solid State and Materials Research Dresden, Institute for Solid State Research, Helmholtzstraße 20, D-01069 Dresden, Germany

We have investigated the electronic properties of WSe_2 surfaces covered by fluorinated cobalt phthalocyanine ($F_{16}CoPc$) using photoemission spectroscopy. We show that a charge transfer occurs at this interface, which results in the creation of holes in the WSe_2 surface while the Co center of the phthalocyanine is reduced to Co(I). We observe a potential change in WSe_2 approaching the surface as a consequence of the induced positive charges near the surface. In addition, our data allow for a rough estimation of the induced charge density and suggest that the holes might be localized.

DS 44.8 Thu 17:00 P1C

Infrared studies of device relevant interfaces - energetic and morphological insights — •Sabina Hillebrandt[1,2], Sebastian Beck[1,2], and Annemarie Pucci[1,2] — [1]Kirchhoff-Insitut für Physik, Universität Heidelberg, Germany — [2]Innovationlab GmbH, Heidelberg, Germany

Organic electronic devices consist of stacked organic as well as inorganic materials and the device performance is mainly influenced by the interfaces of the layers. The investigation of charge generation, injection and transport at these interfaces is a major key to the basic understanding of the fundamental mechanisms in organic electronics. We use interface layers of metal oxides, i.e. nickel oxide (NiO) or molybdenum oxide (MoO3), and self-assembled monolayers (SAM) to engineer the surface of certain electrode materials in order to improve charge transport at the inorganic/organic interface. With their inherent dipole SAMs can improve the energetic alignment at the interface. Polarization dependent infrared spectroscopic studies reveal the orientation of such SAMs as well as the influence of the interlayers on the orientation of the subsequent organic semiconductor material like fluorinated zinc phtalocyanine (F4ZnPc). Additionally, supported by density functional theory (DFT) calculations, charge transfer between the electrode material and the organic semiconductor can be investigated, giving a deep insight into the energetic and morphological properties at the interface.

DS 44.9 Thu 17:00 P1C

Co-crystal formation and HOMO-LUMO coupling in mixtures of organic semiconductors. Diindenoperylene (DIP), sexithiophene (6T) as donors and hexafluorotetracyanonaphthoquinodimethane (F6TCNNQ) as acceptor. — •Giuliano Duva[1], Paul Beyer[2], Tino Meisel[2], Andreas Opitz[2], Alexander Hinderhofer[1], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen (Germany) — [2]Humboldt-Universität zu Berlin, Department of Physics, Berlin (Germany)

Donor:acceptor (D:A) blended films of organic semiconductors [1] represent a technologically relevant class of materials. Studying the structural and optical properties of the mixtures resulting upon coevaporation is mandatory to control the parameters that govern the final performances of the device. Here we compare two D:A pairs, respectively DIP:F6TCNNQ and 6T:F6TCNNQ. We investigate their structure via X-ray scattering and find the formation of a D:A cocrystal exhibiting π-π stacking of the molecular components. Such structure correlates with the appearance of several new, sub-bandgap electronic transitions at energies specific for each combination. We discuss several models for charge-transfer, in particular a Hückel-like model for molecular orbitals [2], in order to relate the HOMO-LUMO energies of the compounds in the blend to the newly observed transitions. [1] A. Hinderhofer et al. Chem. Phys. Chem. 13 (2012), p.628. [2] H. Méndez et al. Angew. Chem. Int. Ed. 52 (2013), p.7751.

DS 44.10 Thu 17:00 P1C

Interface formation of Titanium and Tantalum thin films onto LiNbO3 — •Uwe Vogel[1], Steffen Oswald[2], Thomas Gemming[3], and Jürgen Eckert[4] — [1]Helmholtz-Zentrum Berlin / IFW Dresden / TU Dresden — [2]IFW Dresden — [3]IFW Dresden / TU Dresden — [4]ÖAW / IFW Dresden / TU Dresden

We present results of detailed chemical interface analyses of sputtered Tantalum and Titanium thin films as potential adhesion and barrier layers onto cleaned SAW-substrate material (LiNbO3) with respect to their temporal (up to 24 h) and thermal stability up to 600°C in vacuum. The main technique for surface clean is a special Helium plasma, the analysis is done using AR-XPS.

DS 44.11 Thu 17:00 P1C

Photo-induced effects in hole-doped $La_{1-x}Sr_xMnO_3$ ($0 < x \leq 0.1$) films probed by Raman spectroscopy — •Christoph Meyer, Sebastian Merten, Bernd Damaschke, and Vasily Moshnyaga — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Perovskite manganite $La_{1-x}Sr_xMnO_3$ (LSMO) displays a variety of structural, electric and magnetic phases with different types of crystallographic distortions, e.g. the Jahn-Teller effect, manifesting themselves in colossal magnetoresistance effect and insulator-metal transition. To monitor and to disentangle the influence of light, temperature and doping on the structure, we grew series of hole-doped LSMO ($0 \leq x \leq 0.3$) epitaxial thin films on $LaAlO_3$ (100) and MgO (100) substrates by metalorganic aerosol deposition and probed them by polarization-dependent Raman spectroscopy. The Raman spectra were studied as a function of the Sr content, temperature and laser power to determine a photo-induced effect. The emergence of the metallic phase, marked by the Raman mode at ~ 430 cm^{-1} and a simultaneous suppression of the Jahn-Teller bands at ~ 510 cm^{-1} and ~ 630 cm^{-1} by increasing the laser power for the insulating LSMO films with $0 < x \leq 0.1$ was observed. The results are rationalized as a photo-induced shift towards metallic phase, equivalent to the increase of Sr-doping $x > 0.15$ in the LSMO phase diagram. Financial support by the DFG via project SFB 1073/B04 is gratefully acknowledged.

DS 44.12 Thu 17:00 P1C

Defect induced photoluminescence of tungsten di-sulfide monolayers — •Aswin Asaithambi[1], Roland Kozubek[1], Guenther Prinz[1], Francesco Reale[2], Cecilia Mattevi[2], Marika Schleberger[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — [2]Department of Materials, Imperial College London, London, UK

The intriguing electronic properties of graphene have renewed the interest in other 2D materials such as transition metal di-chalcogenides (TMDCs) monolayers. TMDCs, similar to graphite, have a layered structure with an indirect bandgap which becomes direct when only a monolayer is present. This leads to strongly enhanced photoluminescence (PL). However, unavoidable defects affect the opto-electronic properties of TMDC monolayers drastically, which makes it necessary to study and characterize their optical related properties.

In this contribution, we present highly sensitive, non-destructive, temperature and power dependent PL measurements to study the defects present in tungsten di-sulfide (WS_2) monolayers. For this purpose, pristine samples of WS_2 were irradiated with Xe^{30+} ions to additionally create defects in the monolayers. Low temperature spectra of pristine samples show two different peaks associated with free and defect-bound excitons recombinations. For higher temperature or power, only the free exciton recombinations dominate the spectrum. For the different defect densities created in the monolayers, we observed changes in the PL spectrum with regard to intensity and FWHM, which will be discussed and compared to data published in literature.

DS 44.13 Thu 17:00 P1C

Growth of oxide microstructures by metalorganic aerosol deposition technique — •Philipp Ksoll, Hannes Gödecke, Christoph Meyer, Marius Keunecke, and Vasily Moshnyaga — I. Physikalisches Institut Göttingen, 37077 Göttingen, Friedrich-Hund-Platz 1

Microstructuring of thin films, usually processed by different lithography tools, is a crucial step for various device applications, e.g. semiconducting electronics, spintronics, photonics, etc. Metalorganic aerosol deposition (MAD) has been shown to be effective technique to grow complex oxide films of high quality. To avoid the complex oxide lithography we developed a MAD method to grow oxide microstructures with a line width down to 1 μm. Recent material realizations include single, e.g. CuO_x, and complex oxides, i.e. manganites $La_{1-x}Sr_xMnO_3$. The microstructures were characterized by different types of microscopies, like Raman, atomic force, scanning electron and energy dispersion x-ray analysis.

Financial support by the DFG via SFB 1073 (TP B04) is acknowledged.

DS 44.14 Thu 17:00 P1C

Relation of sample stoichiometry and growth conditions in $SrCoO_{3-\delta}$ thin films — •Patrick Schöffmann[1], Sabine Pütter[1], Jürgen Schubert[2], Willi Zander[2], Réne Heller[3], Markus Waschk[4], Paul Zakalek[4], and Thomas Brückel[4] — [1]Jülich Centre for Neutron Science (JCNS) am Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Garching — [2]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich GmbH — [3]Helmholtz-Zentrum Dresden-Rossendorf — [4]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH

Strontium cobaltite ($SrCoO_{3-\delta}$) exists in two topotactic phases, depending on the oxygen content. $SrCoO_3$ is a ferromagnetic metal (T_C=305K) with perovskite structure while $SrCoO_{2.5}$ is an antiferromagnetic insulator(T_N=570K) with brownmillerite structure.[1]

We aim at growing thin films of $SrCoO_{3-\delta}$ via molecular beam epitaxy, and thus investigate the influence of growth conditions like the elemental deposition rate of Sr and Co, substrate temperature and oxygen pressure on the sample stoichiometry and surface topography.

For this, we employ in-situ electron diffraction to monitor the sample growth and ex-situ X-ray reflectometry and atomic force microscopy to investigate the structural properties. The stoichiometry is determined by Rutherford backscattering spectrometry.

We provide a comprehensive overview of the samples addressing the requirements to achieve a Sr:Co stoichiometry of 1:1.

[1]C.K. Xie et al., Appl. Phys. Lett 99, 052503 (2011)

DS 44.15 Thu 17:00 P1C

Large area graphene on silicon by carbon ion implantation in copper and subsequent transfer — •Jan Lehnert[1], Daniel Spemann[1], Stephan Mändl[1], Hamza Hatahet[1], Aron Varga[1], and Bernd Rauschenbach[1,2] — [1]Leibniz Institute of Surface Modification (IOM), Leipzig, Germany — [2]Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

Despite of many research efforts on graphene it still attracts much interest due to its promising properties. Especially for practical applications it is necessary to produce large area and high quality graphene films which is still a challenge. In this work we present a synthesis method by use of ion beam implantation, annealing and subsequent transfer. Cu foils (cm in size) which were pre-annealed at 950 °C for 2 h and analysed by SEM, AFM, XRD and XPS measurements before and after annealing have been implanted with 35 keV carbon ions with a fluence of $1 \times 10^{16}\,\mathrm{cm}^{-2}$ at room temperature and subsequently annealed at 850 °C for 2 h to form graphene layers on the Cu surface. Afterwards, the graphene was transferred to a SiO_2/Si substrate by a PMMA free chemical etching process in which the Cu foils were removed by exposure to a mixture of iron(III) chloride ($FeCl_3$) and hydrochloric acid (HCl). Raman spectroscopy at room temperature after the transfer show nearly defect-free monolayer graphene. Furthermore, SEM and AFM measurements were performed to investigate the size and quality of the synthesised graphene. No graphene was observed on unimplanted samples that were treated with the same annealing procedure.

DS 44.16 Thu 17:00 P1C

Morphology and adsorption of organic thin films on MgO/Ag(100) — •Sabrina Pechmann, Daniel Schultheiss, and Rainer H. Fink — Physical Chemistry II, FAU Erlangen-Nuremberg, Erlangen, Germany

Over recent years a vast field of new technological applications for organic thin films on defined and tunable metal-oxide surfaces has gained increasing attention. These systems allow investigation by various electron or photon based techniques, which would be impossible for bulk metal-oxides due to potential charging. Epitaxial MgO/Ag(100) was chosen as model system, as both bulk structures exhibit a comparatively small lattice mismatch [1], which reduces the amount of defects. Growth could be observed in-situ by LEEM, stoichiometry and thin film properties were checked by XPS and LEED-IV. It could be shown, that MgO can be modified by electrons and photons, enabling to tune the surface properties. The MgO surface serves as substrate for semiconducting organic molecules with large, extended pi-systems. For our studies cobalt (II) octaethylporphyrin, its free base equivalent, PTCDA and dihexylquatertiophene were chosen, as all those systems grow in different, highly ordered manners. Therefore their long-range ordered superstructure could be determined by LEED, whereas NEXAFS dichroism offered insight into the molecular orientation. Furthermore, it was possible to metalize octaethylporphyrin by the underlying magnesium [2]. This work is funded by the funCOS research unit (FOR 1878, DFG). [1] Valeri, S. et al., Surf. Sci. 507-510, 311-317, 2002 [2] Schneider, J. et al., Chem. Eur. J. 22, 1744-1749, 2016

DS 44.17 Thu 17:00 P1C

Electrical Characterization of Silver Thin Films for Optimization of Low-Emissivity Glass-Coatings — •Julian Mertens, Roland Sittner, and Matthias Wuttig — 1. Physikalisches Institut A, RWTH Aachen

The increasing use of large window areas in modern architecture makes the improvement of efficient low-emissivity coatings indispensable. Therefore the key property to optimize transparent thin film layer stacks used for glass coatings is given by the infrared reflectance. As the infrared reflectance of the corresponding thin film is directly linked to the goodness of electrical conductivity, it is mandatory to gain an understanding of the dominant scattering mechanisms in metallic thin films that dominate conductivity. Due to its lowest bulk-resistivity, silver is the element of choice. To improve the infrared reflectance of silver thin films different layer systems were used and improved over the last twenty years. However, it is still not understood what kind of scattering mechanisms are responsible for the huge increase of specific sheet resistance as the layer thickness decreases. Mayadas and Shatzkes developed a theory which combines diffusive interface scattering, as well as electron scattering at grain boundaries in a total picture, which makes it possible to distinguish between both scattering mechanisms. To apply this approach, the resistivity of thin silver films, deposited on different seed-layers by DC Magnetron Sputter Deposition, is fitted to said theory. The results enable to separate both scattering mechanisms and help to improve the development of layer stack optimization methods.

DS 44.18 Thu 17:00 P1C

Recombination prefactor in organic bulk heterojunction solar cells — •Jędrzej Szmytkowski — Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gdańsk, Poland

In this work, we report on theoretical studies of reduced bimolecular recombination in organic donor–acceptor bulk heterojunction structures. The values of the Langevin recombination prefactor have been calculated as a function of several quantities, including temperature, external electric field and charge carrier concentration. In addition, an effect of exciton–charge carrier interaction has been taken into account to describe changes of this prefactor. We have also investigated an influence of disorder on the nongeminate recombination in organic systems with an exponential density of states. Presented results can explain mechanisms which cause a loss of photocurrent in organic solar cells.

DS 44.19 Thu 17:00 P1C

Self-Assembly of Di-lithium Phthalocyanine on Different Surfaces — •nhung n.t.t.[1,3], lars s.[2], ha n.t.n.[2], and michael h.[2] — [1]IFW Dresden — [2]TU-Chemnitz — [3]Duy Tan University, Vietnam

Metal phthalocyanines (MPc) behave as semiconductors in their pure form. Therefore doping MPc thin films by oxidizing the ligands and creating an open shell can considerably increase their electrical conductivity [1-2]. These doped organic thin films may play an crucial role in developing new effective materials for nano-devices like insulator-metal-insulator transistor [3] or light emitting devices [4].

In addition, self-assembly structures of di-lithium phthalocyanine (Li2Pc), which have been used as electrolyte in an all-solid state electrochemical cell, lead to a pronounced electric field dependence of the lithium ion transport in channel formation process [5].

Here the self-assembly of Li2Pc on different crystalline surfaces will be investigated by means of scanning tunneling microscopy (STM) in ultra-high vacuum. In the first part Li2Pc is grown by organic molecular beam deposition (OMBD) on Au(111) surface to prepare a crystalline thin film. To get more information on the adsorption process, a small amount of this molecule has been doped at the F16CoPc thin films on Au(111) and HOPG substrates. STM results collected at low temperatures as well as molecular manipulating of Li2Pc by applying voltage pulses to the STM tip illustrate the deposition behavior of Li2Pc. All of the research was performed in TU-Chemnitz.

DS 44.20 Thu 17:00 P1C

Microstructure and Stress Gradients in Diamond Films Revealed by Cross section X-ray nanodiffraction — •Nicolas Wöhrl[1], Hadwig Sternschulte[2], Manfred Burghammer[3], Ju-

raj Todt[4], and Jozef Keckes[4] — [1]Faculty of Physics and CENIDE, University of Duisburg- Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Hochschule Augsburg, Fakultät für Allgemeinwissenschaften, Augsburg, Germany — [3]ESRF, Grenoble, France — [4]Erich Schmidt Institut and Montanuniversität Leoben, Leoben, Austria

Ultrananocrystalline diamond (UNCD) films consist of small randomly oriented diamond grains embedded in an amorphous C:H matrix. Usually, the grain size is determined by X-ray diffraction (XRD) or transmission electron microscopy revealing information only from the total UNCD film or only locally from selected areas with low statistics, respectively. In this work we present the first cross section X-ray nanodiffraction study of diamond multi-layers with varying grain size from microcrystalline to UNCD. For the cross section study the samples have been cut in thin slices by FIB. The X-ray nanodiffraction was performed in transmission geometry at the ESRF in Grenoble using X-ray beam of 30nm in a diameter adjusted parallel to the Diamond-Si interface and the sample scanned in steps from the interface to the growth surface. The 2D XRD patterns recorded by a CCD detector were used to evaluate depth gradients of texture, grain sizes and residual stress in the diamond crystals. The results show complex gradients of microstructure and stresses. [1] J. Keckes et al., Scripta Materialia 67 (2012) 748

DS 44.21 Thu 17:00 P1C

In-depth analysis of nanomorphology in thin films of 6,13-dihydro-6,13-diazapentacene — •Xiaoyan Du[1], Lisa Müller[2], Nicolai Burzlaff[2], and Rainer H. Fink[1] — [1]Physical Chemistry 2 and ICMM Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) Egerlandstr. 3, 91058 Erlangen, Germany — [2]Inorganic Chemistry, Department of Chemistry and Pharmacy Friedrich-Alexander-University Erlangen-Nuremberg Egerlandstr. 1, 91058 Erlangen, Germany

6,13-Dihydro-6,13-diazapentacene (DHDAP) is one of the important pentacene derivatives due to its ability to be easily derivatized, or its environmental stability and its solubility. The performance of organic field-effect transistors (OFETs) based on DHDAP has been found to be extremely sensitive to the substrates nature and temperature, which induces different polymorphs. We employ several complementary microspectroscopic probes to investigate the structure of thermally evaporated films evaporated at different conditions. Detailed analysis of atomic force microscopy (AFM), scanning transmission X-ray microscopy (STXM) and resonant soft X-ray scattering (RSoXS) reveals the dependence of the crystalline domain size on the film preparation conditions. Angle-resolved near edge x-ray absorption fine structure (NEXAFS) spectroscopy sheds lights on the molecular orientation of the molecules close to the substrates. Thus, the structure-property relations offer further insights into the transport properties of the respective OFETs devices. This work is funded by the DFG within GRK 1896.

DS 44.22 Thu 17:00 P1C

Epitaxial thin films of the high-*k* dielectric $SrZrO_3$ — •Corinna Müller, Patrick Salg, Aldin Radetinac, Philipp Komissinskiy, and Lambert Alff — Technische Universität Darmstadt, Germany

$SrZrO_3$ has an orthorhombic perovskite crystal structure with a pseudocubic lattice constant of 4.101 Å, a high-*k* dielectric constant (~ 22), a large optical bandgap ($\sim 5.8\,\mathrm{eV}$), and a low oxygen diffusion constant of $10^{-12}\,\mathrm{cm^2 s^{-1}}$ [1,2]. We have investigated the growth of $SrZrO_3$ thin films fabricated by pulsed laser deposition onto $GdScO_3$ substrates at a substrate temperature of 630-700 °C, laser fluence of 0.32-0.98 $\mathrm{J/cm^2}$, and oxygen partial pressure below 10^{-8} Torr. X-ray diffraction measurements reveal that the crystal structure of $SrZrO_3$ is rather stable against variation of the growth parameters. The 20-70 nm thick films are relaxed and show lattice parameters close to the $SrZrO_3$ bulk values. It is investigated how the Sr:Zr cation stoichiometry of the films depends on laser fluence which is important as Sr and Zr vacancies act as acceptor defects [2].

[1] P. A. Langjahr *et al.*, Mater. Res. Soc. Symp. Proc. **401**, 109 (1996). [2] L. Weston *et al.*, Phys. Rev. B **89**, 184109 (2014).

DS 44.23 Thu 17:00 P1C

Dopant-Drift in Organic Semiconductors in Dependence of Different Parameters — •Seon-Young Rhim[1,3], Lars Müller[1,2,3], Vipilan Sivanesan[1,3], Dongxiang Wang[1], Jakob Bernhardt[1,3], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab Heidelberg — [2]Institute for High-Frequency Technology, TU Braunschweig — [3]Kirchhoff Institute for Physics, Heidelberg University

The increase in the electrical conductivity of organic semiconductors by doping enables the fabrication of organic electronic devices with high performance. We show that besides the already known dopant diffusion due to a concentration gradient, the dopants are subject to a drift caused by certain operating conditions. In this study we use I(V)-Curve measurements, optical microscopy and spatially resolved infrared spectroscopy for the investigation of the dopant movement. For the device preparation different solution-processable organic hole conducting host-materials as Poly(3-hexylthiophen-2,5-diyl) (P3HT) and p-dopants as 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) were utilized. In dependence of the applied voltage and respective current we observe the formation of an undoped region which we analyze in terms of dopant concentration and other operational parameters. Furthermore we compare the conventional doping in solution to the recently applied sequential doping method. The spatial control of the doped and undoped region within an organic semiconductor can be used to produce passive electronic devices with simple structures. As example we introduce a passive resistor and a non-volatile memory device.

DS 44.24 Thu 17:00 P1C

Perforation of CVD silicon nitride by AgAl alloy formation — •Katharina Krügel, Tobias Urban, and Johannes Heitmann — Institut für Angewandte Physik, TU Bergakademie Freiberg, Freiberg, Germany

The alloying of Al and Ag on dielectric silicon nitride layer (Si3N4), deposited by Chemical Vapor Deposition on <100> Silicon substrates, was investigated. Ag and Al were deposited in variable proportions with overall thickness of 1 μm by Physical Vapor Deposition on the Si-substrate with Si3N4 layers of 80 and 100 nm thickness. This setup is similar to industrial photovoltaic application.

The samples were tempered with Rapid Temperature Processing up to 1000°C. By microscopy square-shaped hollows within the metal layer for annealing temperatures higher than 800°C were shown. By preparation of a Focused Ion Beam-cut and following Scanning Electron Microscope investigation a local perforation of the Si3N4 layer was observed. Below this region a pyramidal etching spike is formed with an angle of 52.3° which is equal to the angle between the <100> and <111> plane. These spikes were filled with an intermetallic phase consisting of fcc AgAl- and hcp Ag2Al-phase with local silicon precipitations. The formation of this etching pits can be proven by resistance measurement between metal and silicon. With increasing temperature an electrical contact was formed due to the local etching of the dielectric layer.

Usually Si3N4 has a high chemical and thermal stability. For the first time an etching of the passivation layer only by AgAl was observed.

DS 44.25 Thu 17:00 P1C

Ti2AlN and Ti2AlC MAX-phase synthesis by multilayered PVD coatings — •Frank Burmeister[1], Lukas Gröner[1], Eberhard Nold[1], Eduart Reisacher[1], Francesco Colonna[2], Alexander Fromm[1], Frank Meyer[1], and Chris Eberl[1] — [1]Fraunhofer IWM, Freiburg, Deutschland — [2]Freiburger Materialforschungszentrum, Freiburg, Deutschland

Mn+1AXn phases belong to a group of ternary nitrides or carbides, where M denotes an early transition metal, A denotes mostly a group III or IVA element and X is either nitrogen or carbon. Due to the presence of strong covalent MX bonds and weak ionic MA bonds, these materials often exhibit a high corrosion resistance as well as good electrical conductivity and thermal stability. The phase synthesis and their suitability for industrial applications, e.g. as protective and/or conductive coatings has been studied for crystalline films by others. However, these properties are strongly influenced by the material's microstructure and phase composition. To investigate the evolving microstructure of polycrystalline Ti2AlN and Ti2AlC coatings, AlN-Ti and Al-TiC multilayers were deposited by reactive sputtering using either nitrogen or methane as reactive gases, followed by a subsequent annealing step at 700°C in vacuum. In this way, coatings with a dominant M2AX-phase component were synthesized successfully. The coating*s properties were examined by elemental and phase analysis using XPS, XRD and Raman spectroscopy. The investigations revealed a prominent texture in the coating's microstructure which was ascribed to the multilayered deposition.

DS 44.26 Thu 17:00 P1C

Effects of Molecular Orientation in Acceptor-Donor Inter-

faces between Pentacene and C60 and Diels-Alder Adduct Formation at the Molecular Interface — •Tobias Breuer, Andrea Karthäuser, and Gregor Witte — Philipps-Universität Marburg, Germany

Interfaces between pentacene and Buckminster-Fullerene (C_{60}) have attracted interest due to their application as oligomeric acceptor/donor model system for organic solar cells. As the actual device characteristics in such implementations are crucially controlled by the interface structure, detailed investigations of this interface on a molecular level are mandatory. In this study we analyze the influence of the orientation of the pentacene molecules in highly-ordered crystalline bottom layers on the characteristics of such internal interfaces. We show that the interface structure is driven by temperature-controlled diffusion of C_{60} molecules to the pentacene step-edges in the case of uprightly-oriented pentacene. For lying pentacene in the bottom layer, no step-edge decoration is observed while the wetting of the pentacene layer is enhanced. Furthermore, the stability of the interface against intercalation and re-orientation has been analyzed by means of NEXAFS spectroscopy, showing that the orientation of the pentacene molecules at the interface remains unchanged. Instead, we observe strong indication for chemical modification of the molecular entities by the formation of Diels-Alder adducts between C_{60} and pentacene.
[1] T. Breuer et al., Adv. Mater. Interfaces, 3, 1500452 (2016).

DS 44.27 Thu 17:00 P1C

Combinatorial research on thin film Bi-W-Mo-O-N electrocatalysts for solar water splitting — •Mona Scherbeck[1], Ramona Gutkowski[2], Wolfgang Schuhmann[2,3], and Alfred Schuhmann[1,3] — [1]Chair for MEMS Materials, Institute for Materials, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum, Germany — [2]Analytical Chemistry-Center for Electrochemical Sciences (CES) — [3]Materials Research Department, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum, Germany

The discovery of novel photoabsorbers for solar water splitting with improved properties e.g. photocorrosion resistance, high photocurrents and photovoltages is an important topic. In this contribution, results on Bi-W-Mo-O-N n-type photoelectrodes synthesized by combinatorial reactive magnetron co-sputtering are presented. The material libraries were deposited by varying the sputtering parameters e.g. reactive gas flow, sputtering pressure and temperature to identify dependencies of sputtering parameters on the properties of the thin film material libraries. To further characterize the properties of the material libraries the crystal structure, composition, optical properties, and photoelectrochemical performance were measured with high-throughput methods. The functional properties of these material libraries are correlated to their structure, composition, and processing in phase diagrams.

DS 44.28 Thu 17:00 P1C

The novel Kiel high flux X-ray diffractometer for heavy loads and with focusing option — •Finn Christiansen, Jochim Stettner, and Olaf Magnussen — Institut für experimentelle und angewandte Physik Kiel, Univerversität Kiel

We present a novel X-ray diffractometer, installed at the Kiel rotating anode microfocus X-ray lab source, which is characterized by a flexible and massive design of all components and high X-ray flux. The instrument is especially dedicated for in-situ investigations of solid surfaces, solid-solid and liquid-solid interfaces in complex sample environments (e.g. vacuum and plasma chambers up to 250 kg). Additionally, the diffractometer provides a vertical focusing option for spatially resolved measurements, microcrstals and measurements under grazing incidence with enhanced flux on the sample.
Two different modes are available: In the "high flux mode" a Multilayer Montel mirror provides a vertically and horizontally collimated beam with a diameter of ≈2 mm with $4.3 \cdot 10^8$ Ph/s. The white beam background and CuK_β contributions are strongly suppressed. In the "vertical focusing mode", an additional multilayer mirror, located close to the sample, reduces the spot size at the sample position to 2(h) x 0.1(v) mm^2.
Key parameters for both operational modes like flux, resolution and spot size at the sample position were determined quantitatively. Additionally, we present first X-ray data of model systems, e.g. ZnO surfaces and microcrystals in order to demonstrate the performance of this instrument.

DS 44.29 Thu 17:00 P1C

Influence of Microstructure on the Amorphous to Crystalline Phase Transition in the Phase-Change Material GST124 — •Carl-Friedrich Schön, Nikita Polin, Matthias M. Dück, Christoph Persch, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

Phase-change materials (PCM) are a promising candidate for universal memory, as their optical reflectivity and electrical resistivity change considerably along the nanosecond scale transition between the amorphous and the crystalline state. Because this phase transition is the foundation of device functionality, significant effort has been devoted to its understanding. The microstructure of PCM thin films has been found to heavily impact the properties of the phase transition in GST124. While the investigation of microstructural defects is not relevant for application, it might yield new insights into the fundamental mechanisms of the phase transition.

In this work, the microstructure of GST124 thin films is varied and characterized utilizing x-ray reflectivity (XRR) and scanning electron microscopy (SEM). The effects of the microstructure on the film's properties are then measured by x-ray diffraction (XRD), while the phase transition is investigated with a laser setup featuring a high and low power laser combination, enabling the measurement of the materials reflectivity during crystallization. A higher gas pressure causes an increased incorporation of voids as well as an increased minimum energy to crystallize the sample. This energy shift can be attributed to the change of microstructure, as subsidiary effects can be excluded.

DS 44.30 Thu 17:00 P1C

Texture Optimization and Structure-Property Relationships in Chalcogenide Thin Films — •Matthias Maximilian Dück, Stefan Jakobs, Tobias Schäfer, Carolin Jacobi, Felix Lange, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

Chalcogenides along the pseudobinary line between GeTe and Sb_2Te_3 are currently gaining much attention, since a number of interesting properties can be attributed to certain members of that material group. Amongst these compounds, phase-change materials, thermoelectric materials, topological insulators and superconductors are found. Especially for the latter two, a large correlation between functionality and film quality has been observed. With the incorporation of a new sputter setup in a UHV cluster tool featuring a variety of analytic capabilities, access to a large parameter space for the deposition of chalcogenide systems was gained. This allows to push the boundaries in terms of film quality achieved in the sputter process. That way, a compromise between the strengths of MBE (film quality) and sputter deposition (industrial relevance) is found. This study focuses on the optimization of phase-change material thin films with respect to film quality and texture. The films are thoroughly characterized by a variety of methods, enabling the detailed investigation of film quality, texture and structure-property relationships.

DS 44.31 Thu 17:00 P1C

On the Role of the Interface on the Growth of a Stabilized Bilayer Framework System — •Alexander Mänz, Michael Kothe, and Gregor Witte — Molekulare Festkörperphysik, Fachbereich Physik, Philipps-Universität Marburg, Renthof 7, 35032 Marburg

The nonplanar, π-conjugated PAH titanyl-phthalocyanine (TiOPc) is known for exceptional optical and electronic properties. To utilize and optimize TiOPc based thin film devices a detailed understanding of interface related growth is of great importance. This study links characteristics of inital growth of the TiOPc bilayer framework, deposited via organic molecular beam deposition (OMBD) with the morphology of TiOPc multilayer systems on various substrates. In a first step, the molecular arrangement of TiOPc on Au(111) and Ag(111) substrates from monolayer to multilayer regime is characterized by scanning tunneling microscopy (STM). Consecutively, we analyze the morphology and crystallinity of TiOPc multilayers by means of atomic force microscopy (AFM) and X-ray diffraction (XRD). After completion of the first bilayer on Au and Ag substrates, dewetting leads to formation of separated islands with height of multiples of the bilayer, which are stabilized by the alternating orientation of the titanyl units. Comparative analyses for thin films grown on KCl and HOPG substrates show a similar behaviour, while somewhat different polymorphs were identified in thicker films.

DS 44.32 Thu 17:00 P1C

Development of a new method to probe the electronic structure of organic photovoltaic materials in a bulk heterojunction — •Vincent Lami[1,2], Paul E. Hopkinson[1,2], and Yana

Vaynzof[1,2] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Centre for Advanced Materials, Heidelberg University, Germany

Organic photovoltaic (OPV) cells have attracted remarkable interest as a possible alternative to conventional inorganic technologies. The performance of an OPV device is largely determined by the alignment of the electronic energy levels of its individual components. Despite the importance of energetics, the understanding of the energy level evolution within the device is still limited. Consequently, energy level diagrams of OPVs are typically constructed by measuring the energy levels of the individual materials, without taking into account the interactions between them. Herein, we demonstrate the development of a new experimental technique based on ultra-violet photoemission spectroscopy that allows us to measure the progression of both the energy levels and material composition within the photovoltaic active layer. Our preliminary results obtained on a variety of organic materials are very promising and demonstrate the effectiveness of our new technique.

DS 44.33 Thu 17:00 P1C

Morphological studies of Squaraine-Fullerene blend films — •Angelika Maderitsch[1], Oliya Sadrillaevna Abdullaeva[1], Matthias Schulz[2], Arne Lützen[2], Jürgen Parisi[1], and Manuela Schiek[1] — [1]Energy and Semiconductor Research Laboratory, Institute of Physics, University of Oldenburg, Germany — [2]Kekulé Institute of Organic Chemistry and Biochemistry, Rheinische-Friedrich-Wilhelms-University of Bonn, Germany

Organic photoelectric materials are promising candidates for the development of biocompatible artificial photoreceptors. Currently, we are investigating a photoactive layer consisting of an anilino-squaraine donor (SQIB), a small molecular model organic semiconductor, blended with a fullerene acceptor (PCBM). After annealing at high temperatures the crystalline film shows two distinct structural motifs with different properties.[1] SEM and TEM are applied to gain a deeper insight to the morphology of the photoactive layer. TEM samples are prepared via floating and FIB-milling providing cross section lamellae. The predominant structure (platelets) shows a rather flat surface partly with elongated pinholes and borders between different crystalline orientations. The discontinuously localised second structure (ferns) is less homogeneous and significantly rougher. Voids between ferns seem to consist of very thin PCBM film. The results are compared to those of other methods like AFM, XRD and optical microscopy.

(1) Abdullaeva et al., Langmuir 2016 32 (33), 8533-8542, DOI:10.1021/acs.langmuir.6b02085

DS 44.34 Thu 17:00 P1C

Investigation of Disorder Related Electrical Properties in the Pseudo-Binary Line SnTe-PbTe — •Johannes Reindl[1], Alexander Rochotzki[1], Zheng Zhen[1], Stefan Jakobs[1], and Matthias Wuttig[1,2] — [1]1. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA-FIT, RWTH Aachen University, 52056 Aachen, Germany

The solid solutions of the chalcogenides SnTe and PbTe have been thoroughly investigated in the past under the premise of infrared applications, which exploit the small band gap that can be tuned with stochiometry [1]. Of additional interest is the shift from p-type conduction in SnTe to n-type conduction of PbTe that can be described with a band inversion in SnTe and the crossing of the bands at a specific composition of the alloys [1]. In recent years the investigation of topological insulator states has led to the insight that topology is pivotal in this material system and thus SnTe single crystals have been found to be topological crystalline insulators [2].

For industrial applications of the aforementioned effects it would be beneficial to shift from physical vapor deposition fabrication of single crystals to large scale production processes, like sputtering. However, the unique physical properties might get lost due to the formation of structural defects. This general increase of disorder and the subsequent influence on some key electrical properties will be investigated, with special focus on the region of the band crossing.

[1] Dimmock, J. O. et al., Phys. Rev. Lett. 16, 1193 (1966)
[2] Xu, S.-Y. et al., Nat. Commun. 3, 1192 (2012)

DS 44.35 Thu 17:00 P1C

Surface reconstruction in STO: Experimental and theoretical optical constants — •B. Katter[1], V. B. Zabolotnyy[1], C. Schüssler-Langeheine[2], E. Schierle[2], L. Dudy[1], O. Kirilmaz[1], S. Macke[4], M. W. Haverkort[3], and V. Hinkov[1] — [1]Universität Würzburg — [2]Helmholtz-Zentrum Berlin für Materialien und Energie — [3]Universität Heidelberg — [4]Max-Planck-Institut Stuttgart

Transition metal oxides, like all crystaline solids, can show reconstruction effects at their surface due to breaking of the crystal symmetry. In $SrTiO_3$ missing oxygen at the surface lifts the orbital degeneracy and effectively lowers the symmetry from O_h do D_{4h}, which leeds to anisotropy of the optical constants in the surface layer. We have implemented a matrix formalism to study $SrTiO_3$ with surface reconstruction using resonant X-ray reflectometry. This allows us to extract the optical constants of the anisotropic system from experimental data. These in turn can be compared to crystal field calculations, which helps to understand the orbital reconstruction on a microscopic level.

DS 44.36 Thu 17:00 P1C

Substrate roughness effect on c-axis preferred orientation of ZnO layers — Sebnem Yazici, •Mariana V.G.Oliveira, and Matthias Wuttig — I. Institute of Physics, Physics of New Materials, RWTH Aachen University, 52056 Aachen, Germany

Improved TCO materials are needed for a range of applications, such as photovoltaics and flat panel displays. Understanding how to control the production processes and thus structure and properties is of fundamental importance. In this work, we have investigated how the roughness of the substrate effects the c-axis texture formation of ZnO thin films. To obtain the substrates, SiNx under layers were deposited on Si wafers, before ZnO layer deposition. Rough SiNx was a good candidate due to its amorphous structure, avoiding epitaxy influence. The roughness dependence of SiNx layers on different operating pressures and thickness were investigated. Generally, thicker films and films that were deposited at higher operating pressures ended up with higher roughness values. Layers of ZnO with thickness of 50nm were deposited onto 10, 20, 30 nm thick SiNx layers and on bare Si wafer as a reference sample. Structural characterization using X-ray diffraction (Bragg-Brentano, rocking curve) was carried out to compare the reference and rough underlayer samples.

DS 44.37 Thu 17:00 P1C

Combined local electrical and optical measurements of individual semiconductor nanosheets — •Andreas Kolditz, Christian Strelow, Tobias Kipp, and Alf Mews — University of Hamburg, Institute of Physical Chemistry, Grindelallee 117, 20146 Hamburg, Germany

Tin(II) sulfide or tin(II) selenide are very attractive IV-VI semiconductor materials because of the natural abundance and low toxicity. In particular, two-dimensional (2D) nanosheets of these materials are promising for photovoltaics as well as for light-emitting applications. We investigate the optical and electrical characteristics of individual 2D nanosheets by combining scanning electrostatic force microscopy (EFM) and Kelvin probe force microscopy (KPFM) with electrical transport and fluorescence measurements. This combination allows us to investigate the effect of band bending on the photo current and also the effects of external charging on the fluorescence properties of individual structures. In first EFM measurements on SnSe nanosheets under local illumination we observed a separation of the photoexcited electrons and holes within the nanosheets. In detail the EFM measurements showed positive excess charges at the excitation area and negative excess charges distributed everywhere else.

DS 44.38 Thu 17:00 P1C

Interactions at the interface of Cobalt phthalocyanine and graphene covered metal surfaces: Influence of fluorination of CoPc — •David Balle, Malgorzata Polek, Reimer Karstens, Peter Grüninger, Hilmar Adler, Thomas Chassé, and Heiko Peisert — Institute of Physical and Theoretical Chemistry, Auf der Morgenstelle 18, 72076 Tuebingen, University of Tuebingen, Germany

The unique electronic, optical and magnetic properties of transition metal phthalocyanines (TMPc) have recently led to increasing research efforts and make them suitable candidates for possible organo-electronic devices. Interactions at interfaces, like charge transfers, can drastically change said properties, though, and need to be carefully investigated.

Graphene buffer layers present an effective way to manipulate or prevent such transfer processes. To function as such a buffer layer, interaction between the graphene layer and the substrate must be controlled, though. Properties of strongly bound and coupled graphene on Ni(111) are severly affected, while an intercalated, uncoupled graphene layer can influence interactions between the substrate and the organic layer. Variations of other electronic interface parameters, such as fluorination of the phthalocyanines, also have an impact, leading to a persisting interaction at the interface for $CoPcF_{16}$ while the corresponding interaction is blocked for CoPc on intercalated graphene on Nickel.

Investigations were carried out using mainly X-ray absorption and photoemission spectroscopies (XAS, PES).

DS 44.39 Thu 17:00 P1C

Study of manganites with Resonant X-ray Reflectivity — •Michael Dettbarn[1], Volodymyr B. Zabolotnyy[1], Abdul-Vakhab Tcakaev[1], Benjamin Katter[1], Jorge Enrique Hamann-Borrero[2], Kirill Miller[1], Michael Zapf[1], Andreas Herklotz[3], Diana Rata[4], Enrico Schierle[5], Feizhou He[6], Ronny Sutarto[6], Kathrin Dörr[4], Jochen Geck[7], George A. Sawatzky[8], Michael Sing[1], Ralph Claessen[1], and Vladimir Hinkov[1] — [1]Universität Würzburg and Röntgen Center for Complex Material Systems (RCCM), Würzburg — [2]IFW, Dresden — [3]ORNL, Oak Ridge, USA — [4]Martin-Luther-Universität Halle-Wittenberg, Halle — [5]HZB, Berlin — [6]CLS, Saskatoon, Canada — [7]TU Dresden, Dresden — [8]UBC, Vancouver, Canada

Perovskite manganites such as $LaMnO_3$ are known to reveal a non-trivial behavior of the manganese L-edge resonant absorption, due to a complicated interplay between Hund's first rule, spin-orbit coupling and crystal field splitting. Using Resonant X-ray Reflectivity (RXR), together with cluster calculations, we study the optical properties of $LaMnO_3$ and $Pr_{0.5}Ca_{0.5}MnO_3$ samples. We are investigating the resonant behavior of the Mn ions depending on varying mechanisms such as doping, oxygen stoichiometry overshoots and distortions of the MnO_6 octahedra, the latter being induced by either the Jahn-Teller effect or epitaxial strain. The layer-resolved nature of RXR enables us to derive the separate concentrations of the Mn valencies, which allows for different conclusions about interfacial correlation effects in the presence of orbital and magnetic ordering.

DS 44.40 Thu 17:00 P1C

Photoluminescence imaging of few-layer transition metal dichalcogenides — •Victor Funk, Michael Förg, and Alexander Högele — Ludwig-Maximilians-Universität, München, Deutschland

Transition metal dichalcogenides (TMDs) are novel two-dimensional semiconductor materials with unique optoelectronic properties (1). A crucial step in the fabrication of mono- and multilayer TMD devices is the classification of the number of layers of TMD crystals exfoliated on a polydimethylsiloxane (PDMS) stamp for transfer (2). We report a simple and reliable method for the identification of individual monolayers by means of two-dimensional photoluminescence imaging. Our techniuqe, established for four representative materials of TMD semiconductors and calibrated with layer-sensitive Raman spectroscopy, enables rapid characterization of the crystal layer thickness prior to subsequent transfer onto target substrates.

(1) T. Cao et al., Nature Communications, 3, 887 (2012) (2) A. Castellanos-Gomes et al., 2D Materials, 1, 2053 (2014)

DS 44.41 Thu 17:00 P1C

Photo-Degradation studies of PDTSTzTz (KP115) for application in OVP — •Andreas Früh[1], Ulf Dettinger[1], Heiko Peisert[1], Hans-Joachim Egelhaaf[2], and Thomas Chassé[1] — [1]Eberhard-Karls-University, Institute for Physical and Theoretical Chemistry, Auf der Morgenstelle 18, D-72076 Tübingen, Germany — [2]Belectric OPV GmbH, Landgrabenstr. 94, D-90443 Nürnberg, Germany

Organic photovoltaic (OPV) offers a possible solution for the future energy demands and combines challenging design requirements with flexibility. On the other hand the limited life time of such devices remains a challenge. UV-Vis and FTIR spectroscopy as well as AFM and REM microscopy were used to study the photo-oxidation of the Low-Band-Gap Polymer Poly[4,4'-bis(2-ethylhexyl)dithieno[3,2-b:2',3'-d]silole]-2,6-diyl-alt-[2,5-bis(3-tetradecylthiophen-2-yl)thiazole-[5,4-d]thiazole-1,8-diyl] (PDTSTzTz) as pristine film and blended with PC[60]BM. For pristine PDTSTzTz films in ambient air, an UV induced radical mechanism was recently suggested [1]. In this work we study the photo-oxidation in dry synthetic air as a function of the wavelength of the light and compare the results to irradiation under standard Air Mass 1.5 conditions. The results point to a different degradation mechanism for lower wavelengths. The degradation of the different monomer units of the polymer backbone as well as the side chains is monitored by IR spectroscopy. [1] H. S. Silva et al., J. Mater. Chem. A, 4 (2016) 15647-15654.

DS 44.42 Thu 17:00 P1C

Preparation of Epitaxial PMN-PT Films on Si-based Templates for Electrocaloric Studies — •Robert Kuhrt[1,2], Michael Mietschke[1,2], Christian Molin[4], Sylvia Gebhardt[4], Matthijn Dekkers[3], Kornelius Nielsch[1,2], and Ruben Hühne[1] — [1]IFW Dresden, Germany — [2]Technische Universität Dresden, Germany — [3]Solmates B.V., Enschede, Netherlands — [4]Department of Smart Materials and Systems, Fraunhofer Institute for Ceramic Technologies and Systems, Dresden, Germany

Ferroelectric materials that show a strong electrocaloric (EC) effect near a phase transition are subject of current research. These materials show a temperature change when applying an electric field adiabatically which makes them suitable for solid state coolers. One prominent example are $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT) compounds, which show a high EC effect over a broad temperature range close to room temperature. An integration of these materials into semiconductor architectures might open up new opportunities for cooling sensors or other device structures.

Therefore, epitaxial 0.9PMN-0.1PT films were grown on (001)-oriented $SrTiO_3$ buffered Si wafers by pulsed laser deposition with conducting interlayers as electrodes. Epitaxy, phase purity and surface topography were studied using XRD and AFM. The ferroelectric properties were determined by temperature dependent global polarization measurements as well as local piezo response force microscopy.

DS 44.43 Thu 17:00 P1C

Simulating Interferometric Spectra using Multiple Matrix Methods — •Kai Alexander Schwenzfeier[1], Andreas Erbe[2], and Markus Valtiner[3] — [1]MPIE, Düsseldorf, Germany — [2]NTNU, Trondheim, Norway — [3]TU-BAF, Freiberg, Germany

The analytical equations used for evaluating Surface Forces Apparatus (SFA) data were derived on the basis of a number of simplifications, but the actual impact of these simplifications is largely unknown. Especially the influence of mirror materials has completely been neglected.

By simulating SFA spectra for different interferometer layouts and different mirror materials and analysis of those spectra using the analytical equations it is possible to estimate the relative error done by using those equations.

The optical properties of the mirror material have a great impact on the peak shape as well as position of the resulting interference patterns. Especially with 10-20 nm thin mirrors and gold as mirror material the determination of the fringe order as one integral part of the analytical equations breaks down.

Our findings illustrate the need to reevaluate SFA data with respect to mirror materials and thicknesses with a suitable analysis tool. We developed a new software tool based on multiple matrix methods, that addresses these issues and allows the simulation of interferometer pattern based on the physical properties of the interferometer layers. Our simulation tools can be applied not only to SFA analysis but to general interferometry applications with white light.

DS 44.44 Thu 17:00 P1C

X-Ray Reflectivity Investigation of Structure and Kinetics of Photoswitchable Lipid Monolayers — •Malte Jacobsen[1], Kuntal Chatterjee[1], Björn Haushahn[1], Chen Shen[1,2], Sven Festersen[1], Jonas Warias[1], Benjamin Runge[1], Franziska Reise[3], Thisbe Lindhorst[3], Beate Maria Klösgen[2], Olaf Magnussen[1,4], and Bridget Murphy[1,4] — [1]Institute for Experimental and Applied Physics, CAU Kiel, Germany — [2]SDU Odense, Denmark — [3]Institute of Organic Chemistry, CAU Kiel, Germany — [4]Ruprecht Haensel Laboratory, CAU Kiel, Germany

The mechanical and dynamic properties of phospholipid membranes are important for biological functions such as switching of embedded proteins. To investigate these biologically relevant properties we study model systems in which amphiphilic photoswitchable glycoconjugates have been integrated into biomimetic phospholipid membranes. The structure and kinetics of the switching process in a lipid Langmuir film are measured using Langmuir isotherms and in situ X-ray reflectivity at LISA diffractometer P08, PETRA III. We have modified glycolipids to contain an azobenzene photoswitch between the chain and head group and successfully embedded them in a monolayer of DPPC. We can reversibly change the azobenzene-glycolipid orientation between trans- and cis-conformation by illumination with UV and blue light.

Strong changes in membrane conformation upon switching have been observed, and a critical point has been discovered above which the membrane expands rather than compresses upon switching. This work is funded by SFB 677 and BMBF 05K13FK2.

DS 44.45 Thu 17:00 P1C

Investigation of Charge Carrier Distribution in OLEDs by Means of Photoluminescent Molecular Probes — •Thomas Ferschke[1], Lars Jäger[2], Wolfgang Brütting[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, Julius Maximilian University, 97074 Würzburg — [2]Institute of Physics, University of Augsburg, 86135 Augsburg — [3]ZAE Bayern, 97074 Würzburg

The charge carrier distribution in organic thin film devices is essential for optimizing their operation characteristics. Recently, it has been shown that these current densities can be determined by means of photoluminescence (PL) studies on single guest dye molecules. [Nothaft M. *et al.*, *ChemPhysChem* **12**, 2590–2595 (2011)] Here, this concept is applied to common Alq_3/α-NPD OLEDs by utilizing molecular dopant ensembles in combination with μ-PL. Tetraphenyldibenzoperiflanthene (DBP) is intentionally embedded as dopant (0.1 v-%) via co-evaporation at defined positions within the Alq_3 emission layer. Upon charge injection an effective reduction in the DBP PL is observed which can be attributed to electron - exciton interaction. The macroscopic current density related to the respective PL reduction scales with the distance from the injecting electrode in qualitative agreement with a SCLC model. The validity of this model and thus, variations in vertical charge carrier distribution are studied as a function of current density as well as of temperature. Since at reverse bias PL quenching of DBP near the Alq_3/α-NPD interface is observed, a comparative study of the interfacial charge density is performed by means of integral impedance spectroscopy. [Brütting W. *et al.*, *Org. Electron.*, **2**, 1-36 (2001)]

DS 44.46 Thu 17:00 P1C

Introducing band gap states in MoS_2 monolayers by triangular defects — Tommy Lorenz[1], •André Niebur[1,2], Sibylle Gemming[2,3], Artur Erbe[2], and Gotthard Seifert[1] — [1]Theoretical Chemistry, TU Dresden, 01062 Dresden, Germany — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden - Rossendorf e.V., 01314 Dresden, Germany — [3]Theoretical Physics, Faculty of Sciences, TU Chemnitz, 09107 Chemnitz, Germany

Triangular defects in MoS_2 monolayers and their influence on the crystal and electronic structure have been studied using the density-functional based tight-binding (DFTB) method. Systems with different defect sizes and concentrations have been compared to find out how these parameters affect the electronic properties of MoS_2 monolayers. The density of states (DOS) calculations show the presence of additional states in the HOCO-LUCO-Gap of pristine MoS_2 even for small defects in a low concentration. Band structure calculations and orbital plots characterize these states as localized mid-gap states. From the projected densities of states can be seen that these states mainly arise from d-orbitals of the molybdenum atoms at the defect edges and their number increases with an increasing defect size. Due to the fact that the molybdenum d-states dominate the valence and conduction band edges of MoS_2, the additional states which arise in the band gap may impact the electronic transport through the layer. Analyses of the orbital's degree of (de-) localization show that this influence seems to be quite small for low defect concentrations but increases for higher ones.

DS 44.47 Thu 17:00 P1C

Time-resolved THz spectroscopy on 1T-TaS_2 — •Simon Lange[1], Lara Wimmer[1], Georg Herink[1], Kai Rossnagel[2], and Claus Ropers[1] — [1]4th Physical Institute - Solids and Nanostructures, University of Göttingen, Friedrich-Hund-Platz 1, Germany — [2]Institute for Experimental and Applied Physics, University of Kiel, Leibnizstraße 15, Germany

Transition metal dichalcogenides (TMDCs) are a highly interesting class of materials due to their two-dimensional behaviour, which leads to multiple phenomena, like Mott and Peierls transitions, superconductivity and charge and spin density waves. A prominent representative of TMDCs, 1T-TaS_2, shows various different charge density wave (CDW) phases associated with periodic lattice distortions.

Here, we present an optical pump/terahertz probe setup in a transmission geometry for characterizing the ultrafast response of materials in the spectral range of 0.5 to 3 THz and at temperatures between 130 to 300 K.

Using this setup, in temperature-dependent measurements, we observe the phase transition between the commensurate (C) and nearly-commensurate (NC) charge density wave phases and its hysteresis in a 1T-TaS_2 thin film. We identify three characteristic phonon modes in the insulating C phase, which vanish in the metallic NC phase [1]. In time-resolved measurements (see also Ref. [2]), we optically induce this transition and track the evolution of the phonon modes.

[1] L. Gasparov, Phys. Rev. B, 66, 094301 (2002)

[2] N. Dean et al., Phys. Rev. Lett. 106, 016401 (2011)

DS 44.48 Thu 17:00 P1C

Ultrafast laser-triggered electron emission from diamond coated metal tips — •Alexander Tafel, Peter Hommelhoff, and Jürgen Ristein — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen

Sharp metal tips are widely used in electron microscopy as cold cathodes utilizing the outstanding beam quality of field emitted electrons from a nm sized virtual source. Nanocrystalline diamond with negative electron affinity exhibits excellent electron field emission properties and allows nm thin coating. The combination of the unique properties of sharp tips and nanodiamond are used in this work for building a high brightness femtosecond electron source.

Tungsten tips are etched electrochemically with resulting tip radii < 20 nm. Nanodiamond seeding is used to achieve high nucleation densities required for thin but dense films. Diamond films are grown using microwave enhanced chemical vapour deposition.

Ultrafast electron emission from diamond coated samples is investigated by few-cycle infrared pulses. Here, we present first experimental results and compare electron emission from diamond coated tips to bare tungsten tips.

The goal of this research is to develop a source of ultrashort and intense electron bunches for use in 4-D electron microscopy, dielectric laser acceleration and ultrafast electron diffraction.

DS 44.49 Thu 17:00 P1C

Improving the photovoltaic performance of hybrid photovoltaics by inorganic interfacial modification — •Yvonne J. Hofstetter[1,2], Paul E. Hopkinson[1,2], Artem A. Bakulin[3], and Yana Vaynzof[1,2] — [1]Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany — [2]Centre for Advanced Materials, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany — [3]Cavendish Laboratory, Cambridge University, JJ Thomson Ave, Cambridge, UK

Bilayer organic-inorganic hybrid photovoltaic devices offer the possibility to modify the organic-inorganic interface, and thus to influence the efficiency of photo-induced charge separation. Various organic modifiers have been investigated, whereas inorganic modifiers have remained unconsidered for the most part. Here, we introduce an inorganic modifier, caesium carbonate, as an interlayer in a model poly(3-hexathiophene)/ZnO system. Upon modification, we observe an improved energy level alignment at the hybrid interface resulting in a significantly increased open circuit voltage, and suppressed formation of interfacial bound charge pairs resulting in reduced interfacial recombination losses and an increased short circuit current. These improvements add up to a twelve fold enhancement in power conversion efficiency which demonstrates the significant potential of applying inorganic modifiers in hybrid photovoltaics to improve the performance.

DS 44.50 Thu 17:00 P1C

Combinatorial Synthesis of Ni-based Nanoparticles by Sputtering into Ionic Liquids — •Christina Eberling, Gesa Zahn, Christoph Somsen, and Alfred Ludwig — Institute for Materials, Ruhr-Universität Bochum, 44780 Bochum, Germany

Nanomaterials are of great interest for different applications, especially for catalysis, for example in fuel cells. To realize low-cost hydrogen fuel cells, commonly used rare and expensive metals must be replaced by new potential catalysts. High-throughput and combinatorial approaches offer a good possibility to identify promising material combinations in a fast and efficient way. By using combinatorial co-sputter deposition techniques, unary, binary and multinary metal alloys nanoparticles (NPs) can be synthesized with different composition. As a substrate, we use a micromachined cavity array wafer. The cavities are filled with an ionic liquid (IL) that can be handled under vacuum conditions due to its very low vapour pressure. In first experiments, we focused on the fabrication of Ni-based alloy NPs with different compositions in the IL 1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([BMim][Tf2N]), especially Ni-Co and Ni-Mn. Transmission electron microscopy (TEM) measurements show that non-agglomerated, crystalline NPs with a diameter of 3 to 6 nm could be synthesized. In addition, thin films were deposited under the same sputtering conditions and analysed using energy dispersive X-ray spectroscopy (EDX) and X-ray diffraction (XRD) in order to compare elemental distribution and crystal structure of thin films with those of NPs.

DS 44.51 Thu 17:00 P1C

Understanding Epitaxial Growth of Perfluoropentacene on Graphite — •Felix Widdascheck and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7, D-35032 Marburg, Germany

Understanding and controlling the growth of organic molecular films is crucial for their use in optoelectronic devices. A common approach is to use different substrates in order to mediate the growth and control the orientation and polymorph in the film. Therefore, the substrate-molecule interface is of particular importance as this controls the initial stage of film growth. In this regard an interesting model system are perfluoropentacene (PFP) films which grow epitaxially on graphite and exhibit a new, substrate induced π-stacked polymorph. [1, 2] Here, we report on a STM study of the PFP/Graphite interface and the initial stage of film growth. Using single crystalline graphite and tip assisted removing of PFP molecules the adlayer structure and the azimuthal orientation of the first two monolayers were determined with high precision. It is found that the first monolayers act as a precursor for further growth, already resembling the multilayer structure, while a dislocation pattern was identified, which is attributed to the misfit between the locally dense packed film and the substrate lattice.

[1] I. Salzman et al., ACS Nano (2012), 6, 10874
[2] R. Félix et al., Cryst. Growth Des., Article ASAP, DOI: 10.1021/acs.cgd.6b01117

DS 44.52 Thu 17:00 P1C

Growth of pinholes in metal electrodes of organic photovoltaic cells — •Daniel Fluhr[1], Burhan Muhsin[2], Rolf Öttking[2], Roland Rösch[2], Stefan Krischok[1], and Harald Hoppe[2] — [1]Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena) & Laboratory of Organic and Macromolecular Chem- istry (IOMC), Friedrich Schiller University Jena, 07743 Jena, Germany

Lifetime is still a major problem of organic photovoltaic (OPV) cells. There are many reasons for solar cell degradation varying from shunts induced by impurities or electromigration over photoinduced oxidation of active layer materials to corrosion and delamination of the metal contact both induced by oxygen or water ingress. One issue concerns so-called pinholes through the metal back electrode of the device. These pinholes offer pathways for ingress of water and oxygen which may attack the metal-organic interface by introducing delamination through formation of insulating metal oxides or hydrogen evolution. As charge injection and extraction is suppressed at delaminated areas, the active area taking part in power conversion - and hence the overall efficiency becomes reduced. We investigated the influence of different environmental conditions on the reduction of the active area of the OPV cell. Spatially resolved measurements give information on location and size of insulated areas induced by pinholes in the metal back contact. Time resolved measurements during degradation of the devices revealed the dynamics and rate of growth of these individual defects.

DS 44.53 Thu 17:00 P1C

3D-Analysis of InGaN-Quantum Wells — •Maximilian Ries — Schwarzschildstraße 8

Modern LEDs (light emitting diodes) are frequently made of III-nitride structures, with applications ranging from lightning, optoelecetronics to life sciences and health care. To allow excellent performances, complex heterostructures must be fabricated with high precision. This study introduces a 3D analysis based on Raman and photoluminescence (PL) spectroscopy of InGaN quantum well (QW) structures. Simultaneous excitation and measurement of PL and Raman modes with a home-built setup allow for non-destructive and efficient determination of QW thickness and In-content, providing valuable information on device performance.

DS 44.54 Thu 17:00 P1C

Development of quantitative Reflectance Anisotropy Microscopy — •Timo Seemke, Eugen Speiser, Johannes Falkenburg, Maciej D. Neumann, and Norbert Esser — Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Department Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany

Reflectance anisotropy microscopy (RAM) is a technique that monitors the optical anisotropy of surfaces with spatial resolution and provides information about crystal orientation and local strain on the surface.

Often, technologically relevant materials are not transparent, thus transmittance based polarization- or phase microscopy methods are not an option for measuring spatially resolved, low amplitude surface anisotropy. Common reflectance based methods depend on beam-splitting elements that do not fully conserve polarization states. Other common methods make use of a Foster prism polarizing beamsplitter, that detect only the depolarization by the surface and do not measure the anisotropy quantitatively. A third widely used approach is to separate the incoming and outgoing light beam by using a small angle of incidence to the surface, which severely limits the use of high spatial resolution optics.

We present a new RAM setup for quantitative and spatially resolved measurements of optical anisotropy with a signal to noise ratio comparable to common, non-spatially resolved Reflectance Anisotropy Spectroscopy (RAS) methods. Spatial resolution in the micrometer range was achieved in a spectral range from UV to near IR. RAM measurements on wide-bandgap oxide- and nitride-semiconductors surfaces as well as on periodic microstructures will be discussed.

DS 45: Transport: Spintronics, Spincalorics and Magnetotransport (jointly with HL, MA)

Time: Friday 9:30–11:30 Location: HSZ 03

DS 45.1 Fri 9:30 HSZ 03

Search for magneto-hydrodynamics in the delafossite metals $PdCoO_2$ and $PtCoO_2$ — •Nabhanila Nandi[1], Pallavi Kushwaha[1], Seunghyun Khim[1], Philip J.W. Moll[1], Burkhard Schmidt[1], Thomas Scaffidi[2], Markus König[1], and Andrew P. Mackenzie[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Department of Physics, University of California, Berkeley, California 94720, USA — [3]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom

Electrical resistance is conventionally determined by the momentum-relaxing scattering of electrons by the host solid and its excitations. Hydrodynamic fluid flow through channels, in contrast, is determined by geometrical factors, boundary scattering and the viscosity of the fluid, which is governed by momentum-conserving internal collisions. In almost all known materials, however, the signatures of viscosity in electron flow cannot be resolved, because the rate of momentum-relaxing collisions dominates that of the momentum-conserving ones that give the viscous term. In previously published work, we reported experimental evidence that there is a regime in restricted channels of the ultra-pure two-dimensional delafossite metal $PdCoO_2$ in which the resistance has a large viscous contribution. In this talk I will report on our current work in which we extend our experiments to magneto-hydrodynamics, discussing data both from $PdCoO_2$ and a second delafossite metal, $PtCoO_2$.

DS 45.2 Fri 9:45 HSZ 03

Fe_3O_4 thin films: controlling and manipulating an elusive quantum material — •xionghua liu, chun-fu chang, aurora diana rata, alexander christoph komarek, and liu hao tjeng — Max Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, 01187 Dresden, Germany

Fe_3O_4 (magnetite) is one of the most elusive quantum materials and at the same time one of the most studied transition metal oxide materials for thin film applications. The theoretically expected half-metallic behavior generates high expectations that it can be used in spintronic devices. Yet, despite the tremendous amount of work devoted to preparing thin films, the enigmatic first order metal-insulator transition and the hall mark of magnetite known as the Verwey transition, is in thin films extremely broad and occurs at substantially lower temperatures as compared to that in high quality bulk single crystals.

In this work, we investigate systematically the effect of oxygen stoichiometry, thickness, strain, and microstructure on the Verwey transition in epitaxial Fe_3O_4 thin films on a variety of substrates. We have been able to determine the factors that affect negatively the Verwey transition in thin films. We have succeeded in finding and making a particular class of substrates that allows the growth of magnetite thin films with the Verwey transition as sharp as in the bulk. Moreover, we are now able to tune the transition temperature and, using tensile strain, increase it to substantially higher values than in the bulk.

DS 45.3 Fri 10:00 HSZ 03

Spin-switching via quantum dot spin valves — •Niklas M. Gergs[1], Scott A. Bender[1], Rembert A. Duine[1,2], and Dirk Schuricht[1] — [1]Institute for Theoretical Physics, Utrecht University, Utrecht, The Netherlands — [2]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

We theoretically investigate a spin-valve transistor setup, ie, correlated transport through a quantum dot positioned between two spin-polarised nano magnets. This causes the dynamical generation of a magnetic field on the dot even in the absence of external fields [1].

Here we consider the back action of the quantum dot onto the attached nano magnets via exerted spin torques. This may be used to switch the nano magnets reliably from a parallel to an anti-parallel alignment and vice versa. All operations are done in the Coulomb-blockade regime of the quantum dot, so that the charge transport through the setup is strongly suppressed.

[1] M. Braun, J. König, J. Martinek, Phys. Rev. B 70, 195345 (2004)

DS 45.4 Fri 10:15 HSZ 03

Strong non-equilibrium effects in spin torque systems — •Tim Ludwig[1], Igor S. Burmistrov[2,3], Yuval Gefen[4], and Alexander Shnirman[1] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]L.D. Landau Institute for Theoretical Physics RAS, Kosygina street 2, 119334 Moscow, Russia — [3]Laboratory for Condensed Matter Physics, National Research University Higher School of Economics, 101000 Moscow, Russia — [4]Department of Condensed Matter Physics, Weizmann Institute of Science, 76100 Rehovot, Israel

We consider a problem of persistent magnetization precession in a single domain ferromagnetic nano particle under the driving by the spin-transfer torque [1]. We find that the adjustment of the electronic distribution function in the particle renders this state unstable. Instead, abrupt switching of the spin orientation is predicted upon increase of the spin-transfer torque current. On the technical level, we derive an effective action of the type of Ambegaokar-Eckern-Schön action for the coupled dynamics of magnetization (gauge group SU(2)) and voltage (gauge group U(1)).

[1] T. Ludwig, I. S. Burmistrov, Y. Gefen, and A. Shnirman, arXiv:1610.09944 (2016)

DS 45.5 Fri 10:30 HSZ 03

Spin-charge coupled dynamics driven by a time-dependent magnetization — •Sebastian Tölle[1], Ulrich Eckern[1], and Cosimo Gorini[2] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Faculty of Physics, University of Regensburg, 93040 Regensburg, Germany

The spin-charge coupled dynamics in a thin, magnetized metallic system are investigated. The effective driving force acting on the charge carriers is generated by a dynamical magnetic texture, which can be induced, e.g., by a magnetic material in contact with a normal-metal system. We consider a general inversion-asymmetric substrate/normal-metal/magnet structure, which, by specifying the precise nature of each layer, can mimick various experimentally employed setups. Inversion symmetry breaking gives rise to an effective Rashba spin-orbit interaction. We derive general spin-charge kinetic equations which show that such spin-orbit interaction, together with anisotropic Elliott-Yafet spin relaxation, yields significant corrections to the magnetization-induced dynamics. To highlight their physical meaning, the spin pumping configuration of typical experimental setups is analyzed in detail. In the two-dimensional limit the build-up of a DC voltage is dominated by the spin galvanic (inverse Edelstein) effect. A measuring scheme that could isolate this contribution is discussed.

DS 45.6 Fri 10:45 HSZ 03

Emergent magnetic ordering in transition metal atomic contacts — •Martin Keller, Florian Strigl, Elke Scheer und Torsten Pietsch — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

MD simulations and DFT calculations predict the development of local magnetic order at reduced dimensions in some paramagnetic transition metals (Pt, Pd, Ir), especially in atomic configurations [1,2,3]. This unusual property allows us to investigate the influence of the local magnetic properties on the conductance of atomic contacts without the effect of magnetic leads. Therefore atomic contacts of these metals are a model system to understand the origin of magnetoconductance and the role of spin-polarization of the conduction electrons. Herein we discuss recent results of Pt, Pd and Ir in the context of a microscopic model that successfully describes the observed magnetoconductance signature in these atomic contacts and chains [4]. Additionally, electronic transport spectroscopy is used to evaluate magnetic excitations in the electronic system of the contact, i.e. the presence of i) a zero-bias anomaly which is described by Kondo physics and ii) conductance fluctuations in the atomic contact, which indicate the formation of a magnetically ordered state. We will compare the three transition metals with respect to their different electronic structure and the role of spin-orbit coupling in the contacts.

[1] Phys. Rev. Lett. 92, 057201 (2004)
[2] Phys. Rev. B 78, 014423 (2008)
[3] Phys. Rev. B 81, 054433 (2010)
[4] Nature Comm. 6, 6172 (2015); Phys. Rev. B 94, 144431 (2016)

DS 45.7 Fri 11:00 HSZ 03

Electron transport through the helical systems: chiral magnetoresistance effect — •Volodymyr V. Maslyuk, Rafael Gutiérrez, and Gianaurelio Cuniberti — Institute for Material Science and Max Bergmann Center for Biomaterials, Dresden University of Technology, Hallwachstr. 3, 01069 Dresden, Germany

Recently, the chirality-induced spin selectivity (CISS) effect [1] has been discovered in which electron transport through systems with helical symmetry shows the different transmission for the electrons with different spin-polarizations. In this work, we show that CISS can be utilized in the new class of magnetic field sensors via novel chiral magnetoresistance effect (CMR) [2]. We present a theoretical investigation of the electron transport through the poly-GLY in helical form placed between one magnetic and one nonmagnetic leads by using the DFT and NEGF approach. We obtain that MR of the order 2

[1] Göhler B., Hamelbeck V., Markus T. Z., Kettner M., Hanne G. F., Vager Z., Naaman R., and Zacharias H., Science 331, 894 (2011)
[2] Kiran V., Mathew S.P., Cohen S.R., Delgado I.H., Lacour J., Naaman R., Adv. Mater. 28, 1957 (2016)

DS 45.8 Fri 11:15 HSZ 03

A Landauer-Büttiker approach for hyperfine mediated electronic transport in the integer quantum Hall regime — •Aniket Singha[1], M. Hamzah Fauzi[2], Yoshiro Hirayama[2], and Bhaskaran Muralidharan[1] — [1]Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India — [2]Graduate School of Science, Tohoku University, Aoba-ku, Sendai-980-8578, Japan

The interplay of spin-polarized electronic edge states with the dynamics of host nuclei in quantum Hall systems presents rich and non-trivial transport physics. Here, we develop a Landauer-Büttiker approach to understand various experimental features observed in integer quantum Hall set ups featuring quantum point contacts. Such approach entails a phenomenological description of spin resolved inter-edge scattering induced via hyperfine assisted electron-nuclear spin flip-flop processes along with a self consistent simulation framework between the nuclear spin dynamics and edge state electronic transport in order to gain insights into the nuclear polarization effects on electronic transport vice-versa. In particular, we show that the hysteresis noted experimentally in the conductance-voltage trace as well as in the resistively detected NMR lineshape results from a lack of quasi-equilibrium between electronic transport and nuclear polarization evolution. In addition, we present circuit models to further facilitate a clear understanding of the electronic transport processes occurring near the quantum point contact.

DS 46: Ion and Electron Beam Induced Processes

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

DS 46.1 Fri 9:30 CHE 89

Tuning of magnetic and structural properties of $Fe_{60}Al_{40}$ thin films by ion irradiation — •Jonathan Ehrler[1,2], Rantej Bali[1], Roman Böttger[1], Jörg Grenzer[1], and Kay Potzger[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]Dresden University of Technology, Helmholtzstrasse 10, 01069 Dresden, Germany

The effects of ion implantation on the structural and magnetic properties of $Fe_{60}Al_{40}$ films, possessing A2 and B2 structure respectively, have been investigated by means of X-ray diffraction and Vibrating sample magnetometry. The studies show that the magnetic properties of the 250 nm thick $Fe_{60}Al_{40}$ films depend on the structural order only. The chemical disorder induced evolution of ferromagnetism comes along with an abrupt disappearance of the (100)-superlattice peak.

The irradiation of paramagnetic B2 $Fe_{60}Al_{40}$ with H^+, He^+ or Ne^+ ions with different fluences at low temperatures led to an increase of saturation magnetization (M_S) going along with a lattice expansion induced by structural disorder. This effect did not appear for proton irradiation at elevated temperatures (250 °C) where the ordered B2 phase was retained. Upon low temperature hydrogen implantation of disordered A2 $Fe_{60}Al_{40}$ films, on the other hand, unlike for helium or neon irradiation, the lattice parameter and M_S decreased indicating a little ordering. This might offer the possibility of H^+ irradiation induced ordering of chemically disordered alloy thin films well below the ordering temperature.

DS 46.2 Fri 9:45 CHE 89

Material processing via ion beam treatment — •Martin Becker, Angelika Polity, and Peter J. Klar — Institute of Experimental Physics I, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

In order to deposit polycrystalline thin films on different substrates, sputtering methods are the most established techniques. This broad acceptance is due to the homogeneity and reproducibility of the grown layers with high deposition rates. Conventional RF and DC sputtering, however, are subject to limitations based on substrate heating and volatile impurities to be incorporated into the growing films, both issues being significantly reduced in ion beam sputter deposition (IBSD). Films with high crystalline quality can be produced with an independent control of ion energy, beam direction and current density.

We report on the development of a system for the ion beam processing of semiconductors. In order to deposit thin layers of desired material by IBSD as well as to modify their properties by prior or simultaneous ion beam treatments, different sputter geometries come into play, whose discussion will be part of this presentation. An optimization of the crystalline and optical properties is carried out for oxide-based materials. In addition to binary materials, the advantages of forming ternary materials via dual source operation are discussed. On this basis, composition gradients were produced. Within this framework, self-designed ion sources are characterized according to the requirements of different material science processes.

DS 46.3 Fri 10:00 CHE 89

Ultrafast electronic response of graphene to a strong and localized electric field — •Richard A. Wilhelm[1], Elisabeth Gruber[2], Rémi Pétuya[3], Roland Kozubek[4], Bernhard C. Bayer[5], Anke Hierzenberger[4], Valerie Smejkal[2], Florian Libisch[2], Iñigo Adalzabal[7], Andrey K. Kazansky[3,8], Arkady Krasheninnikov[1], Marika Schleberger[4], Stefan Facsko[1], Andrei G. Borisov[6], Andres Arnau[3,7], and Friedrich Aumayr[2] — [1]HZDR — [2]TU Wien — [3]DIPC, San Sebastian — [4]Uni Duisburg-Essen — [5]Uni Wien — [6]CNRS, Paris — [7]CFM, San Sebastian — [8]IKERBASQUE, Bilbao

Ion transmission through thin solid films revealed many interesting properties of ion-solid interaction mechanisms, among them is ion equilibrium charge state and the ion stopping force. Using a well defined target such as free-standing graphene, ion transmission can also provide insights into processes occuring in the target material. Here we use slow highly charged ions and inverstigate their charge exchange and energy loss due to transmission through graphene. In a joint theoretical and experimental effort we find that large current densities of at least 10^{12} A/cm^{-2} are sustained by graphene without rupture, even though this current is only active for a few femtoseconds on a nm^2 sized area, it's value is about 3 orders of magnitude higher than established DC breakdown current densities. Our study shows that especially highly charged ions are well suited to investigate material properties under extreme conditions on a femtosecond time scale.

DS 46.4 Fri 10:15 CHE 89

Epitaxial nitride thin films by ion mass and ion energy selective ion-beam assisted deposition — •Philipp Schumacher[1], Michael Mensing[1], Jürgen W. Gerlach[1], Stephan Rauschenbach[2], and Bernd Rauschenbach[1,3] — [1]Leibniz-Institut für Oberflächenmodifizierung, 04318 Leipzig — [2]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart — [3]Fakultät für Physik und Geowissenschaften, 04103 Leipzig

Ion-beam assisted deposition (IBAD) is a versatile tool for the synthesis of thin films, as it offers several degrees of freedom to modify the properties of the fabricated material. Ion sources for IBAD typically provide a blend of ion species with broad distributions of ion kinetic energy in the ion beam. For a fundamental understanding of ion-assisted growth processes, however, it is required to evaluate the influence of ion mass and ion kinetic energy, separately. In this contribution, first a novel setup for hyperthermal IBAD of GaN including a dedicated quadrupole mass filter is presented. The deposition of the model material GaN using only one ion species (N^+ or N_2^+) while independently defining the ion kinetic energy is accomplished. Second, results on GaN thin films synthesized by ion mass and ion energy selective IBAD on both 6H-SiC(0001) and Al_2O_3(1-102) substrates are presented. Atomic force microscopy is applied to analyze the surface topography. The thin films are shown to be epitaxial as determined by reflection high-energy electron diffraction and x-ray diffraction. The properties of the deposited thin films are compared with respect to the utilized separated parameters.

DS 46.5 Fri 10:30 CHE 89

Ion Induced Surface Pattern Formation by ion implantation — •Hans Hofsäss, Kun Zhang, and Omar Bobes — Fakultät für Physik, Universität Göttingen, Göttingen, Germany

Recently Bradley and Hofsäss introduced ion implantation as an additional effect contributing to pattern formation. The theory is briefly introduced and the calculation of implantation curvature coefficients, based on the linear continuum models for pattern formation and the crater function formalism are described. The calculations use Monte Carlo simulations, taking into account contributions due to erosion, implantation, recoil redistribution and the dynamic layer thickness effect. We are now able to quantitatively predict pattern formation or surface stability for a variety of ion-target systems and a broad range of irradiation conditions. Pattern formation on a-C surfaces by C^+ and Ne^+ ion irradiation as well as N^+ ion irradiation of Si and Si_3N_4 demonstrate that ion implantation can be crucial for pattern formation.

DS 46.6 Fri 10:45 CHE 89

Chemical Diffusion of Potassium Ions in thin film PrMnO3 — •Karl-Michael Weitzel[1], Johannes Martin[1], Melanie Gräf[1], Thilo Kramer[2], and Christian Jooss[2] — [1]Philipps-Universität Marburg — [2]Universität Göttingen

The transport of potassium through praseodymium-manganese oxide (PrMnO3) has been investigated by means of the bombardment induced ion transport (BIIT) technique. To this end potassium ions are attached to the front side of a 250 nm thick sample of PrMnO3. Most of the potassium ions become neutralized at the surface of the PrMnO3. Part of the potassium ions diffuse through the PrMnO3. Ex situ analysis of the sample by time-of-flight secondary ion mass spectrometry (ToF-SIMS) reveals pronounced concentration profiles of the potassium indicative of chemical diffusion. Two distinctly different diffusion coefficients have been derived, i. one assigned to bulk diffusion and ii. another one assigned to diffusion along grain boundaries. The latter conclusion is supported by transmission electron microscopy of thin lamella cut out from the sample which reveals twin grain boundaries reaching through the entire sample.

DS 47: Organic-Inorganic Hybride Interfaces

Time: Friday 9:30–11:45 Location: CHE 91

DS 47.1 Fri 9:30 CHE 91

Hybrid organic-inorganic nano-structures studied by HR-PES and HR-TEM — •Olga Molodtsova[1,2], Sergey Babenkov[1], Irina Aristova[3], Andrei Hloskovsky[1], Denis Vyalikh[4], Dmitry Smirnov[5], Karina Schulte[6], and Victor Aristov[1,3,7] — [1]DESY, Hamburg, Germany — [2]ITMO, Saint Petersburg,Russia — [3]ISSP RAS, Chernogolovka, Russia — [4]TU Dresden, Germany — [5]BESSY, Berlin, Germany — [6]Max-lab, Lund, Sweden — [7]TU Bergakademie, Freiberg, Germany

Morphology and the electronic properties of hybrid organic-inorganic systems, composed of metallic nanoparticles which are self-organized in organic semiconductor thin film of phthalocyanines complexes were studied by transmission electron microscopy and photoelectron spectroscopy using synchrotron radiation.

DS 47.2 Fri 9:45 CHE 91

STM and PES Investigations of Organic-TMD Heterointerfaces: Self-Assembly and Energy Level Alignment — •Thorsten Schultz[1], Yuli Huang[2,3], Zhibo Song[2,3], Zijing Ding[2], Lain-Jong Li[4], Dongzhi Chi[2], Patrick Amsalem[1], Andrew Wee[3], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Germany — [2]Agency for Science, Technology and Research, Singapore — [3]National University of Singapore — [4]King Abdullah University of Science and Technology, Saudi Arabia

The growing interest in two-dimensional transition metal dichalcogenide (TMD) materials brings additional opportunities for interfacing with organic molecules to fabricate flexible organic/inorganic devices. However, the complex interfacial properties at the organic-TMD heterointerfaces, including the growth behavior and energy level alignment (ELA) that determine the device performance, are still not well understood. Combining scanning tunneling microscopy/spectroscopy (STM/STS) with photoemission spectroscopy (PES), we are able to probe the self-assembly of fluorinated fullerene C60F48 on single-layer WSe2 deposited on a graphite substrate and its interfacial electronic properties. From our studies it is found that the interfacial dipole together with charge transfer play critical roles in determining the phase evolution of the C60F48 molecules adsorbed on the surface, as well as the ELA at the C60F48/WSe2/graphite heterointerface.

DS 47.3 Fri 10:00 CHE 91

Energy Level Control at ZnO/Organic Semiconductor Interfaces — •Raphael Schlesinger[1], Sylke Blumstengel[1], Stefanie Winkler[2], Johannes Frisch[1], Jens Niederhausen[1], Ruslan Ovsyannikov[2], Antje Vollmer[2], Fritz Henneberger[1], and Norbert Koch[1,2] — [1]Humboldt-Universität zu Berlin, Institut für Physik — [2]Helmholtz-Zentrum Berlin - BESSY II

Hybrid inorganic organic systems (HIOS) are promising candidates for future (opto-)electronic devices by taking advantage of the complementary beneficial properties of two different material classes. However, inadequate interfacial energy level alignment is an intrinsic obstacle to superior device function. Hence, to design efficient HIOS devices, understanding and controlling HIOS energy level alignment is a key factor.

In this contribution we employ molecular electron donor or acceptor interlayers to tune the work function (ϕ) of ZnO between 2.2 eV (by using the organometallic donor [RuCp*mes]$_2$) and 6.4 eV (by using F4TCNQ). Only for molecular acceptor adsorption, significant adsorption induced upward band bending of up to 0.9 eV is found within ZnO. Exploiting the huge ϕ modifications of ZnO, up- and downward HIOS energy level readjustments are shown, which realize ultimately low electron- or hole-injection barriers. Moreover, by using an OSC whose gap matches that of ZnO, the energy level offsets at the HIOS interface could be eliminated. This enables highly efficient, non-quenched energy transfer across the HIOS interface, which is usually inhibited by unfavorable energy level alignment.

DS 47.4 Fri 10:15 CHE 91

Structure of van der Waals bound Hybrids of Organic Semiconductors and Transition Metal Dichalcogenides: the Case of Acene Films on MoS2 — •Tobias Breuer, Tobias Massmeyer, Alexander Mänz, Steffen Zoerb, Bernd Harbrecht, and Gregor Witte — Philipps-Universität Marburg, Germany

Transition metal dichalcogenides (TMDC) are important representatives in the emerging field of two-dimensional materials. At present, their combination with molecular films is discussed as it enables the realization of van der Waals bound organic/inorganic hybrids which are of interest in future device architectures. Here, we discuss the potential use of molybdenum disulfide (MoS$_2$) as supporting substrate for the growth of well-defined, crystalline organic adlayers. By this means, hybrid systems between the TMDC surface and organic compounds can be prepared, allowing for the profound investigation of mutual optical and electronic coupling mechanisms. As model system, we choose pentacene and perfluoropentacene as prototypical organic semiconductors and analyze their film formation on MoS$_2$(001) surfaces. In both cases, we observe smooth, crystalline film growth in lying molecular configuration, hence enabling the preparation of welldefined hybrid systems. By contrast, on defective MoS$_2$ surfaces both materials adopt an upright molecular orientation and exhibit distinctly different film morphologies. This emphasizes the importance of highly ordered TMDC surfaces with low defect density for the fabrication of well-defined hybrid systems.

[1] T. Breuer et al., PSS RRL (2016), DOI: 10.1002/pssr.201600320

15 min. break.

DS 47.5 Fri 10:45 CHE 91

Real-Time Investigation during Au sputter deposition on polymer and SiOx surfaces. — •Matthias Schwartzkopf[1], André Rothkirch[1], Björn Beyersdorff[1], Calvin Brett[1], Marc Gensch[1], Wiebke Ohm[1], Oleksandr Polonskyi[2], Alexander Hinz[2], Thomas Strunskus[2], Adrian Haussmann[3], Franziska Löhrer[3], Volker Körstgens[3], Franz Faupel[2], Peter Müller-Buschbaum[3], and Stephan Roth[1,4] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]CAU zu Kiel, Kaiserstr.2, D-24143 Kiel — [3]TUM, James-Franck-Str. 1, D-85748 Garching — [4]KTH, Teknikringen 56-58,SE-100 44 Stockholm

The reproducible low-cost fabrication of functional polymer-metal-nanocomposites remains a major issue in applied nanotechnology. In order to obtain full control over the nanostructural evolution at the metal-polymer interface, we employed the combination of time-resolved surface sensitive X-ray scattering with optical measurements during sputter deposition of gold on thin polystyrene films [1] and SiOx [2]. We correlate the evolution of the metallic layer morphology with changes in the key scattering features. This enabled us to identify the impact of substrate effects on the growth regimes with their specific thresholds and their resulting optical properties. Our study opens up the opportunity to improve nanofabrication of tailored metal-polymer nanostructures for organic electronics like photovoltaic applications and plasmonic-based technologies. [1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015); [2] Schwartzkopf et al., Nanoscale 5, 5053 (2013).

DS 47.6 Fri 11:00 CHE 91

Analytical Study of Solution-Processed Nickel Oxide and its Application in Organic Electronics - (1) Photoelectron Spectroscopy — •Florian Ullrich[1,4], Valentina Rohnacher[2,4], Jakob Bombsch[3,4], Wolfram Jaegermann[1,4], and Eric Mankel[1,4] — [1]TU Darmstadt, Materials Science Institute — [2]University of Heidelberg — [3]TU Braunschweig — [4]InnovationLab

For the fabrication of efficient organic solar cells (OPV) suitable extraction layers are needed. A material fulfilling the requirements and leading to superior efficiencies in comparison to the standard material PEDOT:PSS is nickel oxide (NiO).

In this work we want to contribute to a more detailed understanding of the relations between annealing temperature of solution-processed NiO (sNiO), surface treatments, bulk and surface composition, structure and properties, ability to form self-assembled monolayers (SAMs) and the characteristics of sNiO-based OPV. For that purpose different analytical methods like x-ray photoelectron spectroscopy (XPS) and infrared spectroscopy (IR) were conducted and various OPVs were built and characterized.

In this first part we use XPS to monitor changes of band bending and surface dipoles induced by surface treatments like oxygen plasma (OP) or deposition of SAMs. These information help to explain characteristics of corresponding OPVs and provide valuable hints for the design of more efficient devices. We show how band alignment can controllably be improved by adjusting the work function via varying annealing temperature of sNiO films, OP treatment and SAM molecules.

DS 47.7 Fri 11:15 CHE 91

Analytical study of Solution-processed Nickel Oxide and its Application in Organic Electronics: (2) Infrared Spectroscopy — •Valentina Rohnacher^{1,2}, Sabina Hillebrandt^{1,2}, Florian Ullrich^{2,3}, Jakob Bombsch^{2,4}, Sebastian Beck^{1,2}, and Annemarie Pucci^{1,2} — ^{1}Kirchhoff-Institut für Physik, Universität Heidelberg — ^{2}InnovationLab, Heidelberg — ^{3}TU Darmstadt — ^{4}TU Braunschweig

The performance of organic photovoltaic cells (OPVs) is significantly influenced by the properties of the interfaces between the layers. Increasing the interfacial compatibility especially between the transparent conductive oxide electrode and the organic semiconductor layer can improve the charge carrier transport through the stack and thus the efficiency of the device. Thin films of nickel oxide (NiO) have shown promising characteristics as hole extraction layers in OPVs. In our studies, solution-processed NiO surfaces were passivated by self-assembled monolayers (SAMs) to tune the work function and to reduce the surface reactivity. Infrared spectroscopy gives insight into the composition of the investigated material and can monitor orientation of characteristic vibrations or functional groups. The results show that temperature and plasma treatment dramatically change the surface properties and that especially nickel hydroxide and nickel oxyhydroxide play an important role for the binding mechanism of SAMs. Together with photoelectron spectroscopy and OPV device characteristics a better understanding of the energetic and chemical properties at the interface was achieved helping to improve device performance.

DS 47.8 Fri 11:30 CHE 91

Analytical Study of Solution-Processed Nickel Oxide and its Application in Organic Electronics: (3) Application in Organic Solar Cells — •Jakob Bombsch^{1,2,4}, Sebastian Hietzschold^{1,2,4}, Valentina Rohnacher^{2,4}, Florian Ullrich^{3,4}, Robert Lovrincic^{1,4}, and Wolfgang Kowalsky^{1,2,4} — ^{1}TU Braunschweig — ^{2}Uni Heidelberg — ^{3}TU Darmstadt — ^{4}InnovationLab, Heidelberg

Nickel oxide (NiO) has shown promising properties as a carrier-selective hole contact material with high transparency, and a good matching ionization potential to most donor materials [1,2]. Here we apply solution-processed NiO films as an interlayer in small molecule flat- and bulk-heterojunction solar cells with F4ZnPc and C60 as a donor and acceptor, respectively, and correlate the observed IV-characteristics with annealing temperature, thickness, and surface post-treatment of the NiO layer. While oxygen plasma treatment improves device performance, the application of dipolar self-assembled monolayers lead to strongly S-shaped IV curves. To examine the nature of the barrier introduced, we vary the doping density of the NiO film by adding copper oxide. Together with data from Infrared spectroscopy and Photoelectron spectroscopy measurements, we gain a more fundamental understanding of the impact of NiO surface properties on solar cell performance. [1] Manders, J. R. Et al. Adv. Funct. Mater., 23: 2993-3001 (2013). [2] Schulz, P. et al. Adv. Funct. Mater. 24, 701-706 (2014).

DS 48: Oxide Semiconductors (jointly with HL)

Time: Friday 9:30–12:45 Location: POT 51

Invited Talk DS 48.1 Fri 9:30 POT 51

New Frontiers in Quantum Matter Heterostructures — •Jochen Mannhart — Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Combining the power and possibilities of heterostructure engineering with the collective and emergent properties of quantum materials, quantum-matter heterostructures [1] open a new arena of solid-state physics. Here we provide a review of interfaces and heterostructures made of quantum matter. As we will show, unique electronic states can be engineered in these structures, giving rise to unforeseeable opportunities for scientific discovery and potential applications.

[1] Quantum-Matter Heterostructures, H. Boschker and J. Mannhart, Annual Reviews of Condensed Matter Physics, 8, April 2017.

DS 48.2 Fri 10:00 POT 51

Self-consistent hybrid functional calculations: Electronic and optical properties of oxide semiconductors — •Daniel Fritsch^{1}, Benjamin Morgan^{1}, and Aron Walsh^{1,2} — ^{1}Department of Chemistry, University of Bath, BA2 7AY Bath, UK — ^{2}Department of Materials, Imperial College London, SW7 2AZ London, UK

Owing to limitations of existing approximate exchange-correlation functionals, band gaps of semiconductors and insulators are often severely underestimated in density functional theory calculations. Considerable improvements are possible by including a fraction of Hartree-Fock exchange, constructing a so-called “hybrid” functional. The precise proportion of Hartree-Fock exchange is typically treated as an empirical parameter chosen from intuition and experimental calibration.

A recent self-consistent hybrid functional [1] removes this empiricism and offers a new approach for parameter-free hybrid functional investigations. Moreover, it provides a better starting point for many-body perturbation calculations based on the *GW* approximation. Applying this approach to a range of oxide semiconductors, we report on the electronic and optical properties, and compare them to other theoretical and experimental data.

[1] J. H. Skone *et al.*, Phys. Rev. B **89**, 195112 (2014).

DS 48.3 Fri 10:15 POT 51

Influence of temperature on the creation of Rydberg excitons — •Peter Grünwald^{1}, Julian Heckötter^{2}, Marc Assmann^{2}, Dietmar Fröhlich^{2}, Manfred Bayer^{2}, Heinrich Stolz^{1}, and Stefan Scheel^{1} — ^{1}Institut für Physik, Universität Rostock, Rostock, Germany — ^{2}Experimentelle Physik 2, TU Dortmund, Dortmund, Germany

Solid-state systems are heavily influenced by temperature, changing the crystal structure and thus shifting the energy bands [1,2]. Excitons in semiconductors additionally experience collision ionization, and a decrease of the band edge due to plasma interaction [3]. However, in most semiconductor systems, measuring these effects is difficult because of the limited number of exciton states available. This is different for Rydberg excitons [4], where states up to $n \gtrsim 20$ can easily be generated. Hence, these states can be used to analyze the temperature influence on the excited states and the excitation limit set by finite temperature.

[1] T. Itoh and S. Narita, J. Phys. Soc. Japan **39**, 140 (1975).
[2] P. B. Allen and M. Cardona, Phys. Rev. B **23**, 1495 (1980).
[3] D. Semkat *et al.*, Phys. Rev. B **80**, 155201 (2009).
[4] T. Kazimierczuk *et al.*, Nature **514**, 343 (2014).

DS 48.4 Fri 10:30 POT 51

Excitonic Giant-Dipole Potentials in Cuprous Oxide — •Markus Kurz and Stefan Scheel — AG Quantenoptik makroskopischer Systeme, Institut für Physik, Universität Rostock

Wannier excitons are of great physical interest since they represent the fundamental optical excitation in semiconductors. Recently, the discovery of highly excited Rydberg excitons in Cuprous Oxide (Cu_2O) and their exposure to external fields have shown a plethora of complex physical phenomena [1]. In atomic physics an exotic species of Rydberg atoms in crossed electric and magnetic fields, so-called giant-dipole atoms, have been predicted for two decades [2]. These exotic objects are characterized by an electron-ionic core separation in the range of several micrometers.

In this work, we expand this concept and predict the existence of excitonic giant-dipole states in Cu_2O. Performing a gauge-independent pseudoseparation of the center of mass motion we derive an effective single-particle description of the field-dressed excitonic system obtaining a spatial dependent electron-hole interaction potential. For specific field strengths and field orientations this potential exhibits an outer potential well providing bound excitonic states. Furthermore, we show that the giant-dipole interaction potential gives rise to Abelian and non-Abelian gauge fields acting on the relative motion of the two excitonic constituents.

[1]T. Kazimierczuk *et al.*, Nature (London) **514**, 343 (2014)

[2]O. Dippel, *et al.*, Phys. Rev. A **49**, 4415 (1994)

DS 48.5 Fri 10:45 POT 51

Excitons at $SrTiO_3$ and ZnO interfaces in ellipsometry spectra — •Stefan Zollner[1], C. Rodriguez[1], N. Samarasingha[1], J. Moya[1], N. Fernando[1], P. Ponath[2], K. Kormondy[2], A.A. Demkov[2], and S. Chattopadhyay[3] — [1]New Mexico State University, Las Cruces, NM, USA — [2]University of Texas, Austin, TX, USA — [3]Indian Institute of Technology, Indore, India

Excitonic features in optical spectra of semiconductors and insulators have been studied for many years. In an epitaxial layer on a substrate with a different band gap, the wave functions of electron and hole are strongly modified. In a type-I quantum well, consisting of a narrow-gap semiconductor grown on a large-gap substrate, both electron and hole are confined, which leads to an increase in the dipole overlap matrix element. Therefore, the dominant absorption peak at 4.2 eV is larger in a 20 nm thick $SrTiO_3$ layer on $LaAlO_3$ than in bulk $SrTiO_3$. (The band gap of $LaAlO_3$ is larger than that of $SrTiO_3$.) On the other hand, in a staggered type-II quantum well, either the electron is confined, or the hole, but not both. Therefore, the overlap dipole matrix element (and the excitonic absorption) is strongly reduced, because one quasiparticle resides in the quantum well and the other in the substrate. If a $SrTiO_3$ layer is grown on Si or Ge, the valence band maximum occurs in the substrate, while the conduction band offset is very small. Therefore, the exciton wave function is delocalized, which reduces the dipole overlap matrix element. The real and imaginary part of thin SrTiO3 layers on Si or Ge are much smaller than in the bulk and decrease monotonically with decreasing thickness.

Coffee Break

DS 48.6 Fri 11:30 POT 51

Tuning the refractive index of transparent conducting oxides via oxide/oxide periodic heterostructures — David Caffrey, Emma Norton, Cormac Ó Coileáin, Christopher M. Smith, Igor V. Shvets, and •Karsten Fleischer — School of Physics and CRANN, Trinity College Dublin, The University of Dublin, Ireland

Superlattice structures are a novel method of improving upon the optoelectronic properties of Transparent Conducting Oxide (TCO) structures. The invariability of the refractive index of TCO materials leads to reflection losses cells. The development of a transparent material or structure of tuneable refractive index at the interfaces of transparent devices such as solar would allow for the integration of anti-reflective coatings which would reduce such losses significantly, thus improving device efficiency. Previous attempts to modify the refractive index have been marred by the degradation of the electrical or optical properties of the tuned material. We demonstrate the novel use of a TCO/dielectric superlattice structure to achieve an effective medium of altered refractive index, while maintaining high values of transparency, conductivity and mobility. We demonstrate the efficacy of these superlattice structures on both amorphous $InGaZnO_4$ and ZnO:Al via TCO/SiO_2 and TCO/TiO_2 superlattices. The effective refractive indices of the films were successfully tuned over a range of $\Delta n \approx -0.2$ (SiO_2 inclusion) to $+0.4$ (TiO_2 inclusion) with a decrease in conductivity of less than an order of magnitude. Mobility of the films was also well conserved. We also discuss differences in the carrier injection from the TCO into the dielectric for the SiO_2 and TiO_2 case.

DS 48.7 Fri 11:45 POT 51

Hybrid functional calculations of oxygen mono- and di- vacancies in SrTiO3 — •Masud Alam, Liverios Lymperakis, and Jörg Neugebauer — Computational Material Design department, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck Str. 1, 40237 Düsseldorf, Germany

Perovskite-type oxides ABO3 have attracted considerable interest for their large variety of technologically appealing characteristics such as ferroelectricity, magnetism, as well their dielectric properties. Among these materials, SrTiO3 (STO) serves as a representative model for the class of large bandgap perovskites. Nevertheless, the properties of this material are dominated by the presence of oxygen vacancies which act as n-type dopants. In the present work we investigate the energetics, atomic geometry and electronic structures of oxygen mono- and di-vacancies by employing Heyd, Scuseria, Ernzerhof (HSE) hybrid density functional calculations. Based on these calculations we identify the energy levels and the formation energies of aforementioned point defects as well as the binding energies of the point defect complexes. Our calculations reveal that interactions between single and doubly ionized defects as expected are strongly repulsive. Based on the aforementioned results we will further discuss in details the effect of oxygen vacancies as a function of growth conditions and doping level on the electronic properties of STO.

DS 48.8 Fri 12:00 POT 51

Low temperature absorption study of ferromagnetic EuO thin films — •Marcel Ney[1], Günther Prinz[1], Timm Gerber[2], Martina Müller[1,2], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, Universität Duisburg-Essen, D-47048 Duisburg — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, D-52428 Jülich

Europium Oxide is a ferromagnetic semiconductor with the Curie temperature of 69K. When it is used as a tunnel barrier, it can create up to 100% spin polarized electron currents, for use in spintronic research. This remarkable property raises the question, how the magnetic order at low temperatures affects the band structure of a thin EuO layer.

Thin EuO-layers were grown by molecular beam epitaxy on yttria-stabilized-zirconia-substrates, with different thicknesses. A fourier-transform-infrared spectrometer equipped with a liquid helium continuous-flow cryostat was used to measure the transmission through the EuO thin films.

Spectra measured for decreasing EuO thickness (30nm-3nm) show a shift of the absorption edge of EuO to higher energies due to an increasing quantum confinement along the growth direction. For low temperature measurements below the Curie temperature of EuO, we observed a red shift of the bandgap energy of about $E_a = (0.27 \pm 0.02)$eV. This energy shift is in good agreement with theoretical values and experimentally determined exchange splitting energies for thin europium-oxide layers, already published in the literature.

DS 48.9 Fri 12:15 POT 51

Ozone, oxygen and water interaction with $In_2O_3(111)$ surfaces — •Theresa Berthold[1], Stefan Krischok[1], Marcel Himmerlich[1], Vladimir Polyakov[2], Volker Cimalla[2], Julius Rombach[3], and Oliver Bierwagen[3] — [1]Institut für Mikro- und Nanotechnologien MacroNano, Technische Universität Ilmenau — [2]Fraunhofer-Institut für Angewandte Festkörperphysik, Freiburg — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin

In_2O_3 films are widely used in conductometric gas sensors based on their surface electron accumulation layer (SEAL) whose conductance is influenced by gas adsorption [1]. In this study the chemical composition and electronic surface properties of undoped and Mg-doped $In_2O_3(111)$ films grown by plasma-assisted molecular beam epitaxy are analyzed by photoelectron spectroscopy. We analyze the formation or desorption (by UHV annealing or UV illumination) of adsorbates, the generation of defects as well as the variation in surface band bending, electron concentration, and surface dipole. Towards understanding the gas sensitivity under realistic conditions we study the effect of humidity on the sensor properties by experiments combining water interaction with ozone or oxygen surface oxidation. H_2O partially reverses the depletion/reduction of the SEAL after surface oxidation. Complete depletion of the SEAL is found after plasma oxidation [2]. The experimental results are combined with Schrödinger-Poisson calculations to establish a quantitative analysis of the electron density profile and the density of surface states. [1] J. Rombach et al., Sens. Actuators B, 236, 909 (2016) [2] T. Berthold et al., J. Appl. Phys. (submitted)

DS 48.10 Fri 12:30 POT 51

Gas sensing with sub-micrometer Pt/TiO_2 sensors — •Svenja Herbertz, Mihai Cerchez, and Thomas Heinzel — Solid State Physics Laboratory, Heinrich-Heine-Universität Düsseldorf

Pt/nanoporous TiO_2 hydrogen sensors with active sizes in the millimeter regime are technically well established although the underlying physics is still at debate, due to incomplete understanding of the interplay between oxygen vacancies, titanium interstitials, and hydrogen incorporation in this disordered system. The quest for miniaturization as well as for improved spatial resolution drives the search for sensors operational at the microscale. Here we present a sub-micrometer-sized lateral sensor for atmospheric hydrogen with planar geometry and full compatibility with Si processing technology. A titanium dioxide line of 200 nm width, written with the tip of an atomic force microscope, separates a thin Ti film on an insulating substrate into two metallically disconnected electrodes and forms the active area. It is sensitized by a sub-monolayer platinum sputtering step such that the two Ti electrodes remain disconnected. The device shows a large, selective sensitivity to hydrogen gas.

DS 49: Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond (SYES)

Time: Friday 10:30–13:00 Location: HSZ 02

Invited Talk DS 49.1 Fri 10:30 HSZ 02
Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations — •Weitao Yang — Duke University

Fractional fractional charges and fractional spins provide a clear analysis of the errors of commonly used functionals. We developed a scaling correction scheme by imposing the Perdew-Parr-Levy- Balduz linearity condition. Our novel scheme leads to the significantly improved description of dissociating molecules, transition-state species, and charge-transfer systems. Within many-electron theory, we have formulated the ground-state exchange-correlation energy in terms of pairing matrix linear fluctuations, opening new a channel for density functional approximations. This method has many highly desirable properties. It has minimal delocalization error with a nearly linear energy behavior for systems with fractional charges, describes van der Waals interactions similarly and thermodynamic properties significantly better than the conventional RPA, and captures the energy derivative discontinuity in strongly correlated systems. We also adopted pp-RPA to approximate the pairing matrix fluctuation and then determine excitation energies by the differences of two-electron addition/removal energies. This approach captures all types of interesting excitations: single and double excitations are described accurately, Rydberg excitations are in good agreement with experimental data and CT excitations display correct 1/R dependence.

Invited Talk DS 49.2 Fri 11:00 HSZ 02
Multi-reference density functional theory — •Andreas Savin — Laboratoire de Chimie Théorique, CNRS and UPMC, Univ. Paris VI, Sorbonne University, Paris, France

It is sometimes said that there is no multi-reference density functional theory. The talk presents a personal viewpoint, and will focus on the following points. 1) There are many ways to introduce multi-determinant wave functions into density functional theory. 2) Several variants have been successfully explored. 3) Difficulties inherent to approximations (both for wave functions and density functionals) persist, but can be attenuated.

Invited Talk DS 49.3 Fri 11:30 HSZ 02
Density functionals from machine learning — •Kieron Burke — UC Irvine

Machine learning is spreading to all aspects of our lives. A particular method, kernel ridge regression, has proven very useful for fitting and interpolating in high-dimensional spaces.

Several years ago, in collaboration with the group of Klaus-Robert Muller in computer science at TU Berlin, we demonstrated how to construct a machine-learned density functional on a simple toy problem, non-interacting fermions in a box. We showed both its successes and limitations. We have continued to develop this method (PRL, 2012).

I will report on two recent works. In the first (arXiv:1609.02815), we construct the non-interacting kinetic energy functional for small molecules in 3D using a basis. We avoid the challenge of finding functional derivatives by learning the potential to density map directly, thereby bypassing the need to solve the Kohn-Sham equations.

In the second, we learn the interacting functional directly for the first time. In 1D, we model chains of H atoms of different length, and learn F[n] itself, from highly accurate DMRG calculations. With a novel choice of basis for the densities, we are able to learn the functional to chemical accuracy in the thermodynamic limit (arXiv:1609.03705).

Invited Talk DS 49.4 Fri 12:00 HSZ 02
Taming Memory-Dependence in Time-Dependent Density Functional Theory — •Neepa Maitra — Hunter College of the City University of New York

The exact exchange-correlation functional of time-dependent density functional theory (TDDFT) is known to depend on the history of the densities and the initial states, a dependence which is ignored in almost all of the calculations today that use an adiabatic approximation. The lack of this dependence can sometimes lead to drastically incorrect predictions of the dynamics, as has been shown in several examples recently. We present here a new approach to developing functional approximations that breaks free of the adiabatic approximation, and test the resulting approximations on a number of model systems.

Invited Talk DS 49.5 Fri 12:30 HSZ 02
Quantum Embedding Theories — •Fred Manby — School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, UK

Issues of accuracy in density functional theory can be addressed by making more accurate methods (like coupled-cluster theory) more efficient; or by making density functional approximations more accurate. Efforts in both directions are underway in our group, but in this talk I will focus on a third possibility, namely the development of quantum-mechnical multiscale models that enable the use of a high-accuracy method in a small, physically important region coupled to density-functional theory (or other low-cost methods) to describe the molecular environment.

DS 50: Optics and Light-Matter Interaction with Excitons in 2D Materials (Joint Session HL, DS, O, and TT, organized by DS)

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

DS 50.1 Fri 11:15 CHE 89
Enhanced light-matter interaction in graphene/h-BN van der Waals heterostructures — •Caterina Cocchi[1], Wahib Aggoune[1,2], Dmitrii Nabok[1], Karim Rezouali[2], Mohamed Akli Belkhir[2], and Claudia Draxl[1,2] — [1]Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Laboratoire de Physique Théorique, Faculté des sciences exactes, Université de Bejaia, 06000 Bejaia, Algeria

Investigating the electronic and optical properties of graphene/h-BN heterostructures from first principles, we observe a peculiar nature of their excitations. To this extent, we employ density-functional and many-body perturbation theory in terms of the GW approximation and the Bethe-Salpeter equation. The interaction with h-BN opens a gap in graphene, making the heterostructures semiconducting. These systems absorb light over a broad frequency range, from the near-infrared to the ultraviolet region, exhibiting novel features induced by the stacking. While the specific properties of the building blocks are basically preserved, the inter-layer electron-hole pairs that are formed in the heterostructure can be modulated upon layer patterning. By choosing the stacking arrangement, the electronic coupling between the individual components can be tuned to enhance light-matter interaction. Our results open up perspectives in view of designing new low-dimensional materials with tailored opto-electronic characteristics.

DS 50.2 Fri 11:30 CHE 89
Spectral Focusing of Broadband Silver Electrolumines-

cence in Nanoscopic FRET-LEDs — •Robin Puchert, Florian Steiner, Gerd Plechinger, Felix Hofmann, Christian Schüller, Tobias Korn, Jan Vogelsang, Sebastian Bange, and John Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Universitätsstrasse 31, 93053 Regensburg, Germany

A challenge in LED technology is the use of fluorescence resonance energy transfer (FRET) in spectral conversion. An LED based on FRET effect would show both up- and down-conversion of electroluminescence (EL), since the electrically driven resonance of the light emitting device (donor) couples non-radiatively to the acceptor fluorophore resonance.

FRET-LEDs have already been proposed. However, such devices have yet to be demonstrated. The challenge lies in generating light electrically in close proximity to a dipolar acceptor in order to allow near-field coupling. We present a solution to this problem by combining a lateral LED structure with a two-dimensional transition-metal dichalcogenide overlayer (TMDC). The LED's entire excitation energy is transferred to the 2D crystal overlayer through resonant dipole-dipole coupling rather than by trivial reabsorption. This is quite remarkable given the fact that such an atomically thin TMDC monolayer absorbs only a mere 4 % of light. By using plasmonic silver nanoparticle junctions to generate broad-band EL coming from sub-diffraction localized hotspots, we see dramatic spectral focusing of the EL into the narrow excitonic resonance of the atomically thin overlayer.

DS 50.3 Fri 11:45 CHE 89

Spin-flip transitions induced by time-dependent electric fields in tuned Transition Metal Dichalcogenides magnetic thin films. — •Omar Messaoudi[1,2], Julen Ibañez-Azpiroz[2], Hamid Bouzar[1], and Samir Lounis[2] — [1]Université Mouloud Mammeri de Tizi Ouzou, Tizi Ouzou, Algeria — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

We study from first principles the relativistic electron structure of Transition Metal Dichalcogenides such as MoS_2 and WS_2 on top of which Iron is deposited as a monolayer or as a single impurity. The resulting systems turn out to be magnetic and, in particular, the states near the Fermi level show a non-negligible noncollinear spin-polarization due to the effect of spin-orbit coupling. In these noncollinear states, we analyze the excitations induced by a time-dependent electric field employing a formalism based on the maximally localized Wannier functions [1]. Finally, we analyze the absorption spectrum of circularly polarized light and discuss the possibility of observing a dichroic signal.

[1] J. Ibañez-Azpiroz *et. al*, Phys. Rev. Lett. **109**, 156401 (2012)

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DS 50.4 Fri 12:00 CHE 89

Ab-initio calculations of valley depolarization in single-layer WSe_2 mediated by electron-phonon interaction — Alejandro Molina-Sánchez[1], Davide Sangalli[2], Andrea Marini[2], and •Ludger Wirtz[1] — [1]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [2]Istituto de Strutura della Materia (CNR), CNR, Monterrotondo, Rome, Italy

Circularly polarized light can be used to selectively populate the K^+ and K^- electronic valleys of single-layer WSe_2. Valley depolarization has been measured through time-dependent Kerr experiments (measuring the rotation of a linearly polarized probe pulse applied after a circularly polarized pump pulse) by several groups. However, the depolarization mechanism still remains largely debated. Using an ab-initio implementation of time-dependent many-body perturbation theory (including electron-electron, electron-hole, and electron-phonon interaction), we solve unambiguously the debate about the dominant mechanism that drives the valley depolarization. The decay dynamics and peculiar temperature dependence (observed in recent experiments) is explained in terms of electron-phonon mediated processes that induce spin-flip inter-valley transitions.