Thin Films Division
Fachverband Dünne Schichten (DS)

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Overview of Invited Talks and Sessions

(Lecture rooms H 0111, H 2032, and E 020; Poster B and F)

Invited Talks

DS 13.1	Tue	9:30–10:00	E 020	**Electron transport in beta-gallium oxide** — •Rebecca L. Peterson, Zumrad Kabilova, Cagliyan Kurdak
DS 13.2	Tue	10:00–10:30	E 020	**Deep level defects in bulk and epi-grown β-Ga2O3** — •Lasse Vines
DS 13.3	Tue	10:30–11:00	E 020	**Indium Oxide and its surface electrons – a model system to study gas interaction and metal/semiconductor junctions** — •Marcel Himmerlich, Theresa Berthold, Jonas Michel, Simeon Katzer, Stefan Krischok
DS 13.4	Tue	11:00–11:30	E 020	**Phonons and excitons in Ga_2O_3 polytypes** — •Markus R. Wagner
DS 18.1	Wed	9:30–10:00	H 0111	**Infrared nanopolarimetric analysis of structure and anisotropy of thin films** — •Karsten Hinrichs, Timur Shaykhutdinov
DS 19.1	Wed	9:30–10:00	H 2032	**3D direct-write nanofabrication using an electron beam** — •Jason Fowlkes, Robert Winkler, Eva Mutunga, Brett Lewis, Harald Plank, Philip Rack
DS 19.2	Wed	10:00–10:30	H 2032	**Nanosuperconductivity with Focused Particle Beam Induced Deposition structures** — •Rosa Córdoba, Javier Sesé, José María De Teresa
DS 19.3	Wed	10:30–11:00	H 2032	**Chemistry for ELectron-Induced NAnofabrication** — •Petra Swiderek
DS 19.4	Wed	11:00–11:30	H 2032	**The direct electron beam writing of plasmonic nanostructures** — •Katja Höflich
DS 25.1	Wed	16:00–16:30	H 0111	**Prospects of Engineering Chemistry and Electronic Character of Interfaces in Multifunctional (Bio)Organic-Inorganic Hybrids** — •Maria Losurdo
DS 27.1	Thu	9:30–10:00	H 2032	**Coupling RF-driven acoustic wave devices with nanocavity optomechanics** — •Kartik Srinivasan, Marcelo Wu, Marcelo Davanco, Krishna Balram
DS 27.2	Thu	10:00–10:30	H 2032	**Quantum Spin-Mechanics with Color Centers in Diamond** — •Hailin Wang
DS 27.3	Thu	10:30–11:00	H 2032	**Acoustic Traps and Lattices for Electrons in Semiconductors** — Martin Schuetz, •Johannes Knörzer, Géza Giedke, Lieven Vandersypen, Mikhail Lukin, Ignacio Cirac
DS 27.4	Thu	11:00–11:30	H 2032	**Manipulating single electrons on the fly using a sound wave** — •Christopher Bauerle
DS 37.1	Fri	9:30–10:00	H 2032	**Tunable Electronic Structures, Magnetism, and Axis-Dependent Conduction Polarity in Ge and Sn-based 2D Materials** — •Joshua Goldberger

Invited talks of the joint symposium SYID

See SYID for the full program of the symposium.

SYID 1.1	Mon	9:30–10:00	H 0105	**Data driven R&D for Materials: Cognitive Discovery** — •Alessandro Curioni

SYID 1.2	Mon	10:00–10:30	H 0105	**Rational design and synthesis of Pt-based catalysts for fuel cell applications** — •Younan Xia
SYID 1.3	Mon	10:30–11:00	H 0105	**2D, or not 2D? Materials discovery, data provenance, and workflow reproducibility.** — •Nicola Marzari
SYID 1.4	Mon	11:00–11:30	H 0105	**Generating and assessing data from combinatorial and high-throughput experiments for the design of new materials** — •Alfred Ludwig
SYID 1.5	Mon	11:30–12:00	H 0105	**Novel materials discovery: big-data-analytics methods and infrastructure for building maps of materials** — •Luca Ghiringhelli

Invited talks of the joint symposium SYVC

See SYVC for the full program of the symposium.

SYVC 1.1	Wed	15:00–15:30	H 0105	**Magneto-ionic control of interfacial magnetism** — •Geoffrey Beach
SYVC 1.2	Wed	15:30–16:00	H 0105	**Ionic Control of Materials Beyond Interfaces** — •Dustin Gilbert
SYVC 1.3	Wed	16:00–16:30	H 0105	**Microscopic Mechanisms of Memristive Switching in Metal Oxides** — •Rainer Waser, Stephan Menzel, Regina Dittmann
SYVC 1.4	Wed	17:00–17:30	H 0105	**In-situ and operando SQUID magnetometry under electrochemical control** — •Roland Würschum, Markus Gössler, Gregor Klinser, Eva-Maria Steyskal, Heinz Krenn
SYVC 1.5	Wed	17:30–18:00	H 0105	**Reversible chemistry as a tool for dynamic control of physical properties** — •Robert Kruk, Subho Dasgupta, Bijoy Das, Horst Hahn

Invited talks of the joint symposium SYDM

See SYDM for the full program of the symposium.

SYDM 1.1	Thu	15:00–15:30	H 0105	**Bending, pulling, and cutting wrinkled two-dimensional materials** — •Kirill Bolotin
SYDM 1.2	Thu	15:30–16:00	H 0105	**Ultrafast valley and spin dynamics in single-layer transition metal dichalcogenides** — •Alejandro Molina-Sanchez
SYDM 1.3	Thu	16:00–16:30	H 0105	**Interlayer excitons in layered semiconductor transition metal dichalcogenides** — •Steffen Michaelis de Vasconcellos
SYDM 1.4	Thu	16:45–17:15	H 0105	**Exploring exciton physics in liquid-exfoliated 2D materials** — •Claudia Backes
SYDM 1.5	Thu	17:15–17:45	H 0105	**A Progress Report on Electron Transport in MXenes; A New Family of 2D Materials** — •Michel Barsoum

Invited talks of the joint symposium SYAM

See SYAM for the full program of the symposium.

SYAM 1.1	Fri	9:30–10:00	H 0105	**Bringing Dino-Birds to life – Synchrotron X-ray fluorescence and Raman imaging of ancient materials** — •Uwe Bergmann
SYAM 1.2	Fri	10:00–10:30	H 0105	**Linear and Nonlinear Optical Properties of Cultural Heritage Materials** — •Marta Castillejo
SYAM 1.3	Fri	10:30–11:00	H 0105	**Morphology and topology of multiscale pore networks: Imaging structural alteration and hydric invasion** — •Pierre Levitz
SYAM 1.4	Fri	11:15–11:45	H 0105	**Painting cracks: a way to reveal physical properties of matter** — •Ludovic Pauchard
SYAM 1.5	Fri	11:45–12:15	H 0105	**Finite element analysis and biomechanical interpretation of fossil material properties** — •Emily Rayfield

Sessions

DS 1.1–1.8	Mon	9:30–11:30	H 0111	**Layer Properties: Electronic, Optical and Mechanical**
DS 2.1–2.14	Mon	9:30–13:15	H 2032	**2D Materials: Session I (joint session DS/CPP/HL)**
DS 3.1–3.14	Mon	9:30–13:15	E 020	**Oxide Semiconductors for Novel Devices (Focussed Session): Session I**

DS 4.1–4.10	Mon	10:30–13:00	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials I (joint session O/MM/DS/TT/CPP)**
DS 5.1–5.6	Mon	11:45–13:15	H 0111	**Layer Deposition (ALD, MBE, Sputtering, ...)**
DS 6.1–6.12	Mon	15:00–18:15	H 0111	**Thin Film Applications**
DS 7.1–7.10	Mon	15:00–17:45	H 2032	**Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...): Session I**
DS 8.1–8.6	Mon	15:00–16:30	EW 201	**2D materials (joint session HL/DS)**
DS 9.1–9.9	Mon	15:00–17:15	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials II (joint session O/MM/DS/TT/CPP)**
DS 10.1–10.12	Mon	15:00–18:15	E 020	**Oxide Semiconductors for Novel Devices (Focussed Session): Session II**
DS 11.1–11.14	Tue	9:30–13:15	H 0111	**Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...): Session II**
DS 12.1–12.14	Tue	9:30–13:15	H 2032	**2D Materials: Session II (joint session DS/CPP/HL)**
DS 13.1–13.4	Tue	9:30–11:30	E 020	**Oxide Semiconductors for Novel Devices (Focussed Session): Session III**
DS 14.1–14.5	Tue	10:30–13:00	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials III (joint session O/MM/DS/TT/CPP)**
DS 15.1–15.5	Tue	11:45–13:00	E 020	**Thermoelectric and Phase Change Materials**
DS 16.1–16.7	Tue	14:00–15:45	A 151	**2D materials: Graphene and BN (joint session HL/DS)**
DS 17.1–17.81	Tue	18:15–20:15	Poster B	**Poster Session I**
DS 18.1–18.11	Wed	9:30–13:00	H 0111	**Optical Analysis of Thin Films (Reflection, Ellipsometry, Raman, IR-DUV Spectroscopy, ...): Session I**
DS 19.1–19.9	Wed	9:30–13:00	H 2032	**Lithography I: Focused Electron Beam Induced Processing: 3D Nano-Printing for Material Science (Focussed Session): Morning Session (joint session DS/KFM)**
DS 20.1–20.14	Wed	9:30–13:15	A 151	**2D materials: Chalcogenides I (joint session HL/DS)**
DS 21.1–21.9	Wed	10:30–13:00	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials IV (joint session O/MM/DS/TT/CPP)**
DS 22.1–22.3	Wed	15:00–15:45	H 0111	**Optical Analysis of Thin Films (Reflection, Ellipsometry, Raman, IR-DUV Spectroscopy, ...): Session II**
DS 23.1–23.11	Wed	15:00–18:00	H 2032	**Lithography II: Focused Electron Beam Induced Processing: 3D Nano-Printing for Material Science (Focussed Session): Afternoon Session (joint session DS/KFM)**
DS 24.1–24.10	Wed	15:00–17:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials V (joint session O/MM/DS/TT/CPP)**
DS 25.1–25.7	Wed	16:00–18:15	H 0111	**Organic Thin Films, Organic-Inorganic Interfaces: Session I (joint session DS/CPP)**
DS 26	Wed	18:30–19:30	H 0111	**Annual General Meeting of the Thin Films division**
DS 27.1–27.10	Thu	9:30–13:15	H 2032	**New Twists for Nanoquakes on a Chip - Emerging Applications of Surface Acoustic Waves in Condensed Matter Physics (Focussed Session): Session I**
DS 28.1–28.14	Thu	9:30–13:15	A 151	**2D materials: Chalcogenides II (joint session HL/DS)**
DS 29.1–29.8	Thu	9:30–12:50	EMH 025	**Lithography III: Lithography and Structuring (joint session KFM/DS)**
DS 30.1–30.9	Thu	10:30–12:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VI (joint session O/MM/DS/TT/CPP)**
DS 31.1–31.26	Thu	11:15–13:15	Poster F	**Poster Session II**
DS 32.1–32.1	Thu	12:30–13:00	EW 201	**Invited Talk: Michael Heuken (joint session HL/DS)**
DS 33.1–33.3	Thu	15:00–15:45	H 2032	**New Twists for Nanoquakes on a Chip - Emerging Applications of Surface Acoustic Waves in Condensed Matter Physics (Focussed Session): Session II**
DS 34.1–34.10	Thu	15:00–17:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VII (joint session O/TT/MM/DS/CPP)**

DS 35.1–35.8	Thu	15:00–18:10	EMH 025	**Lithography IV: Lithography and Structuring (joint session KFM/DS)**
DS 36.1–36.6	Fri	9:30–11:00	H 0111	**Organic Thin Films, Organic-Inorganic Interfaces: Session II (joint session DS/CPP)**
DS 37.1–37.10	Fri	9:30–12:30	H 2032	**2D Materials: Session III (joint session DS/CPP/HL)**
DS 38.1–38.9	Fri	10:30–12:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VIII (joint session O/TT/MM/DS/CPP)**

Annual General Meeting of the Thin Films Division

Wednesday 18:30–19:30 H 0111

DS 1: Layer Properties: Electronic, Optical and Mechanical

Time: Monday 9:30–11:30 Location: H 0111

DS 1.1 Mon 9:30 H 0111

Tuning the probability of defect formation via substrate strains in Sr_2FeMoO_6 films — Waheed A. Adeagbo[1], •Martin Hoffmann[2], Arthur Ernst[2,3], Wolfram Hergert[1], Minnamari Saloaro[4], and Petriina Paturi[4] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, Germany — [2]Institute for Theoretical Physics, Johannes Kepler University Linz, Austria — [3]Max Planck Institute of Microstructure Physics, Halle, Germany — [4]Wihuri Physical Laboratory, Department of Physics and Astronomy, University of Turku, Finland

Since oxide materials like Sr_2FeMoO_6 are usually applied as thin films, we studied the effect of biaxial strain, resulting from a potential substrate, on the electronic and magnetic properties and, in particular, on the formation energy of point defects. From our first-principles calculations, we determined that the probability of forming point defects – like vacancies or substitutions – in Sr_2FeMoO_6 could be adjusted by choosing a proper substrate. For example, the amount of anti-site disorder and oxygen vacancies can be reduced with compressive strain to get purer Sr_2FeMoO_6 as needed for spintronic applications, while the formation of oxygen vacancies is more likely for tensile strain, which improves the functionality of Sr_2FeMoO_6 as basis material of solid oxide fuel cells. Hence, this degree of freedom might offer in general an additional possibility to tune the appearance of point defects besides e.g. experimental growth conditions like temperature or gas pressure.

DS 1.2 Mon 9:45 H 0111

Disorder Control in Crystalline $GeSb_2Te_4$ and its Impact on Characteristic Length Scales — •Matthias M. Dück[1], Tobias Schäfer[1], Marc Pohlmann[1], Carl-Friedrich Schön[1], Hannah Niehaus[1], and Matthias Wuttig[1,2] — [1]1. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA-FIT, RWTH Aachen University, Germany

Chalcogenides along the pseudobinary line between GeTe and Sb_2Te_3 (GST) are currently gaining much attention, since a number of interesting properties is observed in this material group, which contains phase-change materials, thermoelectrics, topological insulators and superconductors. Phase-change materials from the GST system have recently been reported to exhibit a disorder-induced metal-to-insulator transition, which is not linked to the transition from the metastable to the stable phase of this material. The MIT has been attributed to the ordering of stoichiometric vacancies, which leads to charge carrier delocalization. The current work is based on reports of a correlation between vacancy layer formation in textured films and their electronic transport properties. A systematic study of low temperature transport in combination with highly textured GST thin films provides further insights in the mechanisms of disorder induced charge carrier localization. In this talk, the relationship between characteristic length scales for atomic arrangement as well as electronic transport in the GST124 system will be elucidated. A comparative analysis of the results reveals the importance of vacancy ordering in this system, as well as the insignificance of grain boundaries for the material's properties.

DS 1.3 Mon 10:00 H 0111

2D protective films for lithium and sodium metal anodes — Hongzhen Tian[1], Zhi W. Seh[2], Kai Yan[2], Zhongheng Fu[1], Peng Tang[1], Yingying Lu[3], Ruifeng Zhang[1], •Dominik Legut[4], Yi Cui[5], and Qianfan Zhang[1] — [1]School of Materials Science and Engineering,Beihang University, Beijing 100191, China — [2]Institute of Materials Research and Engineering Agency for Science, Technology and Research, Innovis, Singapore 138634, Singapore — [3]State Key Laboratory of Chemical Engineering College of Chemical and Biological Engineering Zhejiang University Hangzhou 310027, China — [4]IT4Innovations Center, VSB-TU Ostrava, 17.listopadu 15, CZ 70833 Ostrava, Czech Republic — [5]Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305, USA

Rechargeable batteries based on lithium (sodium) metal anodes have been attracting increasing attention due to their high capacity and energy density, but exhibit drawbacks, such as low Coulombic efficiency and dendrites growth. Lay- ered materials have been used experimentally as protective films (PFs) to address these issues. Here we use first-principles calculations to determine the properties and feasibility of various 2D layered PFs.It is found that the introduction of defect, the increase in bond length, and the proximity effect by metal can accelerate the transfer of Li^+ (Na^+) ion and improve the ionic conductivity, but all of them make negative influences on the stiffness of materials. [1] H. Tian et al, Advan. Ene. Mat. **7**, 1602528 (2017).
This work was supported by CSF grant No. 17-27790S and Path to Exascale project No. CZ.02.1.01/0.0/0.0 /16_013/0001791.

DS 1.4 Mon 10:15 H 0111

Development of mirror coatings for gravitational wave detectors — •Lukas Terkowski[1], Jessica Steinlechner[1,2], Daniel Axmann[1], Jim Hough[2], Iain Martin[2], Sheila Rowan[2], and Roman Schnabel[1] — [1]Institut für Laser-Physik, Universität Hamburg, Luruper Chaussee 149, Gebäude 69, 22761 Hamburg, Germany — [2]SUPA, School of Physics and Astronomy, University of Glasgow, Glasgow, G12 8QQ, Scotland

Gravitational waves are ripples in space caused by massive, accelerated objects in space. They were predicted by Einstein more than 100 years ago and first measured in 2015. When reaching their design sensitivity, current gravitational-wave detectors - as well as all planned, future detectors - will be limited, at their most sensitive frequencies, by thermal noise from the highly-reflective mirror coatings.

To detect more, weaker gravitational waves from a wider range of astrophysical sources, it is necessary to develop new coating materials. Besides low thermal noise, there are also strong requirements on the optical absorption and optical scattering of the coatings, which have to be available in large sizes.

Due to low thermal noise, amorphous silicon seems to be a promising solution for a coating material. However, the optical absorption of commercially available amorphous silicon is currently far higher than the requirement. In this talk we will present our work on improving the optical properties of amorphous silicon by optimizing deposition parameters, to make future gravitational-wave detectors more sensitive.

DS 1.5 Mon 10:30 H 0111

Quantitative AM-FM Mode for Fast, Versatile Imaging of Nanoscale Elastic Modulus — •Florian Johann, Roger Proksch, Marta Kocun, and Ted Limpoco — Oxford Instruments (Asylum Research), Santa Barbara, USA

Nanoscale information on mechanical properties is critical for many advanced materials and nanotechnology applications. Atomic Force Microscopy (AFM) techniques for probing mechanical properties of samples in the nanometer range have emerged over the past decades.

Amplitude-modulated AFM (AM-AFM), also known as tapping mode, is a proven, reliable and gentle imaging method with widespread applications. Previously, the contrast in AM-AFM has been difficult to quantify. Here, we introduce AM-FM imaging, which combines the features and benefits of normal tapping mode with quantitative and high sensitivity of frequency modulated (FM) mode. Briefly, the topographic feedback operates in AM mode while the second resonant mode drive frequency is adjusted on resonance. With this approach, frequency feedback and topographic feedback are decoupled, allowing much more stable, robust operation. The FM image returns a quantitative value of the frequency shift that depends on the sample stiffness and can be applied to a variety of physical models.

DS 1.6 Mon 10:45 H 0111

Layer specific observation of the slow thermal equilibration in ultrathin metallicnanolayers by femtosecond x-ray diffraction — Jan-Etienne Pudell[1], Alexey Maznev[2], Marc Herzog[1], Matthias Kronseder[3], Christian Back[3], Gregory Malinowski[4], •Alexander von Reppert[1], and Matias Bargheer[1,5] — [1]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [2]Department of Chemistry, Massachusetts Institute of Technology, Massachusetts, USA — [3]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [4]Institut Jean Lamour (UMR CNRS 7198), Université Lorraine, Nancy, France — [5]Helmholtz-Zentrum Berlin, Berlin, Germany

We study the ultrafast response of nanometric layers of Gold (Au) on Nickel (Ni) upon optical excitation with femtosecond laser pulses by ultrafast x-ray diffraction (UXRD). We show the experimental results

obtained by exciting a 12 nm Ni film through a 5 nm Au film by 800 nm pulses with about 50 fs pulse duration. Although the pump pulse impinges on Au, the initially deposited energy is essentially transferred to the Ni lattice due to its much larger electron phonon-coupling constant. The most surprising result is the very slow heat transport from Ni into the Au lattice. The Au lattice temperature reaches its maximum only after 80 ps, although bulk heat conductivity estimates would predict less than 1 ps to equilibrate the temperatures of the two ultrathin metal layers. UXRD thus represents a formidable experimental probe to support theoretical developments in nanoscale thermal transport.

DS 1.7 Mon 11:00 H 0111

Revealing Charge Redistribution at Hybrid Interfaces by DRS — •Tino Meisel[1], Marcel Gawek[1], Mino Sparenberg[1], Sergey Sadofev[1], Oliver Benson[1], Emil J. W. List-Kratochvil[1,2], and Sylke Blumstengel[1,2] — [1]Institute of Physics, Humboldt University Berlin — [2]Institute of Chemistry, Humboldt University Berlin

Hybrid inorganic/organic systems (HIOS) combining functional conjugated molecules and inorganic semiconductors are promising candidates for opto-electronic devices such as photovoltaic cells and light emitting diodes. For these applications understanding of the interfacial electronic structure plays a key role. In this work we present differential reflectance spectroscopy (DRS) as a novel experimental tool to reveal ground state charge transfer at hybrid interfaces. As prototypical HIOS conjugated molecules (ladder-type quaterphenyl (L4P), NTCDA, F6TCNNQ) were deposited on top of epitaxial ZnO via molecular beam deposition and DRS was conducted in real time in the course of the organic layer growth. Two types of HIOS interfaces will be discussed: (i) HIOS with negligible interfacial charge transfer (L4P/ZnO). In this case the DR spectra can simply be modelled using the dielectric functions of the individual layers. (ii) HIOS with ground state charge transfer at the interface (F6TCNNQ/ZnO, NTCDA/ZnO). Here, the dielectric function of ZnO is significantly altered by the interaction with the molecules which causes a characteristic fingerprint in the DR spectra. DRS is thus viable tool to uncover interfacial charge carrier redistribution at HIOS interfaces.

DS 1.8 Mon 11:15 H 0111

Non-degenerate valleys in transition metal layered WS_2 — •Omar Messaoudi[1,2], Julen Ibañez-Azpiroz[2], 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 present a comparative first principles investigation of the electronic properties of monolayer WS2 coated with an overlayer of a transition metal (Fe, Co, Mn). Fe outstands as the most prominent candidate where our ab initio calculations reveal that the system is a half-metallic ferromagnet with a gap of 1 eV for the majority spin channel. Furthermore, the combined effect of time-reversal symmetry breaking, due to the magnetic Fe overlayer, and the large spin-orbit coupling induced by W gives rise to non-degenerate K and K∗ valleys. This has a tremendous impact on the excited state properties induced by externally applied circularly polarized light. Our analysis demonstrates that the latter induces a singular hot spot structure of the transition probability around the K and K∗ valleys for right and left circular polarization, respectively. We trace back the emergence of this remarkable effect to the strong momentum dependent spin-noncollinearity of the valence band involved. As a main consequence, a strong valley-selective magnetic circular dichroism is obtained, making this system a prime candidate for spintronics and photonics applications.

DS 2: 2D Materials: Session I (joint session DS/CPP/HL)

Time: Monday 9:30–13:15 Location: H 2032

DS 2.1 Mon 9:30 H 2032

Graphene nanoribbon: electronic band structure, doping and Raman fingerprints — •Boris Senkovskiy[1], Dmitry Usachov[2], Alexander Fedorov[2,3], Gianni Profeta[4], Danny Haberer[5], Felix Fischer[5], and Alexander Grüneis[1] — [1]II. Institute of Physics, University of Cologne, Cologne, Germany — [2]St. Petersburg State University, St. Petersburg,Russia — [3]IFW-Dresden, Dresden, Germany — [4]Department of Physical and Chemical Sciences and SPIN-CNR, University of L'Aquila , Coppito, Italy — [5]Department of Chemistry, University of California at Berkeley, Berkeley, USA

We present the state-of-the-art studies of atomically precise graphene nanoribbons (GNRs) synthesized using on-surface assisted molecular assembly. Using angle-resolved photoemission spectroscopy (ARPES), we obtain the band structure of pristine and boron-doped armchair GNRs of N=7 carbon atoms width. ARPES maps in the full 2D momentum space visualize each sub-band of quasi-1D GNRs and allow to extract effective masses, charge carrier velocities and sub-band energy offsets. Vibration properties of GNRs are probed in-situ by ultra-high vacuum Raman setup. We show how the periodically incorporated boron atoms affect the band structure and the Raman-active modes of GNRs. Particularly, in doped nanoribbons the effective mass of charge carriers is ∼2 times smaller and the peculiar Raman modes are red-shifted and doubled regarding to the pristine system.

[1] Senkovskiy et al. Adv. Electron. Mater. 2017.
[2] Senkovskiy et al. Nano Lett., 2017.
[3] Senkovskiy et al. Phys. Status Solidi RRL, 2017.

DS 2.2 Mon 9:45 H 2032

Valley spin lifetimes reaching 100 ns in monolayer $MoSe_2$ at room temperature — •Maximilian Heithoff, Manfred Ersfeld, Frank Volmer, Robin de Winter, Christoph Stampfer, and Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

We present time-resolved Kerr-rotation measurements on a monolayer of $MoSe_2$ revealing spin lifetimes up to 100 ns at room temperature. This extraordinary long-lived spin signal only weakly depends on temperature between 60 K and 300 K. At lower temperatures, it gets masked by an additional spin signal with significantly larger amplitude but shorter spin lifetimes reaching 8 ns. The latter spin signal exhibits a Kerr resonance which coincides with the photoluminescence spectrum from neutral and charged excitons showing that the spin dynamics at low temperatures are dominated by excitonic effects. In contrast, the long-lived spin signal at higher temperatures shows no resonance in the energy regime of the excitons. The absence of such resonance combined with the long spin lifetimes at room temperature is expected if the spin dynamics at elevated temperatures are not dominated by excitonic effects but by a polarization of resident holes, which is protected even at room temperature due to the large spin splitting in the valence bands of transition metal dichalcogenides.

DS 2.3 Mon 10:00 H 2032

Ultra-high vacuum Raman spectroscopy of Cs doped monolayer graphene — •Martin Hell, Boris Senkovskiy, Joshua Hall, Thomas Michely, and Alexander Grüneis — II. Physikalische Institut, Universität zu Köln

We show that ultra-high vacuum (UHV) Raman spectroscopy is a valuable tool for in-situ characterization of epitaxial graphene on Ir(111) regarding strain, defects and doping level. We study the Cs doping induced changes in the Raman spectrum of epitaxial monolayer graphene for 2x2 and $\sqrt{3}$x$\sqrt{3}$ Cs adsorption geometries for exciting laser energies in a wide range (325nm to 633nm). The combined effects of lattice expansion and dynamic effects lead to characteristic changes in the Raman spectrum that allow us to identify the charge transfer and the electron-phonon coupling strength from the position, width and asymmetry of the G band Raman line. The electronic and structural characterization of Cs doped graphene is complemented by angle-resolved photoemission measurements and scanning tunneling microscopy on identically prepared samples. The high energy resolution of Raman (∼1 wavenumber) allows for a precise determination of temperature induced strain of epitaxial graphene. Finally, we will show new results regarding the UHV Raman and luminescence characterization of transition metal dichalcogenides grown on graphene/Ir(111).

DS 2.4 Mon 10:15 H 2032

Raman spectroscopy of misfit layer compound nanotubes from CrS_2 and TaS_2 — •Felix Kampmann[1,2], Dalit Stolovas[3], Leela S. Panchakarla[3], Gal Radovsky[3], Christian Thomsen[2],

Reshef Tenne[3], and Janina Maultzsch[2] — [1]Institut für Festkörperphysik, TU Berlin, Berlin, Germany — [2]Institut für Physik der Kondensierten Materie, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany — [3]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel

Misfit layer compounds (MLC) offer an interesting approach towards synthesis of novel one-dimensional nanostructures and two-dimensional materials. Understanding their structure and their physical properties has been subject to intense scientific research. The MLCs described by the formula MX-TX_2 consist of a transition metal dichalcogenide (TMD) layer TX_2 and an intercalation layer MX with distorted rock-salt structure. Here M denotes a metal, X is one of the elements S or Se, and T is of the group of transition metals.

In our study the TMD layer CrS_2 or TaS_2 is intercalated by either LaS-, CeS- or GdS- layers. Upon formation of the MLC charge transfer between the sublayers and deformation of the intercalation layer stabilize the otherwise metastable CrS_2. Due to the misfit between the sublayers in at least one direction and the seaming of dangling bonds at the rim atoms, the synthesis of nanotubes and -scrolls is favored. We investigate the vibrational properties of MLC nanotubes via Raman spectroscopy and discuss the results regarding previously published TEM methods.

DS 2.5 Mon 10:30 H 2032

Photoluminescence study of MoS_2 monolayers integrated with photonic nanostructures — •Rajeshkumar Mupparapu[1], Tobias Bucher[1], Antony George[2], Frank Setzpfandt[1], Thomas Pertsch[1], Andrey Turchanin[2], and Isabelle Staude[1] — [1]Institute of Applied Physics, Abbe Center of Photonics, Friedrich Schiller University Jena, 07745 Jena, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany

Interaction of light with MoS_2 monolayers can be enhanced by integrating them with resonant nanostructures [1], and such interaction allows to manipulate their photoluminescence (PL) directionality and polarization. Here, we investigated the PL properties of MoS_2 monolayers integrated with resonant Silicon nanostructures [2] to explore the behavior of PL and valley polarization. Experiments performed on MoS_2-nanostructures reveal a significant PL enhancement [3], dominantly due to the local strain rather than Purcell enhancement. We further studied the valley polarization of MoS_2 flakes under different locally modified environments.

References:

[1]. S. Butun, *et al.*, Nano Lett., 2015, 15, 2700-2704.
[2]. M. Decker, I. Staude, J. Opt. 18, 103001 (2016).
[3]. T. Bucher, *et al.*, CLEO/Europe-EQEC 2017, Munich, EI-4.5, (2017).

DS 2.6 Mon 10:45 H 2032

luminescence at defects in h-BN : excitons at stacking faults and single photon emitters — •Alberto Zobelli, Romain Bourrellier, Sophie Meuret, Michele Amato, Odile Stéphan, Luiz Tizei, and Mathieu Kociak — Laboratoire de Physique des Solides, University of Paris-Sud, CNRS, Orsay, France

h-BN is a promising material for optical application due to a strong exciton in the far UV and bright and stable defect emissions. Here we investigate the spatial localization at the nanometric scale of defects lines in this rich emission spectrum by employing an original cathodoluminescence system (nano-CL) integrated within a scanning transmission electron microscope. We show that high energy emissions are related to crystal folds leading to local changes of the layer stacking order which promote additional excitons. Furthermore, middle band gap emissions present a high spatial localization (˜80 nm) and a typical zero-phonon line plus phonon replica spectroscopic signature, indicating a point defect origin. Finally, by combining our nano-CL system with an Hanbury Brown and Twiss (HBT) interferometer we identify a new bright and stable single photon emitter in the far UV.

DS 2.7 Mon 11:00 H 2032

Density-functional perturbation theory for gated 2D heterostructures — •Thibault Sohier[1], Marco Gibertini[1], Nicola Marzari[1], Matteo Calandra[2], and Francesco Mauri[3] — [1]THEOS and MARVEL, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]IMPMC, CNRS, Université Pierre et Marie Curie, Paris, France — [3]Departimento di Fisica, Università di Roma La Sapienza, Roma, Italy

The ability to perform first-principles calculations of phonons and electron-phonon interactions in gated 2D heterostructures is crucial to the understanding and design of next-generation devices. Yet, standard methods relying on 3D periodic-boundary conditions fail to properly account for the consequences of dimensionality and the field-effect on electron-phonon physics. Here we present an implementation of density-functional perturbation theory using open boundary conditions adequate to the simulation of 2D systems, and with the possibility to add charged planes to emulate the doping of the slab via field-effect. We first illustrate the importance of working in the correct 2D framework with the study of long-wavelength phonons in polar materials, focusing on two mechanisms relevant for the performances of electronic devices: the Fröhlich interaction and the LO-TO splitting. Second, we address the consequences of the field-effect setup by looking at flexural phonons and their coupling to electrons in gated graphene. We observe that unlike isolated graphene, the coupling with flexural phonons in gated graphene is not forbidden by symmetry, but it is strongly suppressed by electronic screening.

15 min. break.

DS 2.8 Mon 11:30 H 2032

Spectroscopic characterization of the silicene multi-layer phase on Ag(111) — •Dmytro Solonenko[1], Sandhya Chandola[2], Eugen Speiser[2], Norbert Esser[2], Dietrich R.T. Zahn[1], and Patrick Vogt[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V., 12489 Berlin, Germany

The formation of so-called "multi-layer silicene" has been suggested to form for supramonolayer Si coverages on Ag(111)[1], but its nature is still controversially discussed including silicene multi-layers, bilayers or Ag-mediated growth of bulk Si with a Ag-terminated $(\sqrt{3}\times\sqrt{3})$R30° reconstruction[2]. However, the experimental results which were shown so far do not allow an unequivocal assignment of this phase to any of the suggested structures. In order to retrieve the structural properties of this $(\sqrt{3}\times\sqrt{3})$R30° structure, we carried out an *in situ* Raman spectroscopy study varying the Si coverage (up to 10 monolayers). Our results show a unique spectral signature, which does not bear any resemblance to monolayer epitaxial silicene[3]. We compare the Raman results to those for the $(\sqrt{3}\times\sqrt{3})$R30° Ag/Si(111) system, yielding the similarities in terms of the overall number of spectral bands and their positions but also suggests fundamental differences, hinting towards the formation of a Si bilayer.

[1] Vogt, P., *et al.*, *Appl. Phys. Lett.* **104**, 021602 (2014). [2] Borensztein, Y., *et al.*, *Phys. Rev. B* **92**, 155407 (2015). [3] Solonenko, D., *et al.*, *2D Mat.* **4**, 015008 (2017).

DS 2.9 Mon 11:45 H 2032

Frictional anisotropy of MoS2 studied with molecular dynamics simulations — •Victor Claerbout[1], Tomas Polcar[1,2], and Paolo Nicolini[1] — [1]Czech Technical University in Prague, Prague, Czech Republic — [2]nCATS, University of Southampton, Southampton, United Kingdom

Transition metal dichalcogenides are considered to be among the best solid lubricants due to their lamellar structure. Tribological research focused upon molybdenum disulfide has revealed its super low friction behavior [1]. However, a full understanding of the mechanism behind this behavior remains lacking. In this contribution we aim to elucidate the phenomena taking place at the nanoscale when two commensurate layers of molybdenum disulfide slide one atop of another. In particular, by means of molecular dynamics simulations, we studied the effect of sliding anisotropy [2] (i.e., the changing frictional behavior upon varying the sliding angle of two commensurate layers) on the energy dissipation due to friction. We simulated different sliding conditions (varying e.g. normal load, sliding speed and system temperature) in order to highlight their effect on the lubricating properties. These results will help on the one hand to identify the fundamental mechanisms that govern friction at an atomistic level, as well as providing guidelines for the design of novel layered materials with improved tribological properties.

[1] J.M. Martin et al., Phys. Rev. B, 48, 10583(R) (1993). [2] Onodera et al., J. Phys. Chem. B, 114, 15832 (2010).

DS 2.10 Mon 12:00 H 2032

Structural changes and phase stability of Ti doped MoS_2 monolayers — •Andrea Silva, Tomas Polcar, Ondrej Hovorka, and Denis Kramer — Faculty of Engineering and Environment, Uni-

versity of Southampton, SO17 1BJ Southampton, United Kingdom

The discovery of graphene and its remarkable properties has renewed interest in inorganic materials and drawn attention to two-dimensional systems. Transition metal dichalcogenides (TMDs) have been known for decades in industry, but only recently their graphite-like layered structure has renewed academic interest. Quantum confinement in the monolayers yields different electronic properties compared to bulk counterparts. Moreover, TMDs are more chemically versatile than graphene, allowing easy functionalization of the layers [1]. Understanding the doping possibilities for TMDs is a key step in exploiting their potential.

In this study, we focus on the Ti doped MoS_2 TMD, a recently proposed new material with enhanced tribological properties [2].

In order to address the challenging task of determining the phase-stability of a new compound, we map energy landscapes obtained with DFT onto a cluster-expansion hamiltonian and iteratively search for low energy orderings of the atoms inside the given host. This methodology allows us to explore the Ti-Mo-S phase space and determine doping possibilities leading to stable phases of the form $Ti_xMo_{1-x}S_2$, quantify miscibility gaps and thermodynamic competition with ternary oxides.

[1] M. Chhowalla *et al.*, Nat. Chem. 5, 263 (2013).

[2] A. Cammarata and T. Polcar, Inorg. Chem. 54, 5739 (2015).

DS 2.11 Mon 12:15 H 2032

Resonance profiles of valley polarization in single-layer MoS_2 and $MoSe_2$ — •Hans Tornatzky[1], Roland Gillen[1,2], Anne-Marie Kaulitz[1], and Janina Maultzsch[1,2] — [1]Institut für Festkörperphysik, TU Berlin, Germany — [2]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Transition metal dichalcogenides (TMDCs) attract a lot of interest due to their unique properties, such as the repeatedly investigated strong photoluminescence from the direct gap in few layered samples. Furthermore, TMDCs have recently become promising materials for spin- and valleytronics as circular polarized excitation leads to the generation of electron-hole-pairs with distinct spin at either K or K^* points in the Brillouin zone. However, questions remain unanswered about the mechanisms of the scattering processes.

In this talk we present photoluminescence measurements with different excitation energies on single-layer MoS_2 and $MoSe_2$ in order to examine the resonance behavior of the conservation of circular polarization in these TMDCs. We find that the circular polarization of the emitted light is conserved to 100 % in MoS_2 and 84 %/79 % (A/A^- peaks) in $MoSe_2$ close to resonance. The values for $MoSe_2$ surpass any previously reported value. However, in contrast to previous predictions, the degree of circular polarization decreases clearly at energies less than the 2 LA phonon energy above the resonance.

Our findings indicate that at least two competing processes underly the depolarization of the emission in single-layer transition metal dichalcogenides.

DS 2.12 Mon 12:30 H 2032

Defect mediated phase transformation of two-dimensional 2H-MoTe2 to the distorted 1T'-MoTe2 — •Tibor Lehnert[1], Mahdi Ghorbani-Asl[2], Janis Köster[1], Hannu-Pekka Komsa[3], Arkady Krasheninnikov[2,3], and Ute Kaiser[1] — [1]Electron Microscopy Group of Materials Science, University of Ulm, Ulm 89081, Germany — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden 01328, Germany — [3]Department of Applied Physics, Aalto University, P.O. Box 11100, 00076 Aalto, Finland

We applied the newly developed Cc-and Cs-corrected SALVE (Sub-Angstrom Low-Voltage Electron Microscopy)[1] instrument, to study the dynamics of extended defects in single-layer 2H-MoTe2. In particular we report atom by atom on the transformation of an area in single-layer MoTe2 from the semiconducting 2H to the distorted and metallic 1T* phase, starting with a single vacancy line of missing Te atoms. We find that the size of the transformed area is defined by the length of the single vacancy line. First-principles calculations are performed to understand the transformation's driving forces.

[1] www.salve-project.de

DS 2.13 Mon 12:45 H 2032

Excitonic transitions in heterostructured Mo and W transition metal dichalcogenides from first principles — •Roland Gillen and Janina Maultzsch — Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Novel two-dimensional materials from the group of layered transition metal dichalcogenides (TMDC) attract scientific interest for their unusual physical properties, such as their strong optical response. Two ways to tailor the electronic and optical properties are (i) the combination of different TMDCs to form lateral and stacked heterostructures and (ii) creation of alloys containing different metal or chalcogen atoms. Recent experiments have suggested long-lived interlayer excitons in stacked heterostructures, with spatial separation of electrons and holes across the layers, allowing for exploitation in solar cells.

Based on recent work [1,2], we show the theoretical absorption spectra of bilayer $MoSe_2$-WSe_2 and MoS_2-WSe_2 heterostructures from solution of the excitonic Bethe-Salpeter equation with GW quasiparticle corrections and inclusion of spin-orbit-coupling. In accordance with experimental observations, we find contributions related to interlayer excitons below the absorption onset of the monolayer materials. Our calculations allow us to estimate the binding energy of these electron-hole pairs to be on the order of 0.2 eV for both studied heterostructures. We will further show recent calculations of the absorption spectra of alloyed $MoWS_2$ materials.

[1] Gillen et al., IEEE JSTQE 23, 1 (2017), [2] Gillen et al., in preparation

DS 2.14 Mon 13:00 H 2032

Suppression of inhomogeneous broadening of excitons and trions in encapsulated $MoSe_2$ monolayers — •Max Waldherr[1], Jacob Goddard[1], Nils Lundt[1], Sefaattin Tongay[2], Kenji Watanabe[3], Takashi Taniguchi[3], Sven Höfling[1,4], and Christian Schneider[1] — [1]Technische Physik, Physikalisches Institut and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]School for Engineering of Matter, Transport, and Energy, Arizona State University, Tempe, Arizona 85287, USA — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan — [4]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

Two-dimensional transition metal dichalcogenides offer a rich platform for the investigation of light-matter coupling effects due to unique effects such as spin-valley locking. In the monolayer limit the optical properties of these materials are highly sensitive to surface effects, hence the exciton and trion resonances undergo inhomogeneous broadening by surface impurities. We present a method to reduce the linewidth of these resonances involving encapsulation between two ultra-thin hexagonal boron nitride layers and thermal annealing in an argon-hydrogen atmosphere. With this technique inhomogeneous broadening is suppressed effectively which manifests in a Lorentzian line shape and improved optical quality. Moreover, the spectral weight of the exciton increases and the linewidths of the exciton and trion reduce to 2.9 and 2.4 meV, respectively.

DS 3: Oxide Semiconductors for Novel Devices (Focussed Session): Session I

The class of semiconducting oxides includes low temperature processed amorphous thin films for bendable electronics and display technology as well as highly crystalline materials such as the wide band group-III sesquioxides being interesting for UV and DUV photo sensors, power electronics and even memristors. This session sets a focus on physical properties of such oxides, their growth methods and heterostructures for demonstrator devices. This focus session is supported by the Leibniz ScienceCampus GraFOx.

Organized by

Dr. Karsten Fleischer School of Physics, Trinity College Dublin, the University of Dublin Dublin 2, Ireland

Dr. Holger von Wenckstern Universität Leipzig Felix-Bloch-Institut für Festkörperphysik Halbleiterphysik Linnéstraße 5 04103 Leipzig, Germany

Prof. Dr. rer. nat. Holger Eisele Experimental Physics Technische Universität Berlin Department for Mathematics and Science Institute of Solid State Physics Hardenbergstr. 36, Sekr. EW 4-1, D-10623 Berlin, Germany

Dr. Oliver Bierwagen Paul-Drude-Institut für Festkörperelektronik (PDI) Hausvogteiplatz 5-7 10117 Berlin, Germany

Time: Monday 9:30–13:15 Location: E 020

DS 3.1 Mon 9:30 E 020

Switching kinetics of VCM-based resistive memories at ultrafast time scales — •Moritz von Witzleben[1], Viktor Havel[1], Karsten Fleck[1], Andreas Kindsmüller[1], Rainer Waser[1,2], Stephan Menzel[2], and Ulrich Böttger[1] — [1]Institut für Werkstoffe der Elektrotechnik II, RWTH Aachen University, 52064 Aachen, Germany — [2]Peter Grünberg Institut (PGI 7), Forschungszentrum Jülich, 52425 Jülich, Germany

Redox-based resistive memories (ReRAM) are likely to overcome the challenges that nowadays memories are facing as they show auspicious properties regarding switching times, scaling, retention and endurance. For their application, fast switching times are mandatory for the writing process whereas their resistive state must be retained during many read-out operations. This issue is known as voltage-time dilemma and can be overcome by an extremely nonlinear correlation between the switching time and the applied voltage. Therefore, the switching kinetics of $Pt/Ta_2O_5/Ta$ and $Pt/ZrO_2/Ta$ VCM cells are measured over almost 15 orders of magnitude between 10^4 s and 120 ps. The ReRAM cells were incorporated in coplanar waveguide (CPW) structures to provide proper impedance matching at the contact surfaces. Our results indicate that the voltage-time dilemma can be addressed with VCM cells. Furthermore, the switching kinetics at time scales below 10 ns are not limited by conduction mechanisms or electrochemical reactions in the oxide layer or at its interfaces, but RC times play a decisive role due to the capacities of the CPW structure.

DS 3.2 Mon 9:45 E 020

Memsensors: How to design devices with enhanced capabilities in neuromorphic engineering — •Alexander Vahl[1], Jürgen Carstensen[2], Sören Kaps[2], Oleg Lupan[2], Thomas Strunskus[1], Rainer Adelung[2], and Franz Faupel[1] — [1]Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Multicomponent Materials, Kaiserstr. 2, 24143, Kiel, Germany — [2]Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Functional Nano Materials, Kaiserstr. 2, 24143 Kiel, Germany

Memsensors are a class of devices combining resistive switching and sensing properties. Apart from their inherited properties, pinched I-V hysteresis and stimulus dependent resistivity, memsensors have the capability to adapt to an external stimulus. This adaptation shows striking similarities to adaptation in biological neuronal systems, making memsensors ideal candidates for applications in neuromorphic engineering. In addition, the resistive switching is strongly dependent on the external stimulus. We propose a simple equivalent circuit containing two memristors, one in parallel and one in series to a linear sensor. This model allows to understand a multitude of experimental findings and implies a large predictive power for further optimization of memsensing devices and their application in neuromorphic engineering. Based on the model and experimental findings we propose design rules for memsensors that will facilitate further research on memsensitive systems.

DS 3.3 Mon 10:00 E 020

Defect Investigation of $CuBi_2O_4$ Photocathodes for Solar Water Splitting — •Michael Sahre, Marlene Lamers, Matthias Müller, Fatwa F. Abdi, and Roel van de Krol — Institute for Solar Fuels, Helmholtz-Zentrum Berlin, Berlin, Germany

The rise of global warming requires the development of novel sustainable carbon-free energy sources. One promising method is by directly converting water into hydrogen and oxygen using sunlight; the process is usually called "solar water splitting". In such process, a semiconductor is used to absorb the light, separate the photo-generated charge carriers, and produce hydrogen and/or oxygen on its surface. A promising candidate as the semiconductor is $CuBi_2O_4$ due to its suitable bandgap of 1.8 eV (theoretical solar-to-hydrogen efficiency of 24 %) and favorable band positions.[1,2] However, poor charge carrier transport and surface charge transfer limit the photocurrent.[2]

In this work, we attempt to alleviate the above-mentioned limitations by modulating the defects in $CuBi_2O_4$ thin films through various annealing conditions. Time resolved microwave conductivity measurements show an improved charge carrier transport after the high temperature annealing. Simultaneously, this treatment leads to a surface modification and enhanced electron transfer from the semiconductor into the electrolyte, so that the AM1.5 photocurrent is significantly increased. The interplay between the annealing condition, defect formation and photoelectrochemical performance will be discussed.

[1] Chen *et al.*, *J. Mater. Res.* 25 (2010) 3
[2] Berglund *et al.*, *Chem. Mater.* 28 (2016) 4231

DS 3.4 Mon 10:15 E 020

A pulsed laser deposition technique to control the composition of ternary thin films in growth direction demonstrated on the $Mg_xZn_{1-x}O$ alloy — •Max Kneisz, Philipp Storm, Gabriele Benndorf, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Leipzig, Germany

In conventional pulsed laser deposition (PLD) a continuous variation of the composition of ternary thin films in growth direction is not possible since the number of discrete alloy combinations is limited by the amount of targets which can be mounted in the setup. We therefore propose a technique using only a single elliptically-segmented target with two regions of different composition. We control the Mg/Zn ratio of the thin films by varying the radial position of the PLD laser spot on the target and thereby changing the ratio of the path lengths of the laser spot in the different regions. In analogy to our approach for lateral continuous composition spreads [1] (lateral CCS), we call this method vertical CCS. We will show that we are able to control the composition of $Mg_xZn_{1-x}O$ thin films in growth direction quasi continuously or stepwise. Therefore films with varying single Mg-contents are grown using the new technique on highly conductive ZnO:Al buffer

layers. The Mg-content in the films is determined by low temperature photoluminescence spectroscopy. The structural and optical quality is similar to films grown via conventional PLD.
[1] H. von Wenckstern *et al.*, CrystEngComm **15**, 10020 (2013)

DS 3.5 Mon 10:30 E 020

Considerations in the Stability of Multicomponent Oxide Alloys — •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]Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland

Identification of stable crystalline materials for a mixture of two (three) components requires examination of the lowest free energy of approximately 2^N (3^N) configurations, where N is the number of atoms in the unit cell. Cluster expansion-based energy functions offer a numerically efficient approach for estimating the stability of new potential alloys. Combining this approach with the nested sampling algorithm, which is a Bayesian Markov chain Monte Carlo method, allows for a one-shot calculation of the phase diagram as a function of composition and temperature. Our results for stable ternary and quaternary mixtures in various crystalline symmetries of group-III oxides with the formula $(In_xGa_yAl_z)_2O_3$ where $x+y+z=1$ will be presented. The key aspects that determine the stability of these materials will be discussed. 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 3.6 Mon 10:45 E 020

Influence of nitrogen annealing on the properties of spray pyrolysis grown In-doped ZnO thin films — Dilawar Ali[1,2], Muhammad Z. Butt[1], David Caffrey[2], Igor V. Shvets[2], and •Karsten Fleischer[2] — [1]Department of Physics and Centre for Advanced Studies in Physics, GC University Lahore-54000, Pakistan — [2]School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Dublin 2, Ireland

The properties of a low cost transparent conducting oxide (TCO) – spray pyrolysis grown ZnO thin films doped with indium have been investigated. We analyze the optical, electrical, and crystallographic properties as function of In content with a specific focus on post-growth heat treatment of these thin films at 320°C in an inert, nitrogen atmosphere, which remarkably improves the films electrical properties. The effect was found to be dominated by nitrogen induced grain boundary passivation, identified by a combined study using in-situ resistance measurement upon annealing, X-ray photoelectron spectroscopy, photoluminescence and X-ray diffraction studies. We also highlight the chemical mechanism of morphologic and crystallographic changes found in films with high indium content. In optimized growth and post-annealing conditions, ZnO:In with a resistivity as low as $2\times10^{-3}\,\Omega$cm and high optical quality has been obtained using low cost spray pyrolysis.

DS 3.7 Mon 11:00 E 020

Modulation of the In_2O_3 surface electron transport properties by acceptor doping — •Alexandra Papadogianni[1], Julius Rombach[1], Theresa Berthold[2], Stefan Krischok[2], Marcel Himmerlich[2], and Oliver Bierwagen[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5–7, 10117 Berlin, Germany — [2]Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, PF 100565, 98684 Ilmenau, Germany

In_2O_3 is a natively *n*-type transparent semiconducting oxide possessing a surface electron accumulation layer (SEAL) like several other relevant oxides, such as SnO_2 and ZnO. While the SEAL is within the core of In_2O_3-based conductometric gas sensors, it hinders numerous applications of In_2O_3 in electronic devices that require the formation of Schottky contacts. Tunability of the SEAL is hence necessary to unlock the entire spectrum of possible device applications of In_2O_3.
Oxygen plasma treatment of the In_2O_3 surface has been previously shown to effectively deplete surface electrons. Annealing the material, however, has been proven to reverse this effect, which renders this solution unsuitable for devices operating at elevated temperatures. As an alternative, we demonstrate strong reduction of the SEAL by doping with the deep compensating acceptors Mg and Ni performing X-Ray Photoelectron Spectroscopy (XPS) and transport measurements on high quality single-crystalline In_2O_3(111) films grown by plasma-assisted molecular beam epitaxy (PA-MBE). This method also allows for fine-tuning of the electrical transport properties of the SEAL through controllably selecting its degree of depletion.

15 min. break.

DS 3.8 Mon 11:30 E 020

Confining memristive filaments in TiO_2 thin films by Au nanoparticles — •Christian Rodenbücher[1], Nabeel Aslam[1], Dominik Wrana[1,2], Hehe Zhang[1], Hongchu Du[1], Michael Prömpers[1], Dirk Mayer[1], and Susanne Hoffmann-Eifert[1] — [1]Forschungszentrum Jülich, ER-C, ICS, PGI, and JARA-FIT — [2]Jagiellonian University, Institute of Physics, Krakow

The memristive effect in transition metal oxides has attracted much attention promising the design of fast non-volatile and energy-efficient memory devices which additionally would offer the opportunity of hardware-based neuromorphic computing. On the nanoscale, the underlying resistive switching effect was found to be related to conducting filaments evolving during an initial electroforming step. In order to improve the performance of the memristive devices, a control of the filament formation is of high importance. Here, we follow the approach of introducing Au nanoparticles at the Pt/TiO_2 interface of ALD-grown films. Using local-conductivity atomic force microscopy (LC-AFM) we show that the conductivity through the TiO_2 above the nanoparticles is significantly higher than above the surrounding Pt-coated substrate which can be attributed to the different material properties of the two metals (here Au and Pt) forming the interface to the oxide layer. Hence, Au nanoparticles can be used to determine the position of conducting paths as origin for filament formation on the nanoscale. We employ this effect to build up Pt/TiO_2/Pt nanocrossbar devices with embedded Au nanoparticles showing enhanced switching characteristics with significantly reduced forming voltage.

DS 3.9 Mon 11:45 E 020

Epitaxial Stabilization of NbO_2 on TiO_2(110) — •Jos Emiel Boschker[1], Saud Bin Anooz[1,2], Benjamin Kalas[3], Toni Markurt[1], Manfred Ramsteiner[4], Sverre Vegard Pettersen[5], Jostein Kvaal Grepstad[5], Martin Albrecht[1], Péter Petrik[3], and Jutta Schwarzkopf[1] — [1]Leibniz Institute for Crystal Growth, Max-Born-Str. 2, Berlin, D-12489, Germany — [2]Physics Department, Faculty of Science, Hadhramout University, Mukalla, 50511, Yemen — [3]Institute of Technical Physics and Materials Science, Konkoly-Thege Rd. 29-33, 1121 Budapest, Hungary — [4]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, Berlin, D-10117, Germany — [5]Department of Electronic Systems, Norwegian University of Science and Technology, Trondheim, Norway

Niobium oxides have promising physical properties that can be exploited in electronic devices, such as selector and memory devices. Moreover, NbO_2 has attracted considerable scientific interest, as it exhibits a semiconductor-metal transition at 1080K. However, the lack of high quality material complicates fundamental studies of their properties. In this paper, we report on the epitaxial stabilization of NbO_2 thin films grown on TiO_2 substrates by pulsed laser deposition. The anisotropic properties of films grown at different substrate temperatures were determined by various structural and optical methods. The results indicate a phase transition from the rutile structure to a distorted rutile structure with decreasing substrate temperature.

DS 3.10 Mon 12:00 E 020

Characterization of the dielectric function of $RScO_3$ type scandates — •Sergey Kuznetsov[1,2], Martin Feneberg[1], and Rüdiger Goldhahn[1] — [1]Institute of Experimental Physics, Otto-von-Guericke University Magdeburg, Germany — [2]Drexel University Department of Physics, Philadelphia, USA

Due to their high energy band gap and their structural stability towards temperature differences, wide-gap Perovskite structured oxides of type $RScO_3$ are promising candidates for replacing SiO_2 as high-k gate dielectrics. These Sc-based crystals are also among best available bulk substrates for the epitaxial growth of high-quality ferroelectric thin films, however, only limited data on their optical properties is available. Here, we present the results of spectroscopic ellipsometry from the infrared (0.04eV) up to the ultraviolet (6.6eV) at room temperature on $SmScO_3$, $GdScO_3$, $TbScO_3$, and $DyScO_3$ bulk single-crystals. The purpose of the experiments was to determine the in-plane components of the real and imaginary dielectric functions (DF). The analysis revealed 4 phonon modes in the extraordinary DF, and 8 to

9 modes in the ordinary DF. The phonon frequencies are observed to shift systematically with the atomic mass of the rare earth component of the perovskites. This effect was observed in the ordinary and extraordinary DF. Data obtained also indicate the onset of interband absorption at 6 ± 0.1 eV for $GdScO_3$ and $DyScO_3$, and at 5 ± 0.1 eV in the $SmScO_3$ and $TbScO_3$, with a local maximum at 5.4 eV prior to exhibiting similar behavior to the other two samples. A comprehensive overview of the anisotropic dielectric functions will be shown.

DS 3.11 Mon 12:15 E 020

Ferro- and antiferroelectricity in oxygen defficient hafnia and zirconia — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Conventional perovskite ferroelectrics as materials for ferroelectric RAM (FeRAM) suffer from poor CMOS-compatibility and limited scalability. In this sense, the discovery of ferroelectricity in Si:HfO_2 thin films [1] opens new prospectives for HfO_2-based materials because they are CMOS-compatible, and the robust ferroelectric behavior scales down to a film thickness below 10 nm. Recent discovery of ferroelectricity in undoped HfO_2 [2] emphasizes the importance of oxygen deficiency for the desired ferroelectric properties and the quest for a better microscopic understanding.

We present results of our Density Functional Theory combined with an evolutionary algorithm [3] based study of metastable structures in Hf-O and Zr-O solid solutions. We will show suboxides of HfO_2 and ZrO_2, which simultaneously possess a resistive switching capability and (anti)ferroelectricity, i.e. both properties originate from the same structures. We will discuss a possible origin of the ferro-antiferroelectric crossover, observed in $Hf_xZr_{1-x}O_2$ thin films [4].

We acknowledge the support by DFG via SFB 917 "Nanoswitches".
[1] T. Böscke et al, Appl. Phys. Lett. **99**, 102903 (2011); [2] P. Polakowski, J. Müller, Appl. Phys. Lett. **106**, 232905 (2015); [3] http://uspex.stonybrook.edu; [4] J. Müller et al, Nano Lett. **12**, 4318 (2012).

DS 3.12 Mon 12:30 E 020

Direct imaging of reversible massive oxygen transport induced by ionic liquid gating and creation of meso-structures — •Bin Cui, Peter Werner, Tianping Ma, and Stuart Parkin — Max Planck Institute for Microstructure Physics, 06120 Halle, Germany

Ionic liquid (IL) gate induced oxygen migration at the surface of oxide thin films has been proposed to be a powerful tool for manipulating their bulk electronic properties and structures. Advancements in this direction requires an in-depth understanding of the correlation between oxygen transport manner, atomic-scale structural transition, and macroscopic physical responses under IL gating.

Here we directly image the processes of oxygen transport, using in-situ gating, within a TEM, as we induce the transformation between brownmillerite SrCoO2.5 and perovskite SrCoO3. A massive ~0.5 oxygen per formula unit, is observed to be reversibly extracted or injected over several minutes. These changes are consistent with vertical oxygen transport perpendicular to the thin film surface on nanoscale, and lateral transport parallel to the surface on microscale.

Using IL gating through lithographically patterned orifices in resist at the surface of various oxide films with different anisotropic oxygen transport, we show that various three-dimensional metallic structures such as cylinders and rings can be realized.

Our results not only reveal the oxygen transport manner in IL gating, but also provide a roadmap to the complex meso-structures construction in ion-transporting materials from their exterior surfaces.

DS 3.13 Mon 12:45 E 020

Room temperature fabricated all-oxide junction field-effect transistors and inverters on rigid and flexible substrates — •Peter Schlupp, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Leipzig, Germany

Room temperature (RT) fabrication of electronic devices saves energy within the fabrication process and enables the usage of thermally unstable but flexible substrates. One material class that can be fabricated at RT showing promising properties are amorphous (or nanocrystalline) oxide semiconductors (AOS). The most commonly used n-type AOS is indium gallium zinc oxide which is already successfully used as channel material in pixel drivers for active matrix displays [1]. However, because indium is rare and expensive we use n-type zinc tin oxide (ZTO) as channel layer material which shows easily controllable electrical properties [2,3].

We present junction field-effect transistors (JFETs) using p-type amorphous zinc cobalt oxide and nanocrystalline nickel oxide as gate diodes. The ZTO films were grown by magnetron sputtering on glass and flexible polyimide while the p-type layers were grown by pulsed laser deposition. The characteristics of the JFETs and inverters based on them fabricated on both substrates will be discussed. Additionally, their changes after bending the flexible samples will be presented.

[1] Wellenius *et al.*: J. Display Technol. **5**, 438 (2009)
[2] Jayaraj *et al.*: J. Vac. Sci. Technol. B, **26(2)**, 495 (2008)
[3] Schlupp *et al.*: MRS Proceedings **1633**, 101 (2014)

DS 3.14 Mon 13:00 E 020

Surface hole accumulation layer in NiO created by oxygen plasma treatment — •Melanie Budde[1], Carsten Tschammer[1], Theresa Berthold[2], Marcel Himmerlich[2], Stefan Krischok[2], and Oliver Bierwagen[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany. — [2]Institut für Physik und Institut für Mikro- und Nanotechnologien MacroNano, Technische Universität Ilmenau, PF 100565, 98684 Ilmenau, Germany.

Nickel oxide (NiO) is a transparent and semiconducting p-type oxide, which is interesting for various applications, for example photovoltaics, diodes or other electronic devices. However, our high quality NiO layers grown by plasma-assisted MBE are semi-insulating with sheet resistances above 109Ω. Doping of NiO, for example with Lithium, is known to increase its p-type bulk conductivity. In this contribution, we demonstrate the formation of a surface hole accumulation layer generated by oxygen plasma treatment and characterize its conductivity. For this purpose, MBE grown NiO layers on MgO(100) are modified by an oxygen plasma process after growth. The sheet resistance was measured by Van-der-Pauw measurements and a p-type conductivity was confirmed by Seebeck measurements. Furthermore, the results allowed to determine the approximate hole concentration. X-ray photoelectron spectroscopy (XPS) demonstrates a shift of the surface Fermi level towards the valence band maximum, corroborating the formation of a surface hole accumulation layer. The results are compared to published data on p-doped NiO.

DS 4: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials I (joint session O/MM/DS/TT/CPP)

Exploring, understanding, and describing materials with strong electronic Coulomb correlations remain among the big challenges of modern condensed matter physics. Correlated materials are characterized by an extreme sensitivity to external probes such as pressure or temperature, and slight changes in composition, constraints during the growth process (e.g. by heterostructuring) or off-stoechiometries can significantly alter their properties. While the invited lectures will have a focus on correlated electron materials, the symposium will cover the general field of computational materials science and electronic-structure theory.

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Time: Monday 10:30–13:00 Location: HL 001

DS 4.1 Mon 10:30 HL 001

How Derivative Discontinuities in the Energy Yield Interatomic Steps in the Exact Kohn-Sham Potential of Density-Functional Theory — •Eli Kraisler[1], Matthew J. P. Hodgson[1], Axel Schild[2], and Eberhard K.U. Gross[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany — [2]Laboratorium für Physikalische Chemie, ETH Zürich, Switzerland — [3]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Israel

Accurate density-functional calculations hinge on reliable approximations to the unknown exchange-correlation (xc) potential. The most popular approximations usually lack features of the exact xc potential that are important for an accurate prediction of the fundamental gap and the distribution of charge in complex systems. Two principal features in this regard are the spatially uniform shift in the potential, as the number of electrons infinitesimally surpasses an integer, and the spatial steps that form, e.g., between the atoms of stretched molecules. Although both aforementioned concepts are well-known, the exact relationship between them remained unclear. In this talk, we establish this relationship and introduce a new concept: the charge-transfer derivative discontinuity, Δ^{CT}. By numerically solving the many-electron Schrödinger equation, we extract the exact Kohn-Sham potential and directly observe its features, particularly the spatial interatomic steps. For the first time, spatial steps in the exact xc potential of a full configuration-interaction (FCI) calculation of a molecule are presented in three dimensions.

DS 4.2 Mon 10:45 HL 001

Steps in the exact Kohn-Sham potential of ensemble density-functional theory for excited states and their relation to the derivative discontinuity — •Matthew J. P. Hodgson[1], Eli Kraisler[1], Michael T. Entwistle[2], Axel Schild[3], and Eberhard K. U. Gross[1,4] — [1]MPI für Mikrostrukturphysik, D-06120 Halle, Germany — [2]Dep. of Physics, Uni. of York, Heslington, YO10 5DD, UK — [3]Lab. für Physikalische Chemie, ETH Zürich, 8093, Switzerland — [4]Fritz Haber Center for Molecular Dynamics, The Hebrew University of Jerusalem, 91904, Israel

An accurate approximation to the exchange-correlation (xc) part of the Kohn-Sham (KS) potential is essential for any density-functional calculation. Understanding the behaviour of the exact xc potential and developing improved approximations to it are crucial. The focus of calculations within density functional theory is usually on the ground state. However, knowledge of how the system responds to an excitation is important. In this talk we present the exact KS potential of an ensemble of the ground state and the first excited state of a 1D diatomic molecule. For this system, upon excitation, a small amount of charge transfers from one atom to the other. In the corresponding exact ensemble xc potential we find two plateaus: one that forms around the nucleus of the acceptor atom, associated with the derivative discontinuity of that atom, and another that forms around the donor atom and corresponds to a new phenomenon which we term the 'charge-transfer derivative discontinuity'.

DS 4.3 Mon 11:00 HL 001

Koopmans-compliant functionals: A reliable and efficient tool for the prediction of spectroscopic quantities — •Nicola Colonna[1], Ngoc Linh Nguyen[1], Andrea Ferretti[2], and Nicola Marzari[1] — [1]THEOS and MARVEL, EPFL, Lausanne, Switzerland — [2]Centro S3, CNR-Istituto Nanoscienze, Modena, Italy

Commonly used approximate density functionals produce total energies that do not exhibit the expected piecewise-linear behavior as a function of the particle number, leading to a discrepancy between total and partial electron removal/addition energies and poor predictive capabilities of ionization potentials. Koopmans-compliant functionals enforce a generalized criterion of piecewise linearity in the energy of any approximate density functional with respect to the partial removal/addition of an electron - i.e., with respect to charged excitations - from/to any orbital of the system. When used to purify approximate density functionals, Koopmans' corrections lead to orbital-density dependent functionals and potentials that are able to deliver accurate spectroscopic properties. As an example, ionization potentials of a large set of molecules (the GW100 test set), photoemission spectra of organic donors and acceptors and band gaps of 35 semiconductors and insulators are presented, showing very good agreement with experiment or higher-order theories. Being this a functional framework, the straightforward advantages are that forces and other derivatives are also readily accessible, that the computational costs are much reduced, and the numerical parameters are those typical of DFT calculations.

DS 4.4 Mon 11:15 HL 001

Selfconsitent density embedding - a new class of functionals for DFT — •Uliana Mordovina[1], Teresa E. Reinhard[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

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

The proposed density-embedding scheme serves as functional in DFT, which, unlike in usual DFT, can be systematically improved by increasing the size of the active space.

We show convergence toward exact results for 1D systems as well as results for 2D systems.

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

DS 4.5 Mon 11:30 HL 001

Pressure dependence of the effective screened Coulomb interactions in transition metal monoxides — •Swarup Kumar Panda[1], Hong Jiang[2], and Silke Biermann[1,3] — [1]Centre de Physique Théorique, Ecole Polytechnique, France — [2]College of Chemistry and Molecular Engineering, Peking University, China — [3]Collège de France, Paris, France

In transition metal compounds, the magnitudes of the effective Coulomb interaction parameters (Hubbard U) and their pressure dependence are of utmost importance in any realistic many-body simulations for describing their pressure driven insulator-metal transition. One of the powerful methods for calculating the Hubbard U from first

principles is based on linear response theory within the constrained random-phase approximation (cRPA) [1], which provides the full U matrix including off-site elements and its frequency dependence. In this presentation, we apply this method (in its implementation into the Wien2k code [2]) to the transition metal monoxides (FeO, CoO, NiO, and CuO) [3]. Although the pressure induced changes in the bare Coulomb interactions are negligible, the effective screened U grows monotonically with increasing pressure for all of the above monoxides. Finally, I will argue that neither the pressure dependence nor the frequency dependence of U should be ignored in a reliable theoretical description of correlated oxides.

References: [1] Aryasetiawan et al., PRB 70, 195104 (2004) [2] Vaugier et al., PRB 86, 165105 (2012) [3] Panda et al., PRB 96, 045137 (2017)

DS 4.6 Mon 11:45 HL 001

Self-Interaction Corrected SCAN for Molecules: All-Electron Implementation with Numerical Atom-Centered Basis Functions — •Sheng Bi, Igor Ying Zhang, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

The self-interaction error (SIE) is a well-known problem in all semilocal density-functional approximations (DFAs), including the recently proposed "strongly constrained and appropriately normed" (SCAN) functional [1]. The so-called self-consistent Fermi-orbital SIC (FSIC) algorithm proposed by Pederson *et al.* [2] shows promising potential to eliminate the self-interaction error in semilocal approximations, which has been demonstrated for the local-spin-density approximation (LSDA) in a study of molecules.

We present an all-electron implementation of the self-consistent FSIC approach on the SCAN method [1]. Beside a systematic benchmark with respect to a selected molecular test set, we examine the performance of FSIC-SCAN in predicting the geometry of Pentacene, which is a well-documented challenge for standard semilocal DFAs [3]. Finally, we briefly discuss our ongoing work concerned with the implementation of the all-electron FSIC-SCAN approach for solids.

[1] J. Sun, A. Ruzsinszky, and J. P. Perdew, *Phys. Rev. Lett.* **115**, 036402 (2015).
[2] M. R. Pederson and T. Baruah, *Advances In Atomic, Molecular, and Optical Physics* **64**, 153 (2015).
[3] M. R. Pederson, T. Baruah, D. you Kao, and L. Basurto, *The Journal of Chemical Physics* **144**, 164117 (2016).

DS 4.7 Mon 12:00 HL 001

Progress in Fermi-Löwdin orbital self-interaction correction to DFT — •Torsten Hahn[1], Sebastian Schwalbe[1], Simon Liebing[1], Mark Pederson[2], and Jens Kortus[1] — [1]TU Freiberg, Institute for Theoretical Physics, Germany — [2]Johns Hopkins University, Department of Chemistry, USA

The accuracy of density functional theory (DFT) calculations is limited by the so called self-interaction error [1]. The recently proposed Fermi-Löwdin orbital based method [2,3,4] for self-interaction correction (FLO-SIC) is a unitary invariant and size extensive approach to overcome this error. We present the current state of the method and discuss the performance of FLO-SIC DFT applied to atoms and molecules in combination with different exchange-correlation functionals. In addition, this method delivers a description of the chemical bonding as intuitive as Lewis theory that may bridge the gap between DFT and chemical intuition.

[1] J. P. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)
[2] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
[3] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)
[4] T. Hahn et. al., J. Chem. Phys., vol- 143, 224104 (2015)

DS 4.8 Mon 12:15 HL 001

First-principles modeling of mixed-valence compounds from extended Hubbard-corrected functionals — •Matteo Cococcioni and Nicola Marzari — Theory and Simulations of Materials and MARVEL, EPFL, Lausanne, Switzerland

Modeling the electronic properties of mixed valence compounds is central to developing many materials of technological relevance. Unfortunately, most approximate implementations of density functional theory (DFT) fail in capturing the localization of valence electrons on low dispersion states (e.g., of d or f kind) and mis-represent many properties of these systems. Quantitatively predictive first-principles calculations thus require, for these systems, the use of corrective functionals able to improve the description of electronic localization. Using the results of a recent study on materials for cathodes of Li-ion batteries this work shows how an extended Hubbard correction to DFT functionals, including on-site (U) and inter-site (V) interactions (named DFT+U+V) improves considerably on simpler approximations for electronic, magnetic and structural properties and correctly describes localized states even in presence of significant inter-site hybridization. The work also demonstrates that evaluating the effective interaction parameters (U and V) consistently with the electronic and crystal structures, and treating them as material-specific quantities, improves the prediction of thermodynamic quantities and of average voltages. Finally, a novel method to compute these interactions from density-functional perturbation theory is shown to guarantee unprecedented efficiency, accuracy and convergence control.

DS 4.9 Mon 12:30 HL 001

A Kohn-Sham type construction on a lattice with the exact kinetic energy density — •Iris Theophilou[1], Michael Ruggenthaler[1], Florian Buchholz[1], Florian Eich[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

In this presentation we explore a possible formulation of ground state Density Functional Theory by introducing the kinetic energy density as basic quantity in addition to the density. We presently restrict this formulation to the lattice case, and show that for a few site Hubbard interacting model it is numerically feasible to find an equivalent non-interacting system that yields the same density and kinetic energy density. By finding such a non-interacting system we mean here finding the local/on site potential and the non-local site dependent hopping that will give the target density and kinetic energy density. Our hope is that by including the kinetic energy density we will facilitate the functional construction and also put into grounds already existing approximations based on this quantity.

DS 4.10 Mon 12:45 HL 001

Small-Polaron Formation in Polymorphs of Ga_2O_3 and TiO_2 — •Sebastian Kokott, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin 14195, Germany

Transparent oxides are key materials for new devices in photovoltaics and electronics. One important factor influencing the behavior of charge carriers in these materials is the interaction with polar phonon modes. We focus on materials with strong electron-phonon coupling, where small polarons are formed. Although, density-functional theory (DFT) is often used for calculating polaron properties, there are two challenges: Sensitivity of the calculated properties to the errors in exchange-correlation treatment, and finite-size effects in supercell calculations. We have developed an approach [1] to address these issues. The polaron properties are obtained using a modified neutral potential-energy surface from DFT [2]. Based on Pekar′s model [3], we correct for the proper elastic long-range behavior of the polaron in a supercell. With this approach, the influence of the crystal structure on the polaron properties is investigated for rutile and anatase TiO_2, and for the monoclinic β– and orthorhombic ε–Ga_2O_3. We find that in rutile TiO_2 only small electron polarons are stable, while only small hole polarons are found in anatase. On the contrary, small hole polarons exist in both Ga_2O_3 polymorphs but have significantly different binding energies.

[1] S. Kokott, arXiv:1710.03722 (2017)
[2] B. Sadigh et al., Phys. Rev. B **92**, 75202 (2015)
[3] S. I. Pekar, Zh. Eksp. Teor. Fiz. **16** 335 (1946)

DS 5: Layer Deposition (ALD, MBE, Sputtering, ...)

Time: Monday 11:45–13:15 Location: H 0111

DS 5.1 Mon 11:45 H 0111

Atomic Layer Deposition of Titanium Nitride Thin Films for Plasmonic Applications — •Gül Dogan, Umut T. Sanli, Gisela Schütz, and Kahraman Keskinbora — MPI for Intelligent Systems, Stuttgart

Titanium Nitride (TiN) emerged as an alternative to gold as a material for refractory plasmonics, mainly due to their similar optical responses in the visible and near-infrared regions. Atomic Layer Deposition (ALD) offers highly conformal coatings over complex geometries, accurate thickness, atomic smooth interfaces and composition control. Here, we deposited TiN thin films at 350 °C by a plasma-enhanced (PE)-ALD, using TiCl4 and N2-H2 as co-reactants. The deposition rate was 0.03 nm/cycle. The prepared polycrystalline films exhibited a strong (200) preferred orientation. The XPS analysis indicated that the Cl impurity concentration was ~4 at. % and the atomic ratio of Ti to N was ~1:1. A low resistivity of 290 uohm.cm was measured by Four Point Probe (FPP). The optical-resistivity values were determined via Spectroscopic Ellipsometry using a Drude-Lorentz model, which were in agreement with FPP measurements, for ~10 nm grain size. When the grain size was <10 nm, large deviations were observed between optical and electrical resistivity measurements, which was attributed to electron scattering at grain boundaries. Low electrical resistivity in combination with a high carrier concentration and carrier mobility are two important parameters for plasmonic applications. Furthermore, a discrepancy between optical and electrical measurements is a reliable indicator of grain boundary scattering.

DS 5.2 Mon 12:00 H 0111

Atomic Layer Deposition of Iridium: Nucleation and Film Growth — •Paul Schenk[1,2] and Adriana Viorica Szeghalmi[1,2] — [1]Fraunhofer-Institute for Applied Optics and Precision Engineering IOF, Albert-Einstein-Straße 7, D-07745 Jena, Germany — [2]Friedrich-Schiller-University Jena, Institute of Applied Physics, Albert-Einstein-Straße 15, D-07745 Jena, Germany

Ultrathin and smooth metal films are essential for numerous optical systems for spectroscopy and sensing in material, life sciences and astronomy, lightning or automobile components, and other applications. Complex shaped substrates or nano- and microstructured components are increasingly necessary in modern applications. However, the conformal deposition of thin metal layers on such elements, using established coating technologies such as physical vapor deposition (PVD), is challenging. In contrast, atomic layer deposition (ALD) is a highly suitable coating technology for the uniform deposition of thin films onto complex shaped surfaces.

Iridium thin films are of interest for applications in broadband metal wire grid polarizers, mirrors and Fresnel zone plates, or even for medical implants. It is essential to control their morphology and topography as well as the mechanical and optical properties to enable components with a high performance. Therefore, one needs to understand the layer growth from the initial nucleation to the formation of a dense and compact thin metal film. In the presented work, we studied the nucleation and film growth of iridium thin films on various substrate materials with regard to their morphology and properties.

DS 5.3 Mon 12:15 H 0111

Energy and mass selective ion beam assisted epitaxy for deposition of thin nitride films — •Philipp Schumacher[1], Michael Mensing[1], Jürgen W. Gerlach[1], Stephan Rauschenbach[2,3], and Bernd Rauschenbach[1] — [1]Leibniz-Institut für Oberflächenmodifizierung (IOM), Leipzig — [2]University of Oxford, UK — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart

Ion-beam assisted deposition (IBAD) represents a frequently applied concept in thin film growth. For hyperthermal kinetic energies (few 1 eV-few 100 eV), the impinging ions provide energy for enhancing the mobility of adatoms, ideally only on the surface. Thus, ion irradiation induced creation of point defects below the surface is minimized. Therefore, IBAD using hyperthermal ions can be applied for growing thin films, for which a high crystalline quality is required. In general, the versatility of IBAD is limited depending on the type of ion source applied. Typical ion sources generate ion beams which contain a multitude of different ion species, each possessing certain kinetic energies, which are possibly different from one another. In order to define the deposition conditions more precisely, a setup for energy and mass selective ion beam assisted deposition (EMS-IBAD) was created, to be used for the deposition of nitride thin films. The feasibility of EMS-IBAD by applying this setup has exemplarily been shown for the growth of non-polar GaN thin films on $Al_2O_3(1\bar{1}02)$. In this contribution, the EMS-IBAD setup is presented, subsequently a brief characterization of such thin films by x-ray diffraction and reflection high-energy electron diffraction is added.

DS 5.4 Mon 12:30 H 0111

Modifying the texture of epitaxially grown chalcogenide thin films — •Marc Pohlmann, Marvin Kaminski, and Matthias Wuttig — I. Institute of Physics, Physics of New Materials, RWTH Aachen University, 52056 Aachen, Germany

A significant number of chalcogenides offers a unique portfolio property. They can be rapidly switched between the amorphous and crystalline state. This transition is accompanied by large changes in optical and electrical properties, which creates significant application opportunities. Hence, these materials are employed for rewriteable optical data storage and have also recently been introduced as electronic phase change memory devices, trying to close the gap between non-volatile but slow devices (such as Flash memories) and volatile but extremely fast devices, like DRAMs. To improve the application range of these materials, it is mandatory to further improve phase change devices. A promising route to do so is via material optimization. This approach requires an understanding of the material properties on a very fundamental level. Therefore, in the frame of this work, we want to investigate the texture formation of different chalcogenides via RHEED and XRD to obtain MBE-grown thin films of high crystal quality. We employ heterostructures of GeTe, SnTe and Sb_2Te_3 to demonstrate how different textures and surfaces can be achieved on the same substrate.

DS 5.5 Mon 12:45 H 0111

Deposition-Flux dependent Intrinsic Film Stress: Scaling — •Marcel Rost[1], Andreas Jamnig[2], Clarisse Furgeaud[2], and Gregory Abadias[2] — [1]Huygens-Kamerlingh Onnes Laboratory, Leiden University, Leiden, The Netherlands — [2]Institut P, CNRS, Université de Poitiers, Poitiers, France

The growth of polycrystalline films at temperatures above ~0.2 of the melting temperature is accompanied by compressive stress development after film closure. A significant part of this stress has a reversible nature: it disappears when the deposition is stopped and re-emerges upon resumption. Based on the variation of the chemical potential of the surface, the grain boundaries, and the film, we have developed a thermodynamic description that predicts the magnitude of the reversible compressive stress [1], and that agrees so far with published experimental results.

Moreover, in analogy to the often observed scaling in growth phenomena, our model also predicts that the stress jumps are proportional to "deposition flux"/"surface mobility". Here we show the first experimental evidence for this scaling, which delivers additional proof for the validity of our model.

[1] A.Saedi and M.J. Rost; Nature Communications, 7:10733 (2016)

DS 5.6 Mon 13:00 H 0111

Aluminum nitride films prepared by plasma atomic layer deposition using different plasma sources — Małgorzata Kot[1], Franziska Naumann[2], Samiran Garain[1], Emilia Pożarowska[1], Hassan Gargouri[2], •Karsten Henkel[1], and Dieter Schmeisser[1] — [1]Angewandte Physik - Sensorik , Brandenburgische TU Cottbus-Senftenberg, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]SENTECH Instruments GmbH, Schwarzschildstraße 2, 12489 Berlin, Germany

Aluminum nitride (AlN) thin films are promising for versatile applications in optoelectronics, electronics, piezoelectrics, and acoustics due to their remarkable properties such as wide band gap, high dielectric constant, low electrical conductivity, good piezoelectric coefficient and high ultrasonic velocity. We present a comparative study of AlN films grown by plasma-enhanced atomic layer deposition at 350°C silicon wafers in the SENTECH SI ALD LL system using TMA and NH_3 where either a capacitively coupled plasma (CCP) or a direct PTSA (planar triple spiral antenna) source was applied. The films

were characterized by ellipsometry, XPS and electrical measurements. The layer properties are discussed concerning the varied ALD process parameters. In general, the process using the direct PTSA source delivered films with higher refractive index and better homogeneity over the wafer achieving also higher growth rates per cycle (GPC) in reduced total cycle durations. Films with refractive index in the range of 2.05 and permittivity around 8 could be realized with a GPC of 1.54 Å/cycle.

DS 6: Thin Film Applications

Time: Monday 15:00–18:15 Location: H 0111

DS 6.1 Mon 15:00 H 0111

Chalkopyrite thin film solar cells conditioned with RbF — •Tim Kodalle[1], Marc Daniel Heinemann[1], Hasan Arif Yetkin[1,2], Iver Lauermann[1], Rutger Schlatmann[1,3], and Christian Alexander Kaufmann[1] — [1]PVcomB/Helmholtz-Zentrum Berlin, Germany — [2]Technical University Berlin, Germany — [3]Hochschule für Technik und Wirtschaft Berlin, Germany

We investigate the impact of an RbF post deposition treatment (PDT) on the material and device properties of Cu(In,Ga)Se_2 thin-film solar cells in dependence of both the PDT's parameters (e.g. the duration of the PDT) and the copper to group III elemental ratio ([Cu]/([Ga]+[In]) = CGI).

A clear trade-off between increasing open-circuit-voltage (V_{OC}) and decreasing fill factor (FF) with longer RbF-deposition could be observed. We propose a model explaining the gain in V_{OC} by an increased carrier concentration and the formation of an (Rb,Na)-In_xSe_y surface layer during the PDT. Additionally we build a model to explain the decreasing FF based on the generation of additional acceptor-like defects at the buffer/window-interface by temperature-induced alkali-migration during sputtering of the window layer.

Furthermore we investigate the performance of the optimized PDT on absorbers with varied CGI. Here we find, that the PDT is most efficiently when being applied to thin films close to stoichiometry. Thereby we were able to overcome the FF-loss and increase the maximum efficiency up to 17.5%, which is about 1.1% (abs.) higher than the reference value.

DS 6.2 Mon 15:15 H 0111

Metal thin films as plasmonic support for surface enhanced vibrational spectroscopy and optofluidics — •Dimitra Gkogkou, Christoph Kratz, Norbert Esser, Eugen Speiser, and Karsten Hinrichs — Leibniz-Institut für Analytische Wissenschaften -ISAS- e.V., Department Berlin, Schwarzschildstr. 8, 12489 Berlin, Germany

We present metal nanoisland films that exhibit plasmonic resonances in the visible and infrared region of the spectrum. These different resonances correspond to adjacent areas of an Au gradient layer and provide surface enhanced Raman scattering (SERS) and surface enhance infrared absorption (SEIRA) signals, dependable on the thickness of the layer. In that way, all vibrational information of an adsorbed molecule can be acquired by a line scan on a single substrate. Also presented is the integration of this combinatorial substrate with a microfluidic setup that allows for the in-situ investigation of μL volumes. Ultra low detection limits of analytes were achieved, i.e. submonolayer sensitivity demonstrated in situ for monolayer self-assembly.

The presented optofluidic platform is a sensing device that has possible applications in sensitive and label-free biosensing, lab-on-a-chip devices, or molecular imaging tools for biochemical analyses.

DS 6.3 Mon 15:30 H 0111

Fully sprayed, ITO-free, flexible organic solar cells — •Marius Loch[1], Florin Loghin[1], Kamyar Baghvand[1], Paolo Lugli[2], and Markus Becherer[1] — [1]Lehrstuhl für Nanoelektronik, Technische Universität München, Theresienstrasse 90, 80333 Munich, Germany. — [2]Faculty of Science and Technology, Free University of Bozen-Bolzano, Universitätsplatz 5, 39100 Bolzano, Italy

Organic solar cells are a promising candidate for a future of ubiquitous, low-cost solar power harvesting. While this promise is founded on easily scalable, large-area solution processing techniques, most of the scientific research community uses small-scale deposition methods convenient for the lab like spin coating in inert atmosphere and vacuum processing, which are not scalable. In this work, we use an automated spray roboter in ambient conditions to deposit all layers of the solar cell (reflective electrode, transparent electrode, active material blend and blocking layers). The layers are independently optimized and eventually put together in one fully sprayed device. By replacing brittle and expensive indium tin oxide (ITO) with silver nanowires (AgNW) and conductive polymers (PEDOT:PSS) for the transparent electrode, the use of flexible foil substrates is enabled and mechanical stability is studied by bending tests.

DS 6.4 Mon 15:45 H 0111

Effect of cation stoichiometry on electric properties of thin-film varactors with $Ba_xSr_{1-x}TiO_3$ tunable dielectric and highly conducting $SrMoO_3$ electrodes — •Lukas Zeinar[1], Patrick Salg[1], Aldin Radetinac[1], Dominik Walk[2], Philipp Komissinskiy[1], Holger Maune[2], Rolf Jacoby[2], and Lambert Alff[1] — [1]Materials Science, TU Darmstadt, Germany — [2]Microwave Engineering and Photonics, TU Darmstadt, Germany

We present Au/Pt/$Ba_xSr_{1-x}TiO_3$/$SrMoO_3$ varactor heterostructures utilizing single crystalline $Ba_xSr_{1-x}TiO_3$ films grown epitaxially by pulsed laser deposition on a highly conducting thin*film oxide $SrMoO_3$ bottom electrodes with a room-temperature resistivity of 30 $\mu\Omega$cm. The stoichiometry of the dielectric $Ba_xSr_{1-x}TiO_3$ was tuned to achieve the desirable high tunability and low losses of the varactors at room temperature. Influence of the cation stoichiometry of the $Ba_xSr_{1-x}TiO_3$ films on their Curie temperature and room-temperature dielectric permittivity was investigated. The changes of the $Ba_xSr_{1-x}TiO_3$ out-of-plane lattice parameter by 2 % and the corresponding changes of the Ba-Sr and (Ba,Sr)-Ti cation ratios by 6 and 11 %, respectively, were observed by varying the laser energy fluence in the range between 0.3 and 1.4 J/cm^2. Tunability and leakage current of the varactors were investigated by a vector network analyzer at frequencies between 300 MHz and 10 GHz. Fine tuning of the $Ba_xSr_{1-x}TiO_3$ cation stoichiometry allows high relative tunability of the varactors up to 80 % and reduction of the varactor leakage current by up to three orders of magnitude down to 10 nA.

DS 6.5 Mon 16:00 H 0111

The Influence of Crystallographic Order on Ferrimagnetic Response of Spinel $ZnFe_2O_4$ Thin Films — •Vitaly Zviagin, Yogesh Kumar, Chris Sturm, Israel Lorite, Pablo Esquinazi, Marius Grundmann, and Rüdiger Schmidt-Grund — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstr. 5, Leipzig

We present the dielectric function of normal spinel $ZnFe_2O_4$ (ZFO) grown at different pressures and temperatures on $SrTiO_3$ (100) substrate by pulsed laser deposition. Electronic transitions visible in the diagonal element of the dielectric tensor are assigned to transitions involving Fe^{2+}, Fe^{3+} and Zn^{2+} cation 3d and 4s orbitals. Transitions from O_{2p} to tetrahedrally coordinated Fe^{3+} cation, located at $\sim$ 3.5 eV, and between octahedrally coordinated Fe^{2+} cations, located at $\sim$ 0.9 eV, give evidence to disorder in the normal spinel structure. Growth temperature dependent investigation has shown a direct correlation between saturation magnetization at 5 K and the amplitude of the former mentioned transition, likely due to the dominant nature of the oxygen mediated coupling between Fe^{3+} located on two different lattice sites.[1] Annealing films at temperatures greater than 250 °C in argon and oxygen atmospheres facilitates a decrease in the ferrimagnetic response and is explained by reordering of the disordered spinel structure toward ordered normal state. A direct correlation between the disorder cation transition contributions to the dielectric function and room temperature ferrimagnetic response is shown.
[1] V. Zviagin et al., Appl. Phys. Lett. **108**, 13 (2016)

DS 6.6 Mon 16:15 H 0111

Unsupervised Hebbian learning experimentally realized with analogue memristive crossbar arrays — •Finn Zahari, Mirko Hansen, Hermann Kohlstedt, and Martin Ziegler — Chair of Nanoelectronics, Faculty for Electrical Engineering and Information Technology, Kiel University, Germany

Memristive devices are promising candidates to emulate synaptic be-

haviour in neuromorphic circuits in an efficient manner. Even though in the last couple of years a variety of materials and device structures were employed to fabricate memristive devices, there is still a gap between promising computing schemes and their hardware realization with memristive devices. We show that so called double barrier memristive devices can be integrated into crossbar architectures without the need for additional selector devices. These ionic memristive devices show a non-filamentary interface-based resistive switching behaviour with a high I-V nonlinearity and asymmetry as well as self-rectifying and self-limitation characteristics. They are used to realize selector-device-free 16x16 crossbar-arrays with 256 memristive devices. A local Hebbian learning scheme was utilized to perform unsupervised learning of visual patterns to demonstrate the applicability of the selector-free crossbars within a mixed signal circuit consisting of double barrier memristive devices as hardware synapses und software neurons.

Financial support by the German Research Foundation through FOR 2093 is gratefully acknowledged.

15 min. break.

DS 6.7 Mon 16:45 H 0111

Bottom-up Synthesis and Characterization of Mesoporous Al-Modified Hematite Thin Film Photo-Anodes — •Ahmed Chnani and Steffen Strehle — Ulm University, Institute of Electron Devices and Circuits, Albert-Einstein-Allee 45, 89081 Ulm

Hematite (α-Fe2O3) is an earth abundant, low-cost and non-toxic n-type semiconductor being in the research focus for the assembly of efficient photo-anodes in the field of solar fuel production by water splitting. Despite a suitable band structure and sufficient water splitting stability, there are various critical issues that need to be resolved including for instance the short charge carrier lifetime that is significantly misaligned with the optical absorption length, an overall low electrical conductivity as well as a low surface charge transfer kinetics.

In this paper, aluminium is added to hematite as a sustainable strategy to reduce the defect state density while simultaneously increasing the charge carrier concentration. For the studies, thermally evaporated Fe(Al) thin films with roughly 200 nm in thickness were utilized. By rational control of a plain thermal oxidation process under ambient conditions, non-porous to mesoporous Al-modified hematite thin films were prepared. The experiments show that mesoporous thin films show not only efficient light trapping but also an overall increased electrical conductivity and an increased photoactivity in comparison to non-porous thin films, plain hematite electrodes and even in comparison to high-density hematite nanowire arrays. The complete surface band structure was reconstructed to evaluate the surface defect states by utilizing a Kelvin probe as well as ambient photoelectron spectroscopy.

DS 6.8 Mon 17:00 H 0111

Large-scale self-assembling of nanostructures by controlled dewetting of ultra-thin silicon films on insulators — •Marco Salvalaglio[1], Rainer Backofen[1], Meher Naffouti[2,3], Thomas Bottein[2], Mario Lodari[4], Thomas David[2], Abdelmalek Benkouider[2], Ibtissem Fraj[3], Luc Favre[2], Antioine Ronda[2], Isabelle Berbezier[2], David Grosso[2], Marco Abbarchi[2], Monica Bollani[4], and Axel Voigt[1] — [1]TU-Dresden, 01062 Dresden, DE — [2]CNRS - IM2NP, 13397 Marseille, FR — [3]Université de Monastir, 5019 Monastir, TN — [4]IFN-CNR, L-NESS, 22100 Como, IT

Thin solid films are rarely stable when annealed even below their melting temperature. Under the action of surface diffusion, atoms move away from the edges of thin films leading to their retraction and breaking. This process occurs in ultra-thin silicon films on insulator (UT-SOI), limiting their applications in several microsystems. Moreover, the self-assembled structures forming at the end of the process show too large randomness in positioning and size dispersion to be exploited for targeted applications. Here, thanks to a synergistic theoretical and experimental investigation, we illustrate a method to control the dewetting of UT-SOI, delivering nanostructures with determined positions, sizes and shapes [1]. 3D phase-field (PF) simulations, accounting for surface diffusion-limited kinetics, are adopted to enlighten the mechanism underlying the process and assess the outcomes of experiments. Indeed, we demonstrate that a fine control over the final structures is achieved when combining patches with an ad hoc initial patterning of the thin film. [1] M. Naffouti et al., Science Adv. 3, eaao1472 (2017).

DS 6.9 Mon 17:15 H 0111

Growth of large sized 2D molybdenum sulfide flakes at the air-liquid interface — Xiaoling Zeng, Talha Nisar, Marlis Ortel, •Torsten Balster, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen,Germany

Layered transition metal chalcogenides, especially MoS_2, are promising materials for catalysis as well as semiconducting layers in thin film transistors. Since the 1st transistors were produced with mechanically exfoliated MoS_2 flakes, new deposition processes for large area and atomically thin layers are needed to enable new generation electronic devices.

In this investigation, we have developed a cheap, wet chemical deposition process, which takes aadvantage of growth on a liquid surface. For this purpose, a saturated solution of ammonium tetrathiomolybdate (ATTM) in deionized water was prepared by heating and ultrasonication. After two hours of cooling period molybdenum sulfide flakes were formed in solution at the air-liquid interface with a lateral size of more than 150μm. These flakes were transferred onto a SiO_2/Si substrate in a Langmuir-Blodgett like deposition process. The thickness of the flakes ranged from a single monolayer to 5 monolayers as confirmed by AFM and Raman spectroscopy. XPS and TEM reveal, that with post growth thermal treatment flakes of high quality are obtained.

DS 6.10 Mon 17:30 H 0111

Magnetron sputtered refractory metal thin films on NiTi and their influence on the phase transition behaviour of NiTi — •Fabian Seifried[1], Helmut Riedel[2], Harald Leiste[1], Ruth Schwaiger[1], Sven Ulrich[1], Hans Juergen Seifert[1], and Michael Stueber[1] — [1]KIT IAM-AWP, Eggenstein-Leopoldshafen, Germany — [2]TU Wien WWWT, Wien, Austria

In this study, pseudo-elastic Ni 50.8 at.%-Ti alloy sheets of 1000 microns thickness were coated with 10 microns thick refractory metal thin films, by non-reactive d.c. magnetron sputtering. These thin films were characterized with regard to their microstructure and selected mechanical properties. Microstructural characterization of the thin films included X-Ray Diffraction and Scanning Electron Microscopy analyses. Mo thin films grow in a densely packed, (110) textured b.c.c. structure with columnar grains on the NiTi substrate. Ta and Nb thin films grow as well in a dense columnar structure; however they show X-Ray diffraction peaks of various lattice planes of the b.c.c. structures (i.e. no texture). Considering the specific thin film/substrate thickness ratio (1:100) of the samples, the mechanical properties of both the thin films and thin film/substrate composites were investigated on different length scales, using nano- and microindentation techniques. To evaluate the potential impact of the surface coating and the deposition process on the phase transformation behaviour of the NiTi shape memory alloy, differential scanning calorimetry analyses were done. Conclusions and recommendations will be given for potential thin film materials as radiopaque coatings on NiTi substrates for medical applications.

DS 6.11 Mon 17:45 H 0111

Focused electron beam induced multi-tip deposition for energy harvesting fromthe green-house radiaton. — •Koops Hans Wilfried Peter — Ernst Ludwig Strasse 16, Ober-Ramstadt, Germany

A cross -lines grid with 0,5 μm cell-width is proposed to harvest IR radiation from the green house gases in the earth atmosphere. According to NASA-measurements 340 W/m^2 reach the earth in the IR-regime. A nanogranular Pt/C material can be used in a detector-matrix to harvest this energy, by collecting IR quanta with nanocrystalline Pt/C compound material in form of electron-hole Bosons. Very large numbers of Bosons can be stored in such energy layers. Applying a field gadient allows to move the Bosons to the end of the material layer, where the Bosons release an electron each, and the resulting hole can form a new Boson again. Electrons are emitted in a coherent fashion. The small-area experiment shall proove the principle of the energy harvesting capability. Large areas of collector fields shall follow, built with the principle of glass coating machines with massive parallel ion beam sources to deposit the Pt/C absorber structure layers.

DS 6.12 Mon 18:00 H 0111

Modelling of the vertical deflection of ferroelectric bending tongues — •Juliette Cardoletti[1], Aldin Radetinac[1], Julian Walker[2], Philipp Komissinskiy[1], Susan Trolier-McKinstry[2], and Lambert Alff[1] — [1]Technische Universität Darmstadt, Institute of Materials Science, Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany — [2]Materials Research Institute, Pennsylvania State University, University Park, PA, 16802, USA

With the acute need for miniaturisation of devices and components, the use of bending tongues (cantilevers or wider beams) based on piezoelectric ceramics is increasing. Due to its large piezoelectric coefficient, $PbZr_{0.52}Ti_{0.48}O_3$ (PZT) is the most commonly used material, but it is also ferroelectric (*i.e.* the polarisation direction can be switched between discrete crystallographically allowable orientations by an external electric field). This particularity should be taken into account when modelling the vertical deflection of bending tongues.

To date, bending tongue based devices have been modelled from a static and dynamic point of view without simulating the ferroelectric switching occurring in grains [1]. However, various papers attempted to describe ferroelectric switching based on different approaches, for example based on a switching criterion accounting for mechanical work and electrical work contributions to the switching process [2].

The here described modelling program, based on Hwang's switching criterion [2], aims to bridge the gap between the previous approaches by describing the vertical deflection of a bending tongue while taking into account ferroelectric switching at the grain scale.

DS 7: Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...): Session I

Time: Monday 15:00–17:45 Location: H 2032

DS 7.1 Mon 15:00 H 2032

Stoichiometry determination of chalcogenide superlattices by means of X-ray diffraction and its limits — Felix R. L. Lange[1,2], Henning Hollermann[1], Stefan Jakobs[1], •Peter Kerres[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen Germany — [2]JARA-FIT Institute Green-IT, RWTH Aachen University and Forschungszentrum Jülich, 52056 Aachen, Germany

In this study we explore the potential of stoichiometry determination of $GeTe/Sb_2Te_3$ superlattices (CSLs) by means of X-ray diffraction (XRD). For this purpose a series of sputter-deposited CSLs with varying ratios of the GeTe and Sb_2Te_3 layer thicknesses is analyzed. Kinematical scattering theory is applied to link the change in average chemical composition with the specific CSL diffraction features. It is found that the lattice parameters of the reference unit cell of the superlattice follow Vegards law, which allows for a straight-forward model for stoichiometry determination.

DS 7.2 Mon 15:15 H 2032

Revealing the Interfaces of MgO/Co/GaAs(001): A Structural and Chemical Investigation with XPS and XPD — •Karim Shamout[1,2], Philipp Espeter[1,2], Peter Roese[1,2], Richard Hönig[1,2], Ulf Berges[1,2] und Carsten Westphal[1,2] — [1]Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — [2]DELTA - Technische Universit
ät Dortmund, Maria-Goeppert-Mayer-Str. 2, 44221 Dortmund, Germany

We report a synchrotron radiation based x-ray photoelectron spectroscopy (XPS) and x-ray photoelectron diffraction (XPD) study on the system MgO/Co(bcc)/GaAs(001)-$c(8 \times 2)$ and its interfaces. Co substitutes As at the Co/GaAs interface and forms a Co_3Ga alloy in $D0_3$-structure with Ga due to interdiffusion. The GaAs surface reconstruction is lifted in favor of the newly formed alloy that serves as a template for the metastable Co(bcc) structure. No indication for Co oxidation was found at the MgO/Co interface. The MgO film grows amorphously up to a thickness of ≤ 4 ML. After 5 ML of MgO deposition, the amorphous phase crystallizes into a distorted unit cell.
Keywords: Topological insulator, MTJ, TMR, PED, XPD, XPS

DS 7.3 Mon 15:30 H 2032

Ti valence mapping in LAO/STO with Resonant Soft X-ray Reflectometry — •Martin Zwiebler[1], Emiliano Di Gennaro[2], Jorge Enrique Hamann-Borrero[4], Fabio Miletto Granozio[2], Enrico Schierle[3], Eugen Weschke[3], Bernd Büchner[4], George Sawatzky[5], Robert Green[5], and Jochen Geck[1] — [1]Institut fuer Festkörper- und Materialphysik Technische Universität Dresden, 01062 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]IFW Dresden, Helmholtzstraße 20, 01069 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. We performed X-ray reflectivity measurements at the Ti L2,3 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 and interacts strongly with the lattice degrees of freedom. From the polarization dependence of the reflectivity we gain new results on the anisotropy of orbital energies and valence orbital occupation.

DS 7.4 Mon 15:45 H 2032

Investigation of wake-up and local polarization switching behavior in La doped HfO2 structures — •Pratyush Buragohain[1], Tony Schenk[2], Uwe Schroeder[2], and Alexei Gruverman[1] — [1]Dept. of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE 68588, USA — [2]NaMLab gGmbH, Noethnitzer Str. 64, 01187 Dresden

The discovery of ferroelectricity in hafnium oxide (HfO2) based thin films is a promising step towards the realization of ferroelectric based memory devices due to their inherent advantages over conventional perovskite materials, especially their compatibility with existing CMOS technology. Although several studies have reported the integral behavior of the capacitors, an in-depth investigation of the local ferroelectric characteristics has not yet been performed. Here, we will discuss the wake-up behavior and the polarization switching dynamics in ultrathin La-doped HfO2 capacitors investigated by means of Piezoresponse Force Microscopy (PFM). Evolution of the domain structure as a function of the applied voltage confirmed that de-pinning of domains is responsible for the increase in polarization upon field cycling. Step-by-step switching of the polarization coupled with PFM imaging revealed that the domains grow from grain boundaries or pinned domains, if present, following the nucleation limited switching (NLS) model.

DS 7.5 Mon 16:00 H 2032

Revealing the actual structure of the oxygen-rich surface of α-Fe_2O_3(0001) — •Jesús Redondo[1], Petr Lazar[2], Benjamín Mallada[1], Aleš Cahlik[1], Pavel Procházka[3], Martin Vondráček[1], Jan Čechal[3], Pavel Jelínek[1], and Martin Švec[1] — [1]Institute of Physics, Czech Academy of Sciences, Praha, Czech Republic — [2]Regional Center for Advanced Materials and Technologies, Olomouc, Czech Republic — [3]Central European Institute of Technology, Brno, Czech Republic

The surface of metal oxides reconstructs in many ways depending on the crystallographic planes and preparation procedures. In the case of iron oxides, the surface reconstruction of α-Fe_2O_3(0001) is still controversial. Under oxidizing conditions, it partially reconstructs in the so-called "biphase" structure, which traditionally has been explained by the coexistence of small islands of FeO and Fe_2O_3(0001). Furthermore, other phases are present, and there is no recipe to obtain large domains of single phases on the surface, which hinders an unambiguous interpretation of spectroscopic and microscopy data.

In this work, we present a procedure to obtain micrometer-sized domains of single stoichiometry under reducing and oxidative conditions. This has allowed us to thoroughly characterize the two main phases of the α-Fe_2O_3(0001) by means of STM, AFM, LEEM, μLEED, XPS, and NEXAFS. Moreover, we have solid evidence that that the "biphase" structure may, in fact, be a novel 2D material rather than a truncated bulk. Complementary DFT calculations support the model of an O-Fe-O trilayer (FeO_2) on the surface.

15 min. break.

DS 7.6 Mon 16:30 H 2032

Effect of stress on structural properties of Fe/Cr multilayers. — •Magnifouet Tchinda Gladice Claire, Dacosta Manu, Meny Christian, and Pierron-Bohnes Véronique — 23 rue du Loess, 67200 Strasbourg

Cr/Fe/Cr tri-layers were deposited by sputtering with an average total thickness of 100nm on MgO(100) and STO(100) substrates. In order to have good epitaxy, the first chromium was deposited at high temperature (400°C), iron at 400°C, 300°C, 200°C and room temperature and; the capping chromium at room temperature. X-ray diffraction is used to study the structure of Cr/Fe/Cr tri-layer. Both the specular scan and pole figure mapping showed good epitaxy of the films along the [100] direction when the temperature of the deposited iron is low (200°C and room temperature). Presence of the residual strain was quantified by *sinus2 * method*. This method revealed that the values of the free lattice stress parameter determined on the tri-layers are sometimes low or high compare to the massive one as I will show it during the presentation.

DS 7.7 Mon 16:45 H 2032

Effect of alkali post-deposition treatments on the formation of the CdS buffer layer / Cu(In,Ga)Se2 thin-film solar cell absorber interface — •Jakob Bombsch[1], Enrico Avancini[2], Romain Carron[2], Thomas Kunze[1], Evelyn Handick[1], Roberto Félix[1], Raul Garcia-Diez[1], Yuefeng Zhang[1,4], Stephan Buecheler[2], Regan Wilks[1,3], and Marcus Bär[1,3] — [1]Renewable Energy, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Berlin, Germany — [2]Laboratory of Thin Films and Photovoltaics, Empa-Swiss Federal Laboratories for Materials and Science and Technology, Dübendorf, Switzerland — [3]Energy Materials In-Situ Laboratory Berlin (EMIL), HZB, Berlin, Germany — [4]Department of Physics, Xiamen University, Xiamen, China

Cu(In,Ga)Se2 (CIGSe) - based devices are considered to be high-efficient alternatives to silicon-wafer based solar cells. The performance of chalcopyrite-based thin-film solar cells has recently been improved by performing alkali post-deposition treatments (PDT), where the highest efficiency so far has been reached using an RbF PDT. We used soft and hard x-ray photoelectron spectroscopy to study the impact of NaF/RbF PDT on the chemical and electronic properties of low temperature processed CIGSe absorbers as a function of alkali content. Evidence for the presence of Cu(II) - scaling with RbF - is found at the absorber (surface). Further, the (wet chemically) deposited CdS buffer layers contain a significant fraction of a sulfate. Finally, in our contribution, we will present and discuss the impact of the PDT on the electronic structure of the CdS/CIGSe interface.

DS 7.8 Mon 17:00 H 2032

Defects investigation in black anatase — •Dmitry Zyabkin[1], Juliana Schell[3], Ulrich Vetter[1], Haraldur Pall Gunnlaugsson[3], Hilary Masenda[2], Peter Schaaf[1], and the ISOLDE Collaboration[2] — [1]Chair materials for Electronics, Institute of Materials Engineering and Institute of Micro- and Nanotechnologies MacroNano®, Gustav-Kirchhoff-Str. 5, 98693 Ilmenau, Germany — [2]School of Physics, University of the Witwatersrand, Johannesburg 2050, South Africa — [3]European Organization for Nuclear Research (CERN), CH-1211 Geneva, Switzerland

Black anatase has been considered as the promising material for dye-sensitized solar cells and efficient water splitting under light exposure [1]. While defects play the essential role in the enhanced photocatalytic activity it has received plenty of attention to expand studies of their roles as well as further advancing of light absorption [2]. Thin films were obtained by means of reactive sputtering and treated at room and 573K temperatures. The current Mössbauer study was done on black anatase thin films at the ISOLDE mass separator at CERN. Implantation of ^{57}Mn ($T_{1/2}$ = 1.5 min) was accomplished at ion energies of 50 keV, with the measurements performed online within an interval from 301 to 735K. Hyperfine parameters are given relative to the centre of the spectrum of α-Fe at RT.

[1] S.Zhang *et al.* Energy Environ. Sci., 2013,6, 1443-1464
[2] F.Amano *et al.* J. Phys. Chem. C, 2016, 120 (12), pp 6467-6474

DS 7.9 Mon 17:15 H 2032

Friction behavior of graphene on polished steel surfaces — •Dogus Ozkan[1], Cem Kincal[2], Egemen Sulukan[3], Yaman Erarslan[4], Baris Yağci[5], and Oğuzhan Gurlu[6] — [1]National Defense University, Naval Academy, Istanbul-Turkey. — [2]Istanbul Technical University, Istanbul-Turkey — [3]National Defense University, Naval Academy, Istanbul-Turkey — [4]Yildiz Technical University, Istanbul-Turkey — [5]Koç University, KUYTAM, Istanbul, Turkey — [6]Istanbul Technical University, Istanbul-Turkey

Application of graphene in tribological problems is gaining importance. In this work, single/multi-layer graphene was growth on copper foils by CVD and transferred on to different polished steels samples, which had different surface roughness (Figure). Lateral force microscopy (LFM) was used to investigate the influence of graphene on the friction behaviour of polished steel surfaces. Effects of surface roughness on the adhesion of single/multi layer graphene was also looked upon. Elastic properties of single/multilayer graphene on steel surface were characterized by AFM in force modulation mode (FMM). Results showed that graphene reduced friction coefficient of steel surface when compared to bare steel surface under different load conditions.

DS 7.10 Mon 17:30 H 2032

Supramolecular Heterostructures - expanding molecular self-assembly beyond 2D — •Vladimir Korolkov[1], Kenji Watanabe[3], Takashi Taniguchi[3], Matteo Baldoni[2], Elena Besley[2], Nicholas Besley[2], and Peter Beton[1] — [1]School of Physics and Astronomy, The University of Nottingham, UK — [2]University Park — [3]University of Nottingham, University Park

For a long time the molecular self-assembly has been limited to engineering 2D molecular structures on surfaces. Here we demonstrate a successful approach that extends self-assembly into 3D by creating supramolecular heterostructures - layered organic materials stabilized by hydrogen bonds in plane and by van der Waals interactions between layers. SHs are formed by growing sequential layers of bi- and mono-component two-dimensional supramolecular arrays. The heterostructures are formed on hexagonal boron nitride by depositing of cyanuric acid/melamine, 5,10,15,20-tetrakis(4-carboxylphenyl) porphyrin, trimesic acid and terephthalyc acid. We analyzed this heterostructures with ambient Atomic Force Microscopy that routinely achieve 0.1 nm resolution. AFM has confirmed that there is a clear epitaxial arrangement between these layers. We demonstrate that heterostructure formation may be used to control the functional properties of supramolecular layers through a shift of the fluorescence peak position.

1 - Korolkov et al. Nature Chemistry, 2017

DS 8: 2D materials (joint session HL/DS)

Time: Monday 15:00–16:30 Location: EW 201

DS 8.1 Mon 15:00 EW 201

Predicting and Understanding Quantum Spin Hall Insulators with the Help of Compressed Sensing/SISSO — Carlos Mera Acosta[1,2], Runhai Ouyang[1], Adalberto Fazzio[2], Matthias Scheffler[1], Luca Ghiringhelli[1], and •Christian Carbogno[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]University of São Paulo, São Paulo, Brazil

Quantum Spin Hall insulators (QSHIs), i.e., two-dimensional insulators with conducting edge states protected by time-reversal symmetry, have attracted considerable scientific interest in recent years. In this work, we perform first-principles calculations to compute the Z_2-invariant for 220 functionalized honeycomb-lattice materials. Using the recently developed sure independence screening and sparsifying operator (SISSO) method [1], we derive a "map of materials", in which metals, trivial insulators, and QSHIs are spatially separated. The axes of this map are defined by physically meaningful descriptors, i.e., non-linear functions that only depend on the properties of the material's constituent free atoms. First, this yields fundamental insights into the mechanisms driving topological transitions. Second, we are able to predict the topological character of materials that are not part of the originally investigated set just from their position on the map (predictive power greater than 95%). By this means, we are able to predict 89 yet unknown QSHIs.

[1] Runhai Ouyang *et al.*, *arXiv:1710.03319* (2017).

DS 8.2 Mon 15:15 EW 201

Superconductivity and electron-phonon properties of intrinsic and doped antimonene — •Andrei Lugovskoi, Mikhail Katsnelson, and Alexander Rudenko — Institute for Molecules and Materials, Radboud University Nijmegen, Nijmegen, The Netherlands

Antimonene is a recently discovered elemental 2D phase of Sb with buckled honeycomb structures. The material was successfully obtained experimentally, and posses interesting set of properties. It was shown to have high stability on base of both experimental observations and *ab initio* modeling, and is also predicted to have interesting optical properties and strain tunable band gap. At the same time, superconductivity in doped phosphorene and graphene was recently observed experimentally, which opens new opportunities for the application of 2D materials.

We present the *ab initio* calculations of electron-phonon coupling properties and critical superconducting temperature in both n- and p-doped antimonene at experimentally achievable carrier concentrations. The effects of small strains and bias voltage on the critical temperature are also considered. Required quantities are obtained by using density functional theory implementation of electron-phonon Wannier-Fourier interpolation in EPW and QE codes. Critical temperature at various carrier densities is estimated using McMillan-Allen-Dynes equation.

The work is a part of the research program "Two-dimensional semiconductor crystals" (prj. 14TWOD01), which is partly financed by the Netherlands Organization for Scientific Research (NWO).

DS 8.3 Mon 15:30 EW 201

Dielectric Engineering of Intra-excitonic Correlations in a van der Waals Heterostructure — •Philipp Steinleitner[1], Philipp Merkl[1], Alexander Graf[1], Philipp Nagler[1], Christian Schüller[1], Tobias Korn[1], Rupert Huber[1], Samuel Brem[2], Malte Selig[3], Gunnar Berghäuser[2], and Ermin Malic[2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [3]Department of Theoretical Physics, Technical University of Berlin, Berlin, Germany

Atomically thin transition metal dichalcogenide monolayers promise novel optoelectronic applications due to their direct bandgap in the optical range. Reduced Coulomb screening, in combination with the two-dimensionality, stabilizes excitons, even at room temperature. Due to the extreme confinement perpendicular to the plane of the material, excitons are particularly sensitive to the local surrounding environment. Thus, capping the monolayer with a dielectric material allows one to non-invasively change their hydrogen-like structure. Here we report how an insulating hexagonal boron nitride cover layer influences the intra-excitonic 1s-2p transition. Using time resolved pump/THz probe techniques, we trace both optically bright and dark exciton states and are able to extract quantitative information about transition energies and linewidths. We find that the cover layer redshifts the 1s-2p transition and leads to a decrease of its linewidth. Using microscopic modelling, we show that our experimental data also support the formation of dark excitons from an initially bright population.

DS 8.4 Mon 15:45 EW 201

high-throughput search of novel 2d materials for electronic and optoelectronic applications — •davide campi, thibault sohier, antimo marrazzo, marco gibertini, nicolas mounet, and nicola marzari — Theory and simulation of materials (THEOS) and national center for computational design and discovery of novel materials (MARVEL), école polytechnique fédéral lausanne, ch-1015, lausanne, switzerland

2D materials provide a novel paradigm and toolbox for materials scientists to discover or engineer new properties and functionalities. However, the handful of 2D materials intensively studied up to now represent only a few of the manifold possibilities. In this work we present the results of an applications-oriented screening that, using state-of-the-art first-principles simulations and automatized high-throughput calculations through the AiiDA platoform[1], identifies new promising candidates for field effect transistors (FET), photocatalytic water splitting and nanoporous crystalline membranes, selected among the hindreds of 2D materials (1844)[2] discovered by performing a "computational exfoliation" of a dataset of more than 100000 bulk parent structures.

[1] G.Pizzi, A.Cepellotti, R.Sabatini, N.Marzari and B.Kozinsky, Comp. Mat. Sci. 111, 218 (2016). [2] N.Mounet, M.Gibertini, P.Schwaller, D.Campi, A.Merkys, A.Marrazzo, T.Sohier, I.E.Castelli, A.Cepellotti, G.Pizzi and N.Marzari, in press (2018).

DS 8.5 Mon 16:00 EW 201

Spin- and valley-dependent transport through a 2D semiconductor with magnetic substrate — •Gerhard Fechteler, Andor Kormányos, and Guido Burkard — University of Konstanz, Germany

Motivated by recent theoretical [1] and experimental [2,3] works, we study spin- and valley-dependent electron scattering in monolayers of transition metal dichalcogenides through a region with an underlying magnetic substrate. The valley splitting and changes in the parameters such as Fermi velocity and effective electron mass induced by the magnetic substrate lead to novel spin- and valley selection possibilities compared to gated structures [4]. Neglecting Rashba spin-orbit coupling (SOC), we study the Fermi energy and incident angle dependence of spin and valley selective scattering processes. Moreover, we find pronounced and tuneable Goos-Hänchen shifts. In the presence of Rashba SOC, we find that the transmitted and reflected electron beams are split due to spin mixing in the scattering region. Such a spin-dependent scattering can prove useful for the design of novel spintronic devices. [1] J. Qi et al., Phys. Rev. B 92, 121403 (2015). [2] C. Zhao et al., Nat. Nanotechnol. 12, 757-760 (2017). [3] D. Zhong et al., Sci. Adv. 3, e1603113 (2017). [4] H. Ghadiri et al., J. Phys.: Condens. Matter 29, 115303 (2017).

DS 8.6 Mon 16:15 EW 201

Electron quantum optics in anisotropic pseudospin one systems — •Yonatan Betancur Ocampo and Dario Bercioux — Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal, 4 20018 Donostia-San Sebastián, Spain

We proposed the development of electron quantum optics devices through heterojunctions formed by anisotropic and relativistic pseudospin one materials. Based on our theoretical calculations, we found that the probability transmission, reflection and refraction law present atypical behavior. We have shown that collimation effect, Veselago lenses, and beam splitters are enhanced using pseudospin one particles. Moreover, novel quantum optics devices could be designed such as asymmetric Veselago and diverging lenses. Our findings suggest that these devices can be built from the strain-engineering of Lieb lattices.

DS 9: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials II (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Monday 15:00–17:15 Location: HL 001

DS 9.1 Mon 15:00 HL 001

Non-adiabatic Dynamics in Single-Electron Tunneling Devices with Time-Dependent Density Functional Theory — •Niklas Dittmann[1,2,3], Janine Splettstoesser[2], and Nicole Helbig[3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany — [2]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Gothenburg, Sweden — [3]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

The recent advance of various single-electron sources in solid-state setups has sparked interest in the investigation of electronic transport at the single-particle level. In our recent work (N. Dittmann, J. Splettstoesser, N. Helbig, arxiv:1706.04547), we put forward time-dependent density-functional theory to calculate the dynamics of interacting electrons in single-electron tunneling devices. As a physical system, we analyze a single-electron source which is built by a quantum dot tunnel-coupled to a nearby electron reservoir and driven by a time-dependent gate voltage. By using analogies with quantum-transport theory, we extract a time-nonlocal exchange-correlation potential for a Hubbard U on-site interaction on the quantum dot. The time nonlocality manifests itself in a dynamical potential step, which we explicitly link to physical relaxation time scales of the electron dynamics. Finally, we discuss prospects for simulations of larger mesoscopic systems.

DS 9.2 Mon 15:15 HL 001

Dissipative exchange-correlation functional in QED-TDDFT — •Camilla Pellegrini[1], Ilya Tokatly[2,3], and Angel Rubio[2,4] — [1]Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, E-20018 San Sebastian, Spain — [3]IKERBASQUE, Basque Foundation for Science, 48001 Bilbao, Spain — [4]Max Planck Institute for the Structure and the Dynamics of Matter, Luruper Chausse 149, 22761 Hamburg, Germany

Time-dependent density functional theory has been recently extended to treat many-electron systems coupled to quantized electromagnetic modes. Here we discuss the implications of this approach for the theory of open quantum systems. In particular we show that in the limit of continuous spectrum of photon modes, QED-TDDFT naturally leads to time-dependent density functional theory for dissipative systems coupled to the Caldeira-Leggett bath. We consider the application to the Ohmic spin boson model and show that the developed approximation to the exchange-correlation functional describes the natural linewidth of the electronic linear density response function.

DS 9.3 Mon 15:30 HL 001

Electric and magnetic response properties of solids from the current density — •Rubén Rodríguez Ferradás[1], Pina Romaniello[2], and Arjan Berger[1] — [1]LCPQ, University of Toulouse, France — [2]LPT, University of Toulouse, France

The evaluation of the macroscopic polarization and magnetization of solids is problematic when periodic boundary conditions are used because surface effects are artificially removed. This poses a problem unless surface effects can be reformulated in terms of bulk quantities [1-5]. In this work we show the advantage of calculating electric and magnetic response properties of solids using the current density as basic variable. An efficient approach to calculate the current density is time-dependent current-density-functional theory. We will show results for optical properties of solids using a recently developed functional [6]. We will also discuss how the magnetization can be described within this framework.

[1] F. Kootstra, P.L. de Boeij, and J.G. Snijders, J. Chem. Phys. 112, 6517.

[2] J.A. Berger, P.L. de Boeij, and R. van Leeuwen, Phys. Rev. B 71, 155104 (2005).

[3] P. Romaniello and P.L. de Boeij, Phys. Rev. B 71, 155108 (2005).

[4] J.A. Berger, P. Romaniello, R. van Leeuwen, and P.L. de Boeij, Phys. Rev. B 74, 245117 (2006).

[5] J.A. Berger, P.L. de Boeij, and R. van Leeuwen, Phys. Rev. B 75, 035116 (2007).

[6] J.A. Berger, Phys. Rev. Lett. 115, 137402 (2015)

DS 9.4 Mon 15:45 HL 001

Coupling Maxwell's equations to the time-dependent Kohn-Sham equations: near-field effects and electromagnetic backreaction — •Rene Jestaedt[1], Micael Oliveira[1], Angel Rubio[1,2,3], and Heiko Appel[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, USA — [3]Nano-bio Spectroscopy Group and ETSF, Universidad del País Vasco, 20018 San Sebastián, Spain

Induced currents in large molecular and condensed matter systems are non-negligible and can affect the conductivity and the optical properties of the system. In the present work, we have implemented the real-time propagation of Maxwell's equations in Riemann-Silberstein representation to use standard unitary propagation techniques in the TDDFT code octopus [1]. The Maxwell and the Kohn-Sham system are coupled via a predictor-corrector method to obtain a self-consistent time-evolution of the total system [2]. Explicitely solving the microscopic Maxwell's equations also allows us to determine the optical properties of the system directly from the Maxwell fields. We show near-field effects of a full Maxwell-matter and matter-Maxwell coupling for plasmon excitations in metallic nanoparticles [2,3] and for ring-currents in organic molecules [2].

[1] Alejandro Varas et al., J. Phys. Chem. Lett. 2015, **6**, 1891-1898 / [2] R. Jestädt et al., (to be submitted) / [3] X. Andrade et al., Physi. Chemistry Chem. Physics 2015, **17** 31371-31396

DS 9.5 Mon 16:00 HL 001

Enhanching excitation energy and charge transfer with strongly correlated light-matter interaction — •Christian Schäfer[1], Michael Ruggenthaler[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

Förster excitation energy and charge transfer are fundamental processes of chemical reactions and connected to interesting quantities such as correlation. Often this correlation is taken as fixed property of the system.

In the current work, we present how the coupling to cavity photons in a minimal realistic molecular system can drastically alter transfer characteristics, e.g. renders the excitation transfer to be distance independent [1,2]. The photonic interaction can imprint fermionic correlation on arbitrary distances.

The exact real-space description is suited to describe transfer and correlation in a unprejudiced ab-initio picture and allows us to extend our insights beyond common quantum-optical approximations.

[1] X. Zhong et al., Angew Chem Int Ed Engl. **56(31)**, 9034 (2017). [2] M. Slootsky et al., PRL **112**, 076401 (2014).

DS 9.6 Mon 16:15 HL 001

Effects of electronic correlations on the magnetic properties of organometallic molecules — •Sumanta Bhandary and Silke Biermann — Centre de Physique Thèorique, Ecole Polytechnique, 91128 Palaiseau, France

The realm of molecular spintronics relies on the external accessibility of molecular magnetic states. In correlated organometallic complexes, a delicate balance between the crystal field, Coulomb repulsion and

dynamical hybridization between metal center and organic ligands dictates the electronic and magnetic properties and often poses challenges for an accurate theoretical modelling. We have employed density functional theory (DFT), the GW approach and Anderson's impurity model (AIM) technique to study the ground state electronic and magnetic properties of transition metal-based porphyrin and phthalocyanine molecules, both in the gas phase [1] as well as while adsorbed on surfaces. Our study reveals that the dynamical correlation effects are important in order to accurately estimate spin-transition energies, magnetic anisotropy energies as well as the ground state electronic configurations in the molecular complexes. We have explored the manipulation of surface molecule interactions to externally influence the electronic and magnetic properties of the molecular system.

[1] S. Bhandary, M. Schüler, P. Thunström, I. di Marco, B. Brena, O. Eriksson, T. Wehling, and B. Sanyal, Phys. Rev. B **93**, 155158 (2016).

DS 9.7 Mon 16:30 HL 001

Structural, electronic and optical properties of cubic and tetragonal $SrTiO_3$: a DFT study including many-body effects — •Vijaya Begum, Markus E. Gruner, and Rossitza Pentcheva — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg.

$SrTiO_3$ (STO) is of fundamental interest as a substrate material in oxide electronics. The bulk undergoes a phase transition from the cubic to a tetragonal structure at T=105 K accompanied by characteristic antiferrodistortive rotations of the TiO_6 octahedra. We present a systematic comparison of the performance of the gradient corrected exchange correlation functional (GGA), the strongly constrained and appropriately normed (SCAN) meta-GGA and the hybrid functional HSE06 with respect to the electronic, structural and optical properties of cubic and tetragonal STO. For the tetragonal structure, SCAN gives a significantly improved description of the structural properties, comparable to HSE06, at a computational cost similar to GGA. The experimental band gap can be reproduced within SCAN with an on-site Hubbard term ($+U$), whereas within GGA the gap is underestimated even for very high U values. We calculate the optical spectrum for both phases, including many-body effects and excitonic corrections within the GW+Bethe-Salpeter equation approach, and compare this to previous theoretical results for the cubic phase [PRB 87, 235102 (2013)] and experiment [PRB 93, 075204 (2016)]. Funding by the DFG within SFB1242, project C02 is gratefully acknowledged.

DS 9.8 Mon 16:45 HL 001

Unveiling the mysterious magnetic state of superconducting iron under pressure — •Matteo d'Astuto — Institut NEEL CNRS/UGA UPR2940 25 rue des Martyrs BP 166 38042 Grenoble cedex 9 FRANCE — IMPMC, UMR CNRS 7590, Sorbonne Universités-UPMC University Paris 06, MNHN, IRD, 4 Place Jussieu, F-75005 Paris, France

Compressed iron undergoes a transition from bcc to hcp crystal structure with a loss of ferromagnetism. The magnetic state of the hcp phase has been debated for many decades and experiments give seemingly contradictory results. Mössbauer measurements find no magnetism, however x-ray emission spectroscopy finds remnant magnetism and Raman mode splitting suggests symmetry breaking due to antiferromagnetism. These paradoxical results are consistent with either a paramagnetic state with spin fluctuations faster than Mössbauer timescales or an antiferromagnetic state, afmII, which is undetectable with Mössbauer spectroscopy. We performed neutron powder diffraction measurements in the hcp phase and do not observe afmII order down to 1.8 K, while confirming the existence of a local magnetic moment in the hcp phase with x-ray emission spectroscopy and find it is intrinsic to this phase (1). This local magnetic moment disappears at 30–40 GPa, exactly the same pressure region where superconductivity disappears.

(1) B. W. Lebert, T. Gorni J.-P. Rueff, S. Klotz, M. Casula, A. Juhin, J. M. Ablett, F. Baudelet, T. Straessle, T. Hansen, A. Polian, P. Munsch, G. Le Marchand, Z. Zhang, M. d'Astuto, article in preparation.

DS 9.9 Mon 17:00 HL 001

Frist-principle and experimental characterisation of the electronic properties of CaGaSiN3 and CaAlSiN3: impact of chemical disorder — •Jan Minar[1], Ondrej Sipr[2], Robin Niklaus[3], Jonas Hausler[3], and Wolfgang Scgnick[3] — [1]New Technologies Research Center, University of West Bohemia, Pilsen, Czech Rep., — [2]FZU, Academy of Sciences, Czech Rep — [3]Department of Chemistry, University of Munich, Munich, Germany

We report a detailed investigation of the electronic, mechanical and optical properties of the recently discovered nitridogallosilicate CaGaSiN3 which has potential as a LED-phosphor host material. We focus on chemical disorder effects, originating from the Ga/Si site, and compared them to those of isostructural CaAlSiN3. We calculate the elastic moduli and the Debye temperature in terms of quasi harmonical approximation. Spectral properties like the joint density of states (JDOS) are evaluated and the absorption, reflectance and energy loss function are obtained from the dielectric function. The optical band gap of CaGaSiN3 from experiment is compared to the electronic band gap in terms of electronic DOS and band structure calculations. All properties are evaluated for different ordering models of Ga/Si while the experimentally observed substitutional disorder is accounted for by utilizing the Coherent Potential Approximation (CPA). We conclude a shrinking of the band gap for both CaGaSiN3 and CaAlSiN3 due to atomic disorder, which is unfavorable for potential phosphor applications [1]. R. Niklaus, J. Minar, J Häusler, W. Schnick, Physical Chemistry Chemical Physics 19 (13), 9292 (2017)

DS 10: Oxide Semiconductors for Novel Devices (Focussed Session): Session II

The class of semiconducting oxides includes low temperature processed amorphous thin films for bendable electronics and display technology as well as highly crystalline materials such as the wide band group-III sesquioxides being interesting for UV and DUV photo sensors, power electronics and even memristors. This session sets a focus on physical properties of such oxides, their growth methods and heterostructures for demonstrator devices. This focus session is supported by the Leibniz ScienceCampus GraFOx.

Organized by

Dr. Karsten Fleischer School of Physics, Trinity College Dublin, the University of Dublin Dublin 2, Ireland

Dr. Holger von Wenckstern Universität Leipzig Felix-Bloch-Institut für Festkörperphysik Halbleiterphysik Linnéstraße 5 04103 Leipzig, Germany

Prof. Dr. rer. nat. Holger Eisele Experimental Physics Technische Universität Berlin Department for Mathematics and Science Institute of Solid State Physics Hardenbergstr. 36, Sekr. EW 4-1, D-10623 Berlin, Germany

Dr. Oliver Bierwagen Paul-Drude-Institut für Festkörperelektronik (PDI) Hausvogteiplatz 5-7 10117 Berlin, Germany

Time: Monday 15:00–18:15 Location: E 020

DS 10.1 Mon 15:00 E 020

Defect and interface formation in $SrTiO_3$ homoepitaxial thin film growth — •Laura Bogula, Toni Markurt, Martin Albrecht, and Jutta Schwarzkopf — Max-Born-Str. 2, 12489 Berlin, Germany

$SrTiO_3$ represents a model system for perovskite materials and is therefore in the focus of fundamental research. Despite many studies, its functional properties and the correlation to atomic defects are not fully understood so far. Moreover, in many $SrTiO_3$ based devices next to the structural quality of the epitaxial film itself also the interface between substrate and film plays a crucial role. Therefore, we have performed a systematic investigation of the influence of different growth and pregrowth conditions on the resulting interface and the structural quality of homoepitaxial films grown by pulsed laser deposition (PLD). Transmission electron microscopy and x-ray diffraction techniques as well as reflection high-energy electron diffraction are applied to characterize films and interfaces. By varying substrate temperature, chamber pressure and oxygen content the optimal growth conditions for a stoichiometric, point defect-poor interface and film structure are specified. We found that on the one hand a high oxygen partial pressure during heat-up prior to film growth leads to an unfavourable surface reconstruction of the substrate causing a non-stoichiometric substrate/film interface. On the other hand, the formation of point defects in the film is correlated to the energetic ion bombardment during film growth which is reduced with a high process pressure.

DS 10.2 Mon 15:15 E 020

The electric field dependence of the permittivity of $SrTiO_3$ — •Julian Stoever, Laura Bogula, Toni Markut, Jos Boschker, Jutta Schwarzkopf, Martin Albrecht, and Klaus Irmscher — Leibniz Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin, Germany

Resistive switching in $SrTiO_3$ belongs to the interesting applications in the fast growing field of oxide electronics. Oxygen vacancy diffusion due to high electric fields in the depletion layer of $SrTiO_3$ Schottky diodes is a commonly used model to describe the resistive switching behaviour. The dependence of the permittivity on the electric field strength has been rarely taken into account for $SrTiO_3$ resistive switching devices. The permittivity of $SrTiO_3$ is strongly dependent on the temperature and the electric field. Additionally, capacitance-voltage and current-voltage characteristics show deviations of the C^{-2}-V relation and the thermionic-emission model, respectively. Theoretical models were developed that assume a non-linear dielectric response of the crystal [Reich et al. Phys. Rev. B, 91 11 (2015)]. Another approach is the introduction of a low-permittivity interlayer, as it was done by Yamamoto et al. [Jpn. J. Appl. Phys. 37 4737 (1998)]. To verify the theoretical approaches, fundamental measurements of the permittivity are necessary. We performed permittivity measurements at different temperatures and electric fields on plate capacitor structures made of insulating $SrTiO_3$. The results will be compared with the behaviour of the Schottky diodes and are important for characterization methods like deep level transient spectroscopy.

DS 10.3 Mon 15:30 E 020

Theoretical description of the current conduction thorough the Schottky barrier in SrTiO3/Pt based resistive switching devices — •Carsten Funck[1], Christoph Bäumer[2], Regina Dittmann[2], Rainer Waser[1,2], and Stephan Menzel[2] — [1]Institute für Werkstoffe der Elektrotechnik II, RWTH Aachen University, 52064 Aachen, Germany — [2]Peter Grünberg Institut (PGI 7), Forschungszentrum Jülich, 52425 Jülich, Germany

The current transport across Schottky contacts is widely investigated in many fields of semiconductor technology. Often this current transport is described with a certain conduction mechanism, which connects the electrical current with an analytical equation. This analytical expressions are frequently used to explain the experimental current through resistive switching devices. Especially, the Schottky emission theory is often applied to $SrTiO_3$ based thin film Schottky contacts. However, this proceeding leads often to physical inconsistencies. Therefore we developed an atomistic fully quantum mechanical model based on density functional theory combined with the non-equilibrium Green's function formalism. This model will be underlined by single band transport simulations. As a conclusion of these models we will show that the often applied Schottky emission theory is insufficient to describe the electrical current in $Nb:SrTiO_3/SrTiO_{3-x}/Pt$ based resistive switching devices. In contrast it will be shown that a thermally assisted tunneling process is responsible for the current transport across the interface, which crosses over into a direct tunneling for higher voltages.

DS 10.4 Mon 15:45 E 020

Pulse kinetic study on HfO_2/TiO_2- bilayer resistive switching memories — •Felix Cüppers[1], Alexander Hardtdegen[1], Susanne Hoffmann-Eifert[1], Moritz von Witzleben[2], and Ulrich Böttger[2] — [1]PGI-7, Forschungszentrum Jülich GmbH, Germany — [2]IWE II, RWTH Aachen University, Germany

Memristive devices based on ultrathin metal oxide layers are promising candidates for future information technology applications. Bilayer oxide stacks of HfO_2/TiO_2 exhibit enhanced switching stability [1] compared to the respective monolayers. However, the origin of the stability is not fully understood. Effects under discussion comprise the intrinsic current limitation by the titanium oxide layer as well as a change in the temperature management during switching. Furthermore, the influence of the intrinsic series resistor on the switching kinetics of the bilayer cell needs further exploration.

In this study, electrical characterization by pulse measurements of bilayer oxide stacks of HfO_2/TiO_2 is done. By variation of time, voltage, state resistance and pulse geometry, different regimes of cell performance are identified and characterized. These results allow a deeper understanding of the kinetics of resistively switching oxide bilayer stacks. [1] A. Hardtdegen et al., "Internal Cell Resistance as the Origin of Abrupt Reset Behavior in HfO_2-Based Devices Determined from Current Compliance Series" *2016 IEEE 8th International Memory Workshop (IMW)*, Paris, 2016, pp. 1-4.

DS 10.5 Mon 16:00 E 020

Electrode Influence on the Resistive Switching Performance in HfOx based RRAM Devices — •Benjamin Krah[1], Stefan Petzold[1], Ulhas Sharath[1], Eszter Piros[1], Tom Blomberg[2], Eric Jalaguier[4], Marko Tuominen[2], Hessel Sprey[3], Sophie Bernasconi[4], Etienne Nowak[4], Philipp Komissinskiy[1], Erwin Hildebrandt[1], and Lambert Alff[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]ASM Microchemistry Ltd., Helsinki, Finland — [3]ASM Belgium, Leuven, Belgium — [4]CEA Leti, Grenoble, France

Resistive switching random access memory (RRAM) is an intensively investigated candidate for DRAM and FLASH replacement. The resistance of an insulator, sandwiched between two electrodes, can be modified by an applied voltage generating a soft breakdown of the dielectric. Hafnium oxide (HfO2) based dielectrics are of high interest due to their proven CMOS compatibility. Recently, we have shown in a simple model device how to achieve all reported switching modes, including conductance quantization [1]. Here, we investigate in the same model device (Pt/HfO2/bottom electrode (BE) and Pt/HfOx/BE) the influence of electrode material on the switching variability and performance. As only additional parameter, the oxygen stoichiometry HfOx is varied. The tested bottom electrodes include TiN, TiWN, WN and W due to their applicability in the semiconductor industry. We found that strong oxygen getter electrodes tend to increase the switching variability and to reduce the reliability. The choice of electrode, therefore, is a crucial parameter for switching performance.

[1] S. U. Sharath et. al., Adv. Funct. Mater. 27, 1700432 (2017)

DS 10.6 Mon 16:15 E 020

Ab initio study of oxygen vacancy formation and migration in HfO_2 under electric field — •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 storage devices investigated so far, resistive random access memories (ReRAMs) stand out because of the high-speed/high-density properties and the low energy required for the writing/rewriting circles. A deep understanding of the role played by point defects and dopants is important for an optimization of the device functionality. We present a density functional theory (DFT) study aimed at investigating the formation energies and the migration energy barriers of oxygen vacancies in monoclinic HfO_2. We look at the dependence of these properties in bulk and film systems on the magnitude of an external electric field. We also study the influence of Yttrium dopants on the diffusion. The nudged elastic band 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 favourable for the application of an external electric field in terms of a capacitor model. - The work is supported by DFG - SFB 917

(Nanoswitches)

DS 10.7 Mon 16:30 E 020

Filament growth and resistive switching in hafnium oxide memristive devices — •Sven Dirkmann[1], Jan Kaiser[1], Christian Wenger[2], and Thomas Mussenbrock[3] — [1]Ruhr-Universität Bochum, Lehrstuhl für Theoretische Elektrotechnik, 44780 Bochum, Germany — [2]IHP, 15239 Frankfurt (Oder), Germany — [3]BTU Cottbus-Senfenberg, Lehrstuhl für Theoretische Elektrotechnik, 03046 Cottbus, Germany

Memristive nanostructures are devices that change their resistance when a voltage is applied to them and maintain their resistance when removing this voltage. In particular, HfO2 based RRAM devices are under investigation due to their scalability (< 10 nm), simple fabrication , fast switching speeds and their compatability with CMOS technology. Here, we report on the resistive switching in TiN/Ti/HfO2/TiN memristive devices. A resistive switching model for the device is proposed, based on important experimental and theoretical findings and validated using 2D and 3D kinetic Monte Carlo simulations. The model is coupled to a field solver and different current transport mechanisms as direct tunneling, trap assisted tunneling, ohmic transport, and transport through a quantum point contact have been taken into account. Important parameter, difficult to measure in experiments, as the shape of the conductive filament, width of the filament constriction, current density and temperature distribution, are calculated. We find that the numerical results are in excellent agreement with experimentally obtained data. This work is funded by the German Research Foundation DFG in the frame of Research Unit FOR2093.

15 min. break.

DS 10.8 Mon 17:00 E 020

Molecular beam epitaxy of Ga2O3 homoepitaxial (010) thin films — •Piero Mazzolini[1], Charlotte Wouters[2], Martin Albrecht[2], and Oliver Bierwagen[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

Due to some of its peculiar properties like its intrinsic wide bandgap (Eg = 4.8 eV) and the possibility to tune its transport properties, gallium oxide is recently attracting large interest especially in the field of power electronic devices. Nonetheless, the future application of Ga2O3 is connected to the possibility to obtain a deep control of its functional properties, i.e. limiting/controlling the presence of defects (e.g. doping). We here present a study on homoepitaxially grown β-Ga2O3 thin films via molecular beam epitaxy on (010)-oriented β-Ga2O3 substrates. We thoroughly study the effect of the in-situ surface cleaning, growth T and metal-to-oxygen flux ratio. The quality of the deposited gallium oxide homoepitaxial thin films is determined employing different in-situ (e.g. RHEED) and ex-situ (e.g TEM, AFM, XRD) characterization techniques.

DS 10.9 Mon 17:15 E 020

Thermal Conductivity of β-Ga_2O_3 Bulk and thin Films — •Martin Handwerg[1], Robin Ahrling[1], Rüdiger Mitdank[1], Günter Wagner[2], Zbigniew Galazka[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, 12489 Berlin, Germany

The transparent conductive oxide β-Ga_2O_3 is of huge interest for high power electronics and optoelectronics because of its high band gap ($E_G \approx 4.7eV$). Knowledge of the thermal conductivity is crucial to design stable applications.

Here, we investigate the thermal conductivity of thin MOVPE grown polycristalline β-Ga_2O_3 films on sapphire-substrates and single-crystalline, electrically conductive β-Ga_2O_3 films on insulating Mg-doped Czochralski-grown β-Ga_2O_3 substrates.

In order to measure the thermal conductivity of films and substrates, we used multiple aspects of the 3ω-method: the differential 3ω-method with a separate measurement of the substrate; a variation of multiple heater lines with different line widths and a 2ω approach.

We observe a reduction of the bulk thermal conductivity in dependence of the crystallinity and film thickness. This reduction can be explained with the reduced mean free path of the phonons due to the film thickness and grain sizes. This result, as well as an observed electrical conductivity reduction with decreasing film thickness, leads to a limitation of thermally influenced applications with films thinner than $\approx$ 150 nm or the need of an improved thermal management.

DS 10.10 Mon 17:30 E 020

Electronic Raman scattering in β-Ga_2O_3 — •Andreas Fiedler[1], Manfred Ramsteiner[2], Zbigniew Galazka[1], and Klaus Irmscher[1] — [1]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5–7, 10117 Berlin, Germany

Currently, β-Ga_2O_3 is in the research focus as a material for power electronic devices because of its anticipated high electric break down field ($\approx$ 8 MV/cm). For such applications, doping control is of outermost importance. Here we report on Raman spectroscopy investigations of highly n-type doped β-Ga_2O_3 single crystals. For degenerate material ($n > 3 \times 10^{18}$ cm^{-3}), we observe Raman lines at about 282 cm^{-1} (with a shoulder at 255 cm^{-1}) and at about 564 cm^{-1}, which cannot be assigned to first-order scattering by phonons. These lines exhibit only a weak temperature dependence and are essentially independent of the shallow donor species (Sn or Si). We attribute the doping induced Raman features to electronic Raman scattering caused by excitation of electrons from an effective-mass like donor impurity band into the conduction band. This assignment is based on the fact that the peak position of the low-frequency line coincides with the ionization energy of effective-mass like donors ($\approx$ 36 meV) and the occurrence of the Raman signals only for doping concentrations exceeding the Mott criterion. Consequently, the high-frequency Raman line at 564 cm^{-1} (= 2 $\times$ 282 cm^{-1}) is explained by second-order electronic Raman scattering.

DS 10.11 Mon 17:45 E 020

Analysis of the conductivity anisotropy of β-Ga_2O_3 using Van der Pauw measurenemts — •Christian Golz[1], Zbigniew Galazka[2], Fariba Hatami[1], W. Ted Masselink[1], and Oliver Bierwagen[3] — [1]Department of Physics, Humboldt-Universität zu Berlin, Newton-Str. 15, D-12489 — [2]Leibniz Institute for Crystal Growth, Max-Born-Str. 2, D-12489 — [3]Paul-Drude-Institute, Hausvogteiplatz 5-7, D-10117

Using Van der Pauw measurements, the conductivity anisotropy of β-Ga_2O_3 was analyzed. The structural asymmetry due to the monoclinic lattice structure of β-Ga_2O_3 translates into anisotropic properties like optical absorption and thermal conductivity. Due to an anisotropic effective mass and anisotropic scattering rates (e. g. due to anisotropic phonon modes), conductivity might be anisotropic as well. Square shaped β-Ga_2O_3 high quality bulk samples oriented in several surface orientations with lithographically processed contacts were analyzed for temperatures between 10 K and 375 K. The results were translated into the conductivity tensor (both diagonal and off-diagonal elements) by comparing them to finite element simulations of the potential in each sample and calculation of a two-dimensional conductivity tensor in the coordinate system of the sample edges. Less than 5% anisotropy were found at and above room temperature, where isotropic conductivity is within the experimental error. Larger anisotropies were found at low temperatures (about 30% at 10 K) and for a samples having a large number of low-angle grain boudaries (anisotropy above a factor of 20 at 50 K, but only 12 % at 365 K).

DS 10.12 Mon 18:00 E 020

Carrier mobility in crystalline MOVPE-Ga2O3-films — •Rüdiger Mitdank[1], Robin Ahrling[1], Martin Handwerg[1], Günter Wagner[2], Zbigniew Galazka[2], and Saskia F. Fischer[1] — [1]AG Novel Matirials, 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

We demonstrate the results of Hall- and van-der-Pauw measurements for Si-doped ß-Ga2O3 MOVPE layers with a thickness 30nm < t < 230 nm between T = 50 K and 300 K. The homoepitaxial layers were grown on isolating substrates with Mg-doping. At high temperature T, the mobility is dominated by scattering of electrons at polar optical phonons, at low T by scattering at ionized impurities. A mobility limit for T = 300K and t >100nm of 140 (cm*cm)/Vs was found in the case of pure electron-phonon interaction. For t < 100 nm the mobility decreases strongly. The reduction of the carrier mobility due to surface scattering and propagation of electron waves in thin films is discussed.

DS 11: Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...): Session II

Time: Tuesday 9:30–13:15 Location: H 0111

DS 11.1 Tue 9:30 H 0111

Ni:SrTiO3 thin films — •Fatima Alarab[1,2], Rostislav Medlin[2], Lucie Prusakova[2], Pavol Sutta[2], Laurent Nicolai[2], Christine Richter[1], Karol Hricovini[1], and Jan Minar[2] — [1]University of Cergy-Pontoise, Paris, France — [2]University of West-Bohemia, New technologies research centre, Plzen, Czech Republic

Strontium titanate (SrTiO3, STO) is a bulk insulator with a band gap of 3,2eV in its cubic phase at room temperature. Specific properties of pure STO like very large dielectric constant and high resistivity make it an interesting material for different applications in microelectronics, optics and in advanced ceramics. By doping with transition metals or oxygen vacancies, STO becomes electrically conductive and the band gap width is modified. Here we report the fabrication, structure and electronic properties of Nickel doped STO (Ni:STO) thin films. The films with different Ni concentrations were prepared by reactive co-sputtering in reactive magnetron units using pure STO and Ni targets. X-ray diffraction, TEM, EELS and XPS techniques were used to characterized the effect of Ni concentration in STO on crystallinity and electronic properties as compared to pure STO. We performed as well calculation of the band structure using SPR-KKR package.

DS 11.2 Tue 9:45 H 0111

Experimental and computational analysis of grain growth in ultrafine-grained thin films — •Ahu Öncü[1], Thorsten Halle[2], and Dana Zöllner[3] — [1]Institute of Experimental Physics, Otto-von-Guericke University Magdeburg, Germany — [2]Institute of Materials and Joining Technology, Otto-von-Guericke University Magdeburg, Germany — [3]B CUBE Center for Molecular Bioengineering, Technische Universität Dresden, Germany

Grain microstructures of polycrystalline solids have an immense impact on materials properties. While investigations of bulk materials it is generally assumed that surfaces or interfaces are negligible. For thin films, surface effects are very important. If during grain growth in such films the average grain size reaches the order of the layer thickness, grain growth slows down or even comes to a halt. Analytic theories of nano- and microcrystalline grain growth of thin films are often in good agreement with numerical results using computer simulations, analytic size distributions or topological correlations between grains rarely capture the experimental features. One reason for this disagreement can be found in the simple fact that the experimental samples are of 3D nature, but are commonly measured in 2D and compared to 2D simulations. In the present work, we analyze the grain microstructures of ultrafine-grained thin metallic films experimentally and compare the results to 3D computer simulations.

DS 11.3 Tue 10:00 H 0111

Structural and magnetic properties of FePt-Tb alloy thin films — •Nataliia Safonova and Manfred Albrecht — Experimental physics IV, Institute of Physics, University of Augsburg, D-86159, Augsburg

Magnetic materials designed for ultrafast all-optical switching of magnetization are of high interest from a fundamental as well as technological point of view [1, 2]. In this study, two series of (FePt)(1-x)Tb(x) ternary alloy thin films with a thickness of about 10 nm were sputter deposited on MgO(100) substrates at 530°C (series I) and 700-770°C (series II). The Tb content x was varied in the range 5 - 28 at.%. Series I reveal limited L10 chemical ordering with an in-plane easy axis at room temperature. By addition of Tb higher than 11 at.%, a loss in crystallinity was observed. It is suggested that Tb is located as an interstitial atom to the FePt lattice, adding elastic stress to the lattice, eventually leading to amorphization of the local Tb environment. At low temperatures a spin reorientation transition (SRT), indicated by the appearance of strong perpendicular magnetic anisotropy (PMA), was observed. The SRT temperature increases linearly with addition of Tb. Higher deposition temperatures of 700-770 °C (series II) promote L10 chemical ordering with (001) orientation and strong PMA of 1.2 MJ/m3 at 300 K. However, with addition of Tb up to 6 at.%, PMA as well as coercivity get strongly reduced.

[1] A. Kirilyuk et al., Rev. Mod. Phys. 82, 2731 (2010).
[2] A. Hassdenteufel et al., Phys. Rev. B 91, 104431 (2015).

DS 11.4 Tue 10:15 H 0111

Structural analysis of epitaxial Ba_2SiO_4 thin films grown on Si(100) — •Julian Koch and Herbert Pfnür — Leibniz Universität Hannover, Inst. für Festkörperphysik, Appelstr. 2, 30167 Hannover

Ba_2SiO_4 is a very promising candidate as a high-k dielectric. Epitaxial films grown in a previous study [1] have shown a dielectric constant of 22.8 ± 0.2, band offsets to p-Si(100) of over 2 eV, a high temperature stability up to desorption at around 750 °C and an acceptable leakage current of 3 mA/cm^2 at -1 V. Unfortunately, these films still feature a high density of interface traps. The primary cause of this is most likely the growth mode of the silicate films, which were produced by heating the Si(100) substrate during the growth of a BaO film, so that a diffusion of Si from the substrate to the film occured turning the BaO into Ba_2SiO_4. This process resulted in an atomically rough interface in a geometric and possibly also in a chemichal sense. Moreover, only the first 5 nm close to the interface turned out to be crystalline.

This study aims to improve the structural quality of the Ba_2SiO_4 films by employing a co-deposition growth method, in which Ba and Si are evaporated simultaneously in an oxygen atmosphere. This eliminates the need for the Si diffusion. The chemical composition and the crystallinity of the films are investigated using XPS and SPA-LEED, respectively. To further investigate the crystalline growth, crystal orientation and thickness HRTEM is used.

DS 11.5 Tue 10:30 H 0111

Ionic and Ferroelectric Behavior of SbSI Films — •Sara Sand, Ka Kan Wong, Susanne T. Birkhold, Eugen Zimmerman, and Lukas Schmidt-Mende — University Konstanz, Konstanz, Germany

Thin film solar cells display many benefits due to their solution-based processing, allowing for inexpensive manufacturing and the possibility of devices on flexible substrates. Recently, perovskite solar cells have dominated this area of research due to their rapidly increasing efficiency, but this material still has many drawbacks due to its toxicity and lack of durability. Antimony sulfoiodide (SbSI) has been identified as a promising material for these applications, because it is much more stable and is similarly defect tolerant. It also has ferroelectric behavior with phase transition around room-temperature and its ionic characteristics. These two properties have been largely discussed in reference to perovskites, but, as of yet, their role in solar cell function is not well understood. The aim of this study is to investigate the ferroelectric and ionic characteristics of SbSI and their impact on solar cell devices. However, SbSI solar cells have not yet been reported in literature, as typical SbSI films possess very uneven surface structures composed of large crystallites. Here we present a novel approach to control the film formation of SbSI. By performing the two-step conversion process of SbSI under elevated pressure within a hot press, even and dense films of SbSI are achieved. Application of these films into devices will allow us to compare ferroelectric and ionic properties of perovskite and SbSI solar cells.

DS 11.6 Tue 10:45 H 0111

Orientation-dependent chemistry and band-bending of Ti thin layers on polar ZnO surfaces — •Patrizia Borghetti[1], Younes Mouchaal[1,2], Zongbei Dai[1], Gregory Cabailh[1], Rémi Lazzari[1], and Jacques Jupille[1] — [1]Sorbonne Universités, Institut des NanoSciences de Paris, F-75005, Paris, France. — [2]Laboratoire de Physique des Couches Minces et Matériaux pour l'Electronique (LPCMME), Université d'Oran 1 31000, Oran, Algeria

Next to its use to create ohmic contacts, the deposition of titanium on ZnO is known to promote adhesion for noble metals in optical coatings for glazings, to enhance the gas sensor properties of ZnO and to set up resistive random access memories. However the detailed mechanism of interface reactivity and the role of the surface orientation of ZnO in terms of species profile and chemical state are not yet resolved. In the present work, orientation-dependent reactivity and band-bending are evidenced by X-ray photoemission spectroscopy upon Ti deposition (1-10 Å) on the polar ZnO(0001)-Zn and ZnO(000-1)-O surfaces [1]. On Zn-ZnO, Ti reduces ZnO to form a Ti oxide, while on O-ZnO, the deposition of Ti gives rise to the formation of a (Ti, Zn, O) compound. A similar chemistry is observed upon annealing the Ti adlayers, although

with very different activation temperatures, 500 K on O-ZnO and 700 K on Zn-ZnO. Those orientation-dependent behaviours are expected to strongly affect applications relying either on thin Ti/ZnO films and partly explain why Ti/ZnO electrical contact properties are quite scattered and depend on annealing treatments and crystal orientation.

[1] P. Borghetti et al., Phys. Chem. Chem. Phys., 2017, 19, 10350.

DS 11.7 Tue 11:00 H 0111

Vertically aligned metal-ceramic nanocomposites: Self-assembly of ultrathin metallic nanowires embedded in oxide matrices — •Marcel Hennes[1], Xiaorong Weng[1], Dominique Demaille[1], Sarah Hidki[1], Emiliano Fonda[2], Yunlin Zheng[1], and Franck Vidal[1] — [1]INSP, UPMC Sorbonne Universités, CNRS UMR 7588, 4 place Jussieu, 75005 Paris, France — [2]Synchrotron SOLEIL, 91192 Gif-sur-Yvette, France

Vertically aligned metal – ceramic thin films constitute a novel class of hybrid materials characterized by the presence of metallic nanopillars embedded in a planar oxide matrix. For the development of these nanocomposites, pulsed laser deposition (PLD) synthesis relying on self-organized growth has recently emerged as a novel technique, complementing conventional template-assisted methods. On the one hand, self-assembly based procedures avoid cumbersome intermediate steps and permit to create arrays of ultrathin nanowires ($d < 5\,\mathrm{nm}$) with extremely high densities ($\rho > 10^{11}/\mathrm{cm}^2$). On the other hand, the metallic and oxide phases exhibit vertical epitaxial coupling, which paves the way for strain engineering and synthesis of artificial multiferroics. In the present contribution, we present results on magnetic nanocomposites and put special emphasis on the possibility to grow alloy wires (Co_xNi_{1-x} and Co_xPt_{1-x}), a simple and efficient strategy to control the magnetic anisotropy of the system. We also address remaining hurdles that have to be overcome to achieve full control of the final thin film nanoarchitecture.

15 min. break.

DS 11.8 Tue 11:30 H 0111

Growth of organic thin films on modified TiO2(110) surfaces — •Konrad Szajna[1], Markus Kratzer[2], Dominik Wrana[1], Wojciech Bełza[1], Benedykt Jany[1], Jacob Genser[2], Franciszek Krok[1], and Christian Teichert[2] — [1]Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow 30-348, Poland — [2]Institute of Physics, Montanuniversitaet Leoben, Franz Josef Straße 18, 8700 Leoben, Austria

The detailed growth morphology of vapor deposited para-hexaphenyl (6P) as model system of small organic molecules on modified TiO2(110) surfaces has been investigated by means of scanning probe microscopy. As substrates, atomically flat, air passivated and rippled ion beam modified TiO2(110) surfaces have been used. On pristine TiO2(110) crystalline needles consisting of flat lying 6P molecules are formed which extend along the [1-10] substrate direction. In contrast, on air exposed and ion beam modified surfaces island growth with an upright standing molecular configuration is favored. [1,2,3] The mechanisms that trigger the transition from flat lying to upright standing structures are discussed. Further the change in the stability of the 6P structures due to ion beam induced substrate rippling was tested by atomic force microscopy and is discussed.[3]

[1] M. Kratzer et al. PCCP 16, 26112 (2014)
[2] D. Wrana et al. JPCC 119, 17004 (2015)
[3] K. Szajna et al. JCP 145, 144703 (2016)

DS 11.9 Tue 11:45 H 0111

Hafnium oxide interface formation during ALD oxide growth on pure Hf films for resistive switches — •Stephan Aussen, Alexander Hardtdegen, Thomas Heisig, Christoph Bäumer, Regina Dittmann, and Susanne Hoffmann-Eifert — Peter Grünberg Institut and JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Oxygen exchange and drift/diffusion processes play a major role in redox-based resistive switching random access memories. Therefore, understanding oxidation/reduction reactions taking place already during the growth process is of utmost importance. In this study we investigate the oxidation behavior of pure Hf during atomic layer deposition (ALD) of stoichiometric oxide films (M′O) as Al_2O_3, TiO_2 and HfO_2 and the switching behavior of the resulting stacks. 25 nm thick sputtered Hf films with a low surface roughness < 0.2 nm were transferred under ultra-high vacuum conditions into an ALD system. Oxide layers were deposited at temperatures between 160 °C and 280 °C from amino-based precursor and O_2-plasma. The resulting stacks were investigated by angle resolved X-ray photoelectron spectroscopy to determine the thickness of the formed interfacial HfO_x layer as well as the valence states of the involved metal cations. The effect of the different ALD processes, e.g. Al_2O_3 as passivation layer, and influence of the temperature on Hf oxidation are discussed. In addition, complementary resistive switching experiments performed on equivalent stacks, i.e. Pt/M′O/HfO_x/Hf, revealed influence of the HfO_x interface formation on the switching behavior.

DS 11.10 Tue 12:00 H 0111

Epitaxial Ag thin films grown on biaxially textured IBAD-MgO template layers — •Sebnem Yazici[1] and Matthias Wuttig[2] — [1]I. Physikalisches Institute, RWTH Aachen, Germany — [2]I. Physikalisches Institute, RWTH Aachen, Germany

The heteropitaxial growth of thin metal films on ceramic substrates is of great scientific and industrial interest, due to their applications in electronic interconnects as well as catalysis and optical coating applications. Therefore, it is very important to examine the growth mechanism of the metal layer including wetting behavior to control crystalline properties and to determine the grain orientations as well as strain relaxations and electron transport mechanisms.

Biaxially ordered films produced by ion beam assisted deposition (IBAD) provides good templates for the heteroepitaxial growth of the functional layers. MgO is a very promising template layer for epitaxial Ag thin film growth since MgO can be deposited with rapid biaxial texture formation via IBAD technique. Besides, very similar in-plane lattice constants of Ag(100) and MgO(100), results in 4-fold symmetric cube-on-cube epitaxy. In this work, Ag thin films were deposited via magnetron sputtering on IBAD-MgO layers in order to study epitaxial relationship and electron transport mechanism of very thin Ag films. Biaxial texture formation in MgO layer depending on MgO layer thickness was investigated. Additionally, effects of post deposition annealing on Ag films grown on IBAD MgO films were analysed regarding crystallinity-texture improvement, stress relaxation and surface roughness via high resolution X-ray diffraction and AFM, respectively.

DS 11.11 Tue 12:15 H 0111

Influences of growth kinetics on interface structure and magnetism in $La_{1/3}Sr_{2/3}FeO_3/La_{2/3}Sr_{1/3}MnO_3$ heterostructures — •Markus Waschk[1], Jörg Voigt[1], Paul Zakalek[1], Juri Barthel[2], and Thomas Brückel[1] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT, 52425 Jülich, Germany — [2]Forschungszentrum Jülich GmbH, Ernst Ruska-Centre for Microscopy with Electrons (ER-C-2), 52425 Jülich, Germany

Transition metal oxide heterostructures like $La_{1/3}Sr_{2/3}FeO_3$/$La_{2/3}Sr_{1/3}MnO_3$ (LSFO/LSMO) has been chosen as a model system to study the interfacial coupling between an antiferromagnet (LSFO) and a ferromagnet with regard to different growth kinetics. Two epitaxial heterostructures (LSFO/LSMO and LSMO/LSFO) were grown with a combination of oxide molecular beam epitaxy and high oxygen sputtering on (001)-oriented $SrTiO_3$ substrates. Subsequent structural analysis with e.g. scanning transmission electron microscopy and energy dispersive X-ray spectroscopy revealed that the interface morphology depends crucially on the growth order. The interface in LSMO/LSFO is dominated by iron interdiffusion from the LSFO into the LSMO layer in at least nine monolayers, where Fe occupies the Mn sites. This leads to significant changes of the magnetic properties within the interface region. In contrast, LSFO/LSMO exhibits a sharp interface. Polarized neutron reflectometry was used to investigate the magnetization profile of both samples and revealed a highly reduced magnetization at the interface for the case of interdiffusion.

DS 11.12 Tue 12:30 H 0111

Room temperature atomic layer deposition for perovskite solar cells — •Malgorzata Kot[1], Lukas Kegelmann[2], Peter Kus[3], Nataliya Tsud[3], Iva Matolinova[3], Steve Albrecht[2], Vladimir Matolin[3], and Dieter Schmeisser[1] — [1]BTU Cottbus-Senftenberg, Konrad-Wachsmann-Allee 17, 03046 Cottbus — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Kekuléstraße 5, 12489 Berlin, Germany — [3]Department of Surface and Plasma Science, Charles University, Prague, 18000, Czech Republic

After few years of efficiency driven research on perovskite solar cells, the focus now is shifting to understand the underlying processes gov-

erning the high efficiency and also to obtain long-term stable devices. Among various deposition methods, atomic layer deposition (ALD) may represent one of the best options, being possible to coat substrates in a very efficient way and at very low temperatures. In our previous work [1] we reported that the efficiency of the solar cell containing aged perovskite film can be enhanced twice while covering the perovskite with a thin ALD alumina film at room temperature. In this work, the chemical, electronic and morphological properties of the fresh perovskite film treated by ALD pulses of the trimethylaluminium and water at room temperature investigated using X-ray Photoelectron Spectroscopy and Field Emission Scanning Electron Microscopy will be discused and correlated with the solar cells performance and stability.

[1] M. Kot et al., ChemSusChem 2016, 9, 3401.

DS 11.13 Tue 12:45 H 0111

Fabrication and structural characterization of diamond coated tungsten tips — •Alexander Tafel[1], Mingjian Wu[2], Erdmann Spieker[2], Peter Hommelhoff[1], and Jürgen Ristein[1] — [1]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen — [2]Department Material Science, Institute of Micro- and Nanostructure Research Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

Coating metal nanotips with a negative electron affinity material like hydrogen terminated diamond promises a high brightness photocathode. Dip seeding in detonation diamond suspensions in combination with nitrogen flow towards the tip apex and subsequent plasma enhanced chemical vapor deposition results in thin and dense diamond films along the tip from shaft to apex. The seeding density can even be controlled locally by the nitrogen flow, which counteracts forces occurring during solvent evaporation. With this technique a homogeneous coating of a complete tip with a dense and 100 nm thin diamond film as well as a selective coating of the tip apex only with 20 nm thin diamond were achieved. (HR)TEM and electron diffraction reveal that columnar nanocrystalline diamond with <110> texture and graphitic tissue between the grains was grown on the tungsten tip. An average of 17 % sp^2-bonded carbon is estimated from the fine structure of the C(1s) electron energy loss spectrum.

DS 11.14 Tue 13:00 H 0111

Formation and thermal stability of co-evaporated lead halide perovskite thin films (ABX_3, A=MA,Cs; B=Pb; X=I,Br,Cl) analysed by in situ XRD — •Paul Pistor, Thomas Burwig, Carlo Brzuska, Rene Csuk, Wolfgang Fränzel, and Roland Scheer — Martin-Luther-Universität Halle-Wittenberg, Halle(Saale), Deutschland

Methyl ammonium (MA) lead halide perovskites (e.g. $MAPbI_3$) are widely used to prepare efficient solar cells. In our group with have built a co-evaporation chamber equipped with a dedicated X-ray diffractometer, which allows us to study the formation and evolution of the different phases during thin film growth and under thermal stress. In this contribution, we show our investigation of the formation of single halide $MAPbI_3$, $MAPbBr_3$ and $MAPbCl_3$ thin films and their thermal decomposition into lead halides at temperatures between 150°C -250°C. Furthermore, the miscibility of $MAPbI_3$ and $MAPbBr_3$ is analyzed in detail. We find a preference for phase segregation if the formation is induced with $PbBr_2$ precursors, in contrast to the case where PbI_2 is used.

Then, $MAPbX_3$ is compared to its inorganic $CsPbX_3$ counterparts, where e.g. a stable cubic perovskite structure is easily obtained for $CsPbBr_3$, while for $CsPbI_3$ two polymorphs with cubic and orthorhombic crystal structure are observed at room temperature. Finally, we find that the inorganic $CsPbX_3$ thin films are thermally more stable and decompose at much higher temperatures (>300°C) through the evaporation of the PbX_2, leaving behind the corresponding cesium halide.

DS 12: 2D Materials: Session II (joint session DS/CPP/HL)

Time: Tuesday 9:30–13:15 Location: H 2032

DS 12.1 Tue 9:30 H 2032

Structural and electronic interactions in vdW heterostructure MoSe2/few-layer-graphene — •minh tuan dau[1], maxime gay[1], daniela di felice[2], céline vergnaud[1], alain marty[1], cyrille beigné[1], gilles renaud[1], olivier renault[1], pierre mallet[3], toai le-quang[3], jean-yves veuillen[3], loïc huder[1], vincent renard[1], claude chapelier[1], giovanni zamborlini[4], matteo jugovac[4], vitaliy feyer[4], yannick dapp[2], pascal pochet[1], and matthieu jamet[1] — [1]INAC-SPINTEC-PHELIQS-MEM, LETI, CEA/CNRS, Univ. Grenoble Alpes, F-38000 Grenoble, France — [2]SPEC, CEA, CNRS, Univ. Paris Saclay, CEA Saclay, 91191 Gif-sur-Yvette cedex, France — [3]Institut Néel, CNRS, Univ. Grenoble Alpes, F-38000 Grenoble, France — [4]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich GmbH, D-52425, Jülich, Germany

We have employed surface-sensitive techniques ranging from atomic resolution (STM-STS) to microscopic scale (synchrotron diffraction, photoemission electron microscopy k-PEEM) in order to probe structural and electronic properties of the van der Waals (vdW) heterojuction: MoSe2/few-layer-graphene grown by molecular beam epitaxy. We find that the crystallographic directions of the MoSe2 lattice align perfectly along the ones of graphene, resulting in only one commensurate configuration. Furthermore, we observe a clear evolution of the band structure of the heterojunction compared to the one of bare few-layer-graphene. Indeed, we evidence a large bandgap opening in few-layer-graphene resulting from significant charge transfer between vdW layers.

DS 12.2 Tue 9:45 H 2032

Interplay of magnetization between graphene and magnetoelectric multiferroics — •Zeila Zanolli — RWTH Aachen Uiniversity, Aachen, Germany

Graphene and magnetoelectric multiferroics are promising materials for spintronic devices with high performance and low energy consumption. We combine the features of both materials by investigating from first principles the interface between graphene and $BaMnO_3$, a magnetoelectric multiferroic. We show [1] that the hybrid systems behaves as a spin filter. Electron charge is transferred across the interface and magnetization is induced in the graphene sheet due to the strong interaction between C and Mn. A remarkably large proximity induced spin splitting of the Dirac cones (300 meV) is achieved and doping can make the high-mobility region of the electronic bands experimentally accessible.

Going further, we investigate spin dynamics at finite temperature using a Monte Carlo approach with exchange coupling parameters fitted from first principles. We find that graphene strongly affects the magnetic properties of the substrate, beyond the interface layer, and induces a softening of the Mn magnetization.

Spin Orbit Coupling calculations reveal that the influence of graphene on the substrate is even more radical and is able to change the direction of the easy axis with respect to the bare $BaMnO_3$ surface. We predict a Rashba splitting of the electronic bands near the K point, and the presence of a Quantum Anomalous Hall effect.

[1] Z. Zanolli, Sci. Rep., 6 (2016) 31346

DS 12.3 Tue 10:00 H 2032

Gate-Dependent Vacancy Migration in Graphene — •Rohit Babar[1] and Mukul Kabir[1,2] — [1]Department of Physics, Indian Institute of Science Education and Research, Pune, India — [2]Center for Energy Science, Indian Institute of Science Education and Research, Pune, India

Graphene based ultrathin devices offer significant advantage due to their high carrier mobility and a gate-tunable carrier density. However, the experimental observations of vacancy diffusion near room-temperature can potentially lead to undesirable void formation and/or edge modification of such devices. Combining transition state theory with first-principles method, we investigate the microscopic vacancy migration mechanism in graphene and its dependence on gate voltage. The intrinsic vacancy diffusion involves a concerted motion of atoms along with an out-of-plane displacement, which is unique to graphene compared with other 2D materials. We further investigate the migration mechanism under gate voltage and find that the activation barrier non-monotonically increases for both electron and hole doping. The trend in activation barrier is explained via collective-phonon stiffening.

We estimate a 10^7-fold decrease in vacancy diffusivity at room temperature. Thus, our findings reveal that the graphene-based devices will not degrade further under device operating condition through vacancy migration.

DS 12.4 Tue 10:15 H 2032

Transition between rhombohedral and Bernal stacking in multilayer graphene flakes — •Fabian Rudolf Geisenhof[1], Felix Winterer[1], and Ralf Thomas Weitz[1,2] — [1]Physics of Nanosystems, Physics Department, Ludwig Maximilians Universität München — [2]NanoSystems Initiative Munich (NIM) and Center for NanoScience (CeNS)

Quantum transport in multilayer graphene is interesting in many aspects. For example, it was shown that in ultraclean samples of graphene bilayers [1] and recently also multilayers [2], the exchange interaction leads to a novel phase, who's nature is currently still under debate. At the heart of answering this question is knowledge of the local stacking order during charge transport experiments. Here, we show that the fabrication process has an impact on the structural properties of the flakes. It can lead to the formation of ripples and even to a non-local transition from ABC to ABA stacking. This transformation has been identified by spatially resolved Raman and scattering SNOM measurements, and we discuss possible reasons.

[1] R.T. Weitz, M.T. Allen, B.E. Feldman, J. Martin, and A. Yacoby, "Broken-symmetry states in doubly gated suspended bilayer graphene", Science 330, 812 (2010)

[2] Y. Nam, D.-K. Ki, M. Koshino, E. McCann and A.F Morpurgo, "Interaction-induced insulating state in thick multilayer graphene", 2D Mater. 3 045014 (2016)

DS 12.5 Tue 10:30 H 2032

Chemical vapour growth and delamination of α-MCl3 nanosheets (M = Ru, Mo, Ti) — •Martin Grönke[1,2], Silke Hampel[1], Peer Schmidt[2], Danny Pohflepp[1], Nadine Bronkalla[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Brandenburg University of Technology Cottbus-Senftenberg, Germany

The two dimensional honeycomb structure of graphene with one monoatomic layer gave an idea to the introduction of other materials with congeneric pattern. Next to carbon based graphene, black phosphorus and binary transition metal chalkogenides, transition metal halides were highly profiled in theory. Among the interest for different materials with strong anisotropic bonding-dependent interactions, resulting frustration effects in honeycomb structures could stabilize new pattern of cooperative magnetic interactions. One candidate to realize a Kitaev Heisenberg (KH) model is the 2D layered honeycomb magnet α-Rutheniumtrichloride (α-RuCl3). Physical properties in nanoscale systems may differ from the respective bulk phase and could even lead to novel physical properties. We herein present to our knowledge the first approach to synthesize phase pure α-RuCl3 crystals on the nanoscale on a substrate via chemical vapour transport (CVT). Beyond that we reveal capabilities to generate thin 2D structures of isostructural compounds like α-MoCl3 and α-TiCl3 on a suitable substrate by means of CVT. Furthermore we show how to increase the number of nanosheets on as grown substrates by different delamination techniques.

DS 12.6 Tue 10:45 H 2032

Suppression of excitonic absorption in few-layer GaSe — •Arne Budweg[1], Dinesh Yadav[1,2], Alexander Grupp[1], Alfred Leitenstorfer[1], Maxim Trushin[1,3], Fabian Pauly[1,2], and Daniele Brida[1] — [1]Department of Physics and Center for Applied Photonics, University of Konstanz, D-78457 Konstanz, Germany — [2]Okinawa Institute of Science and Technology Graduate University, Onna-son, Okinawa 904-0395, Japan — [3]Centre for Advanced 2D Materials, National University of Singapore, 6 Science Drive 2, Singapore 117546

We study the thickness dependent optical absorption of GaSe via highly sensitive differential transmission measurements. Controlling the number of individual layers in a GaSe nanosheet, we observe a suppression of the excitonic transition below a critical value of 8. Ab-initio modelling enables us to attribute this behavior to a fundamental change in the band structure which, in thin GaSe, leads to a valence band shaped as an inverted Mexican hat. The observed modulation of the optical properties is intrinsic and does not require control via external parameters like substrate material or an applied electric field. Therefore GaSe provides attractive resources for the development of functional optoelectronic devices based on a single material.

DS 12.7 Tue 11:00 H 2032

Lateral heterostructures for sensing small molecules: electronic current features — Ganesh Sivaraman[1], Frank C. Maier[1], Fabio A.L. de Souza[2], Rodrigo G. Amorim[3], Wanderla L. Scopel[2], Ralph H. Scheicher[4], and •Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Departamento de Fisica, Univer- sidade Federal do Espirito Santo, Brazil — [3]Universidade Federal Fluminense, Departamento de Física, Volta Redonda/RJ, Brazil — [4]Department of Physics and Astronomy, Materials Theory, Uppsala University, SwedenDe

Using density functional theory based calculations with the non-equilibrium Greens functions approach, we study in detail the structural, transport, and electronic properties of two types of lateral 2D heterostructures. The first is a combination of graphene with hexagonal boron-nitride (G/hBN). The second is a (1T) metallic MoS_2 phase embedded in a (2H) semiconducting MoS_2 phase (1T/2HMoS_2). Our results identify the importance of the interface within these materials and provide the relation to the electronic current flowing across these. Having understood the basic properties of these structures, we further reveal their high potential and relevance in detecting small molecules. On one hand, we show that the G/hBN heterostructure can detect small gas molecules. On the other hand, by opening a small pore in the 1T/2HMoS_2 heterostructure, we can distinguish between DNA nucleotides. Proof of both detection schemes is provided through the distinct electronic properties and the clear electronic current signals for the various molecules and each heterostructure.

15 min. break

DS 12.8 Tue 11:30 H 2032

Thickness dependent electronic and optical properties of TMDCs within many-body perturbation theory — •Philipp Marauhn, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Experimental studies have shown that the spectrum of MoS_2 and other TMDC materials strongly depends on the number of layers of the system. With increasing thickness of a system, the optical absorption spectrum is generally shifted to lower energies.

In this talk we address this behaviour from a theoretical point of view. To investigate the excited electronic states of the TMDCs, we perform three consecutive steps: (i) DFT (ii) *GW* (iii) BSE (Bethe-Salpeter equation). Our results show that both the fundamental quasiparticle gap and the exciton binding energy are significantly reduced when the number of layers is increased. These two effects do not perfectly compensate each other, but lead to an effective shift of the excitation energies towards lower energy. This redshift with increasing number of layers is in agreement with experimental differential reflectance measurements [1]. We also find significant changes in the wave function of some exciton resonances with increasing sample thickness. In multilayer systems, excitons may be composed from electrons and holes situated on different layers, which can be considered as interlayer excitons [2].

[1] Y. Niu et. al., submitted
[2] A. Arora et. al., Nat. Commun., 8(1), 639 (2017)

DS 12.9 Tue 11:45 H 2032

Elasticity theory for two dimensional systems at finite temperatures — •Johannes Häring and Matthias Fuchs — FB Physik, Universität Konstanz, 78457 Konstanz, Germany

According to the Mermin-Wagner theorem many two dimensional systems only exhibit quasi-long-range order. Recently, we developed an elasticity theory for crystals with point defects and applied it to the defect rich cluster crystal [1]. The theory is able to handle long-range translational order. Now we present a method which includes quasi-long-range order.

Furthermore, orientational degrees of freedom are considered as well. As an example results of the helicity modulus and dynamical matrix of the two dimensional XY model are presented. Temperatures range between zero and the Kosterlitz-Thouless transition.

Finally, the influence of topological defects like vortices is discussed.

[1] J.M. Häring, C. Walz, G. Szamel, and M. Fuchs, Phys. Rev. B **92**, 184103 (2015)

DS 12.10 Tue 12:00 H 2032

Ab Initio Study of the Electronic and Optical Properties of Organic-Inorganic two-dimensional Perovskites: The Role of Many-Body Effects — •Maurizia Palummo[1] and Giacomo Giorgi[2] — [1]INFN and Dip. Fisica University of Roma "Tor Vergata" Via della ricerca scientifica 1 Rome Italy — [2]Dip. Ing. Civile e ambientale Univ. Perugia Italy

Organic-Inorganic Halide Perovskites (OIHPs) represent the most relevant breakthrough in the last decade in photovoltaics (PV) Despite the many attractive features, some serious issues remain that prevent their usage in device mass production, such as the fast air/moisture induced degradatio. For this reason, in the last years two-dimensional Ruddlesden-Popper perovskites (2D-RPOIHPs) have emerged as an alternative to 3D bulk for their superior photo- and chemical-stability coupled with high-performance opto-electronic properties and an enhanced hydrophobic nature of the organic part. While the experimental interest towards this 2D class of materials is nowadays well assessed, ab-initio studies focusing on the role of many-body effects are very limited. By means of a coupled GW plus BSE approach on top of DFT-KS simulations, we here study the electronic and optical properties of a 2D-RPOIHP, as a single sheet and also as a periodic QW. A giant band-gap renormalization of the electronic band-gap and the formation of a strongly bound almost 2D excitons are observed. The relationship between the number of layers is discussed.

DS 12.11 Tue 12:15 H 2032

Layered van der Waals crystals with hyperbolic light dispersion — •Morten Gjerding — DTU Physics, Fysikvej building 311, 2800 Kgs. Lyngby

Compared to artificially structured hyperbolic metamaterials, whose performance is limited by the finite size of the metallic components, the sparse number of naturally hyperbolic materials recently discovered are promising candidates for the next generation of hyperbolic materials. Using first-principles calculations, we extend the number of known naturally hyperbolic materials to the broad class of layered transition metal dichalcogenides (TMDs). The diverse electronic properties of the transition metal dichalcogenides result in a large variation of the hyperbolic frequency regimes ranging from the near-infrared to the ultraviolet. Combined with the emerging field of van der Waals heterostructuring, we demonstrate how the hyperbolic properties can be further controlled by stacking different two-dimensional crystals opening new perspectives for atomic-scale design of photonic metamaterials. As an application, we identify candidates for Purcell factor control of emission from diamond nitrogen-vacancy centers.

DS 12.12 Tue 12:30 H 2032

Influence of Hansen solubility parameters on a shear exfoliation process of organophilic layered silica in chloroform — •Michael Huth, Jonas Köhling, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Nanocomposites based on layered silica can be used for several applications, like reinforcement, flame retardant agent, or barrier applications. The understanding of delamination processes of layered silica in organic solvents/polymers is a critical step towards preparing such nanocomposites. In this work, layered silicas with different intercalated molecules are used. Those molecules change the silica surface interaction energies described by Hansen solubility parameters (HSP). HSP of four different synthetic organophilic layered silicas are determined. This allows calculating the dispersibility in chloroform via the Flory-Huggins (F-H) parameter. The F-H parameter can predict the delamination state of organophilic layered silicas in solvents. The delamination state is evaluated quantitatively using atomic force microscopy (AFM). In the case of a high F-H parameter ($\chi > 0.15$), aggregated and unstable layered silica dispersions are found. Whereas in the case of F-H parameters near zero, exfoliated and stable layered silica dispersions are obtained. Additionally, the presence of the surfactant on the surface of fluoromica flakes after exfoliation is proven by Fourier-transform infrared spectroscopy (FT-IR), and density functional theory (DFT) calculations.

DS 12.13 Tue 12:45 H 2032

Theoretical description of photoemission spectroscopy of van der Waals structures — •Bruno Amorim — CeFEMA, Instituto Superior Técnico, University of Lisbon, Av. Rovisco Pais, PT-1049-001 Lisboa, Portugal

I present a general theory to model the angle resolved photoemission spectroscopy (ARPES) of van der Waals (vdW) structures. VdW structures are formed by lattice mismatched and/or misaligned stacked layers of two-dimensional materials and can be commensurate or incommensurate.

The present theory is based on a tight-binding description of the bound electrons and the concept of generalized umklapp processes, being capable of describing both commensurate and incommensurate structures for arbitrary lattice mismatch/misalignment. In this way, the present theory goes beyond previous descriptions of ARPES in incommensurate vdW structures, which are based on continuous, low energy models, which limits their applicability to structures with small lattice mismatch/misalignment.

As an example, I apply the general method to the case of twisted bilayer graphene, obtaining the ARPES bands and ARPES constant energy maps.

The present theory should be useful in correctly interpreting experimental results of ARPES of vdW structures and other system displaying competition between different periodicities, such as density wave phases.

DS 12.14 Tue 13:00 H 2032

Manipulating the Mechanical Properties of Ti2C MXene: Effect of Substitutional Doping — •Poulami Chakraborty[1], Tilak Das[2], Dhani Nafday[1], Lilia Boeri[3], and Tanusri Saha-Dasgupta[1] — [1]Department of Condensed Matter Physics and Materials Science, S.N.Bose National Centre for Basic Sciences, JD Block, Sector-3, Salt Lake , Kolkata 700106, India — [2]Department of Physical Sciences, Indian Institute of Science Education and Research-Kolkata, Mohanpur Campus, PO BCKV Campus Main Office, Nadia * 741252, West Bengal, India — [3]Institute for Theoretical and Computational Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria

Two-dimensional transition metal carbides/nitrides $M_{n+1}X_n$ termed as MXenes have attracted immense interest as potential candidates for Li-ion battery anodes and as a hydrogen storage medium. Our work focuses on the specific case of Ti_2C and Ti_2CO_2 under various tensile strain using density functional theory (DFT). We consider substitutional doping of B and V at Ti and C sites of Ti_2C. We have studied substitutional doping with no surface termination as well as oxygen terminated Ti_2C, i.e., Ti_2CO_2. In-plane stiffness, Young's modulus, and critical strain calculations conclude that B doping is highly effective in improving the elastic properties. This trend is found to hold good even for B-doped and V-doped O terminated systems. However the O passivated compounds are found to have relatively higher critical strain values compared to their pristine counterparts. Thus B doped Ti_2CO_2 , $Ti_2(C_{0.5}, B_{0.5})O_2$, appears to be the best candidate among the studied systems, as compared to pure Ti_2C.

DS 13: Oxide Semiconductors for Novel Devices (Focussed Session): Session III

The class of semiconducting oxides includes low temperature processed amorphous thin films for bendable electronics and display technology as well as highly crystalline materials such as the wide band group-III sesquioxides being interesting for UV and DUV photo sensors, power electronics and even memristors. This session sets a focus on physical properties of such oxides, their growth methods and heterostructures for demonstrator devices. This focus session is supported by the Leibniz ScienceCampus GraFOx.

Organized by

Dr. Karsten Fleischer School of Physics, Trinity College Dublin, the University of Dublin Dublin 2, Ireland

Dr. Holger von Wenckstern Universität Leipzig Felix-Bloch-Institut für Festkörperphysik Halbleiterphysik Linnéstraße 5 04103 Leipzig, Germany

Prof. Dr. rer. nat. Holger Eisele Experimental Physics Technische Universität Berlin Department for Mathematics and Science Institute of Solid State Physics Hardenbergstr. 36, Sekr. EW 4-1, D-10623 Berlin, Germany

Dr. Oliver Bierwagen Paul-Drude-Institut für Festkörperelektronik (PDI) Hausvogteiplatz 5-7 10117 Berlin, Germany

Time: Tuesday 9:30–11:30 Location: E 020

Invited Talk DS 13.1 Tue 9:30 E 020

Electron transport in beta-gallium oxide — •Rebecca L. Peterson[1], Zumrad Kabilova[1], and Cagliyan Kurdak[2] — [1]Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, USA — [2]Department of Physics, University of Michigan, Ann Arbor, Michigan, USA

The sesquioxide semiconductor gallium oxide is currently drawing attention for power electronics and deep ultraviolet optoelectronics applications, due to its ultra-wide bandgap. Gallium oxide has several crystal polytypes. The stable beta-phase has a bandgap of approximately $4.8\,eV$, a monoclinic crystalline structure, and bulk substrates are commercially available. Here, we present our experimental and theoretical work on charge transport in bulk (010) $\beta - Ga_2O_3$, in which the extrinsic tin doping of $10^{18}\,cm^{-3}$ is close to the Mott metal-insulator transition point. A peak electron mobility of $95\,cm^2V^{-1}s^{-1}$ was measured at 185K. Across a wide temperature range, a two-band conduction model applies, consisting of a impurity band in parallel with the conduction band, as was observed previously for n^{++} $(\bar{2}01)\,\beta - Ga_2O_3$ [1]. At low temperature, we find that conduction is via variable-range hoping through the impurity band. At high temperatures, phonon scattering of conduction band electrons dominates, similar to lightly-doped $(100)\,\beta - Ga_2O_3$ [2]. This work was supported by DARPA/SPAWAR under award N66001-14-1-4046. [1] T. Oishi, K. Harada, Y. Koga, and M. Kasu: Japan. J. Appl. Phys. 55, (2016) 030305; [2] A. Parisini and R. Fornari, Semicond. Sci. Technol. 31, (2016) 035023.

Invited Talk DS 13.2 Tue 10:00 E 020

Deep level defects in bulk and epi-grown β-Ga2O3 — •Lasse Vines — University of Oslo, Norway

After the early work on gallium oxide (Ga2O3) in the mid-1900s, a renewed interest has recently emerged on behalf of its prospects in power electronics and UV devices. Particularly, the monoclinic β-Ga2O3 phase attracts interest due to its band gap of ~ 4.8 eV and n-type conductivity, and where promising MOSFET devices have already been demonstrated. However, while controlling charge carrier and defect concentrations is essential for high power and high temperature devices, the understanding of the electrically active defects and dopants is still in its infancy. Here, the present status of controlling electrical properties of β-Ga2O3 will be reviewed, and recent progress in understanding electrically active defects and dopants will be discussed. In particular, recent results combining deep level transient spectroscopy with secondary ion mass spectrometry and ion irradiation on a range of different samples will be shown. The results reveal both intrinsic and extrinsic defects present in the samples, and give insight into the nature new and previously reported energy levels. For example, iron is shown to be an important impurity in bulk samples with an energy level position around 0.78 eV below the conduction band edge, acting as a deep compensating center, while irradiation demonstrate the appearance of a nearby intrinsic defect level, and the results are further supported by density functional calculations

Invited Talk DS 13.3 Tue 10:30 E 020

Indium Oxide and its surface electrons – a model system to study gas interaction and metal/semiconductor junctions — •Marcel Himmerlich, Theresa Berthold, Jonas Michel, Simeon Katzer, and Stefan Krischok — Institut für Physik & IMN Macro Nano, Technische Universität Ilmenau, Germany

The electron accumulation at Indium Oxide surfaces is beneficial for electronic devices that rely on adsorption processes such as gas sensors. However, it is a drawback for electron transport devices since it hinders the fabrication of rectifying metal contacts. In both cases, the manipulation of the electron density by surface reactions is one approach to optimize performance. We analyze the underlying mechanisms of adsorption processes and the formation of metal/semiconductor contacts using model in-situ experiments. For the interaction with O_2, O_3, H_2O, CO and NO_x, a clear correlation exists between adsorbate-semiconductor charge transfer, density of surface charge carriers, and the conductivity of the material. If In_2O_3 is treated by a reactive oxygen plasma, the surface electron layer is fully depleted generating a barrier for interface transport. Photoelectron spectroscopy measurements reveal that adsorption of Pt on these modified surfaces results in sufficient Schottky barriers for rectifying contacts, but fabricated devices fail. It will be demonstrated that the oxygen-rich Pt/In_2O_3 interface is critical in stability and that oxidation of Pt-based contacts is beneficial to enhance electronic barriers and to exploit the effect of electron depletion via oxygen plasma modification. Combining both processes enables performance improvement of In_2O_3 Schottky diodes.

Invited Talk DS 13.4 Tue 11:00 E 020

Phonons and excitons in Ga_2O_3 polytypes — •Markus R. Wagner — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

We present a comparative experimental study of the optical, vibrational and thermal properties of Ga_2O_3 in the alpha-, beta-, gamma-, and epsilon-modification. The anisotropic band gap energies are probed by the observation of deep UV excitation channels using temperature-dependent, polychromatic photoluminescence excitation spectroscopy (PLE). Based on these experiments, we establish an order of the bandgap for the different polymorph of Ga_2O_3. In addition, we investigate the optical phonon modes of the different structural configurations of Ga_2O_3 by polarized and angular resolve micro-Raman spectroscopy. Finally, we compare the temperature-dependent thermal conductivity of the four different Ga_2O_3 polytypes as obtained by 3-omega measurements. The results are discussed considering phonon boundary scattering and size effects due to structural imperfections and reduced dimensionality in ultra-thin films.

DS 14: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials III (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Tuesday 10:30–13:00 Location: HL 001

DS 14.1 Tue 10:30 HL 001

Control and prediction of molecular crystal properties by multilevel strategies — •Jan Gerit Brandenburg — London Centre for Nanotechnology, Department of Physics and Astronomy, University College London, 20 Gordon Street, London, U.K.

Computational material science is a dynamic and thriving area of modern scientific research. Approaches based on the fundamental laws of quantum mechanics are now integral to almost any materials design initiative in academia and industry, underpinning efforts such as the Materials Genome initiative or the computational crystal structure prediction [1]. I will present a hierarchy of quantum chemical methods designed for this purpose, in particular targeting molecular crystals and their property prediction. The methods range from high-level diffusion Monte-Carlo (DMC) to London dispersion inclusive DFT, and thus, cover many orders of magnitudes in computational efficiency [2,3]. I will demonstrate the application to the 6^{th} blind test for organic crystal structure prediction. Comparisons to other state-of-the-art methods indicate both success and remaining challenges in the recent method developments [4].

[1] S. L. Price and J. G. Brandenburg, *Molecular Crystal Structure Prediction*; Elsevier Australia, **2017**.

[2] A. Zen, J. G. Brandenburg, J. Klimeš, A. Tkatchenko, D. Alfè, A. Michaelides, **2017**, *submitted*.

[3] J. G. Brandenburg, E. Caldeweyher, S. Grimme, *Phys. Chem. Chem. Phys.* **2016**, *18*, 15519.

[4] A. M. Reilly, et al. *Acta. Cryst. B* **2016**, *72*, 439.

DS 14.2 Tue 11:00 HL 001

Advances in first-principles and model spin Hamiltonian simulations of point defects in semiconductors for quantum sensors and computing — •Viktor Ivády — Department of Physics, Chemistry and Biology, Linköping University, 581 83 Linköping, Sweden — Wigner Research Center for Physics, Konkoly-Thege Miklós út 29-33, 1121 Budapest, Hungary

First principles simulations play a key role in understanding the physics of point defects in semiconductors, while model spin Hamiltonian approaches are traditionally used to interpret experimental spin dependent observations and describe the spin dynamics of point defects. The development of novel point defect applications, such as quantum bit (qubit) and single photon emitter applications for quantum information processing and quantum sensing, requires detailed understanding of spin-related couplings and addressability of localized defects states in the bath of delocalized electrons that calls for further development and implementation of theoretical tools. Here, I report on my contribution to this field that covers 1) first principles studies for identification of point defect based qubits and single photon emitters , 2) method development for the description of point defects with correlated electron states, 3) implementation of zero-field-splitting calculation for point defect based qubits, 4) development of model spin Hamiltonian approaches for the simulation of optical dynamic nuclear polarization process (ODNP) of point defects, and 5) spin dynamic simulation of existing point defect qubits. As an outlook, I discuss the requirements toward fully-ab initio point defect spin dynamic simulations.

DS 14.3 Tue 11:30 HL 001

Recent advances in first-principles modelling of correlated magnetic materials — •Yaroslav Kvashnin — Department of physics and astronomy, Uppsala University, BOX 516, 75120 Uppsala

Most of modern first-principles electronic structure studies of correlated materials are based on a combination of density functional theory and dynamical mean field theory (DFT+DMFT).

Addressing magnetic materials within DFT+DMFT has certain peculiarities. There are two recipes one can follow: either to account for magnetism within the DFT functional or to introduce it entirely within the self-energy. Both approaches have their flaws and advantages, which are well-known for DFT+U, but are not often discussed for DFT+DMFT. In my talk I will present a systematic comparison of the two methods and demonstrate the evidences favouring the use of non-polarised functionals.

Next, I will demonstrate how the obtained electronic structure information can be used to simulate finite-temperature magnetic properties in real materials. I employ a so-called two-step approach. First, I map the system on a Heisenberg model and extract the effective exchange parameters Jij's from DFT+DMFT. Then the atomistic spin dynamics simulations are used to simulate magnon spectra and predict the magnetic ordering temperatures.

I will demonstrate the power of such an approach by showing a direct comparison with available experimental data for a wide range of different materials.

DS 14.4 Tue 12:00 HL 001

A first-principles approach to hot-electron-induced ultrafast dynamics at metal surfaces — •Reinhard J. Maurer — Department of Chemistry, University of Warwick, Gibbet Hill Road, CV4 7AL Coventry, UK

Low-lying electronic excitations in metals, so-called hot electrons, couple efficiently to molecular adsorbate motion. In doing so, they give rise to a number of curious experimental observations. This includes picosecond-scale energy loss of molecular adsorbate vibration, highly inelastic atomic and molecular scattering from metal surfaces, and light-assisted molecular desorption and chemical transformations, recently coined "hot-electron chemistry". In this talk, I will present a first-principles treatment of hot-electron-induced molecular dynamics based on Density Functional Theory that correctly captures the magnitude and mode-specificity of hot-electron mediated adsorbate-substrate energy transfer [1]. Utilizing our efficient all-electron local-orbital implementation of hot-electron-induced frictional forces based on Time-Dependent Perturbation Theory, [2] I will show how we correctly capture vibrational relaxation in large-scale metal-mounted molecular catalysts as well as the energy loss and coupled electron-nuclear dynamics of small molecular adsorbates in both thermal and laser-heated conditions. [3] We scrutinize our approach in comparison to recent Sum-Frequency Generation (SFG) spectroscopy and molecular beam scattering experiments. [1] Phys. Rev. Lett. 116, 217601 (2016) ; [2] Phys. Rev. B 94, 115432 (2017); [3] Phys. Rev. Lett. 118, 256001 (2017);

DS 14.5 Tue 12:30 HL 001

Temperature effects in spin-orbit physics from first principles — •Bartomeu Monserrat — University of Cambridge, UK — Rutgers University, USA

The spin-orbit interaction drives a number of physical phenomena, including the band inversion in topological insulators and the spin splitting of electronic bands in inversion asymmetric crystals. In this work, we study the effects of finite temperature on such spin-orbit physics, including both thermal expansion and electron-phonon coupling effects [PRB 92, 184301 (2015)].

First, we describe the temperature dependence of the inverted gap in topological insulators. We find that increasing temperature reduces the topological gap in the Bi2Se3 family of materials, and we predict a temperature-induced topological phase transition in Sb2Se3 [PRL 117, 226801 (2016)].

Second, we study the temperature dependence of the spin splitting of electronic bands in both inversion symmetric and asymmetric crystals. We predict a dynamical spin splitting in centrosymmetric crystals and characterise the associated phenomenology in the cubic perovskite CsPbCl3 [arXiv:1711.06274]. In inversion asymmetric crystals, exemplified by the bismuth tellurohalides, we find that increasing temperature suppresses the static spin splitting arising from the Rashba effect [PRM 1, 054201 (2017)].

DS 15: Thermoelectric and Phase Change Materials

Time: Tuesday 11:45–13:00 Location: E 020

DS 15.1 Tue 11:45 E 020

Thermoelectric nanocrystalline SiGe thin films prepared by the combination of AIC and SiO2 reduction — •Marc Lindorf, Anna Zera, and Manfred Albrecht — Institute of Physics, University of Augsburg, Universitätsstraße 1, Augsburg, Germany

Classic thermoelectric materials like SiGe often face low efficiencies for practical applicability while also being held back by industrial inefficient preparation and implementation methods.

In this work, we present a thin film approach for the preparation of nanocrystalline SiGe. The process of aluminum induced crystallization (AIC) is utilized to transform sputter deposited amorphous Si80Ge20 on quartz glass (SiO2) in a polycrystalline state under the presence of Al. Parts of the Al are incorporated into the SiGe leading to p-type doping. The reduction of SiO2 by Al to Si and Al2O3 was used after the catalytic AIC process to remove the remaining metallic Al which otherwise would shortcut the thermoelectric SiGe layer [1].

The AIC processed SiGe thin films were structurally analyzed via Rutherford Backscattering Spectrometry, X-ray Diffraction, and Transmission Electron Microscopy before and after annealing. The Si atoms released by the reduction reaction were incorporated to the SiGe layer without forming a secondary phase. Furthermore, a thermoelectrically promising twin grained microstructure was found for the prepared SiGe. Electrical resistivity and Seebeck coefficient were characterized from room temperature up to 700 K revealing transport properties typical for degenerated semiconductors.

[1] M. Lindorf et al., J. Appl. Phys. 120, 205304 (2016)

DS 15.2 Tue 12:00 E 020

Intermixing of SnTe-GeTe superlattices grown by molecular beam epitaxy — •Kaminski Marvin[1], Pohlmann Marc[1], Meledin Alexander[2], Cojocaru-Mirédin Oana[1], and Wuttig Matthias[1,3] — [1]I. Institute of Physics, Physics of New Materials, RWTH Aachen University, 52056 Aachen, Germany — [2]Gemeinschaftslabor für Elektronenmikroskopie, RWTH Aachen, 52074 Aachen, Germany — [3]JARA-Insitut Energy-efficient information technology (PGI-10), FZ Jülich, 52428 Jülich, Germany

Since its first report in 2013 interfacial phase-change materials (IPCMs) attract plenty of attention. Classical phase change materials (PCM) on the one hand can be switched between the amorphous and the crystalline state. These two states can be switched by joule heating on a ns time scale and differ in orders of magnitude in resistance and up to 20 % in reflectivity. Due to this rare combination of properties PCM are one of the most promising candidates for data storage. IPCMs also switch, if a defined voltage is applied. However, experimental and theoretical results indicate that the switching in IPCMs does not rely on a transition between amorphous and crystalline states, but rather between different crystalline states. The switching in IPCMs is faster and needs less energy than classical PCM.

Here, we present superlattices of SnTe and GeTe layers on Si(111) substrate via MBE. One focus of our work lays on the intermixing of the layers and its dependence on the chosen growth temperatures. Therefore we compare results of different methods like TEM, atom-probe tomography, XRD and RHEED for different growth conditions.

DS 15.3 Tue 12:15 E 020

The Influence of Disorder on the Electrical Properties of SnTe-PbTe Alloys in the Vicinity of the Band Inversion — •Johannes Reindl[1], Zheng Zeng[1], Matteo Cagnoni[1], Alexander Rochotzki[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

Chalcogenide IV-VI compounds are well known to exhibit a plethora of intriguing physical properties, like symmetry protected topological surface states in SnTe or high thermoelectric performance in PbTe. Alloys of these two materials have been utilized for infrared applications because of the tunable small band gap. Furthermore, the combination of SnTe and PbTe yields the model system for the investigation of topological crystalline insulators.

So far research in general was focused on the study of samples with high quality to disentangle the underlying physical phenomena. However, having disorder and defects in the crystal, is not only more feasible or sometimes even beneficial for industrial application, but might also unveil new physical insight. Therefore, with a combination of conductivity, Hall and Seebeck measurements, we investigate the electrical properties of thin films with the stoichiometry being close to the band inversion.

DS 15.4 Tue 12:30 E 020

Modeling of current-voltage characteristics of BFO based memristors — •Max Huber[1,2], Andreas Zienert[3], Jörg Schuster[2], and Michael Schreiber[1] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany — [3]Center for Microtechnologies, Technische Universität Chemnitz, Chemnitz, Germany

Memristors are one of the most promising candidates for next generation memory. They can also be used for nonvolatile logic application, neuromorphic computing and hardware based encryption.

To build high performance devices, one has to know the mechanism behind the resisitive switching. Dependent on the material, the device can show filamentary or interface resistive switching. Despite the increasing interest of the scientific community in studying resistive switching, detailed knowledge of the switching mechanism for many materials is still missing.

We study $BiFeO_3$ (BFO) based memristors which show interface resistive switching. The device is modeled as a serial connection of two head-to-head diodes. To simulate the current-voltage characteristic we solve the drift-diffusion and Poisson's equation selfconsistently and assume the doping profile is constant in time.

DS 15.5 Tue 12:45 E 020

Thermoelectric properties of (Iron) Cobalt Monosilicide — •Lauritz Schnatmann[1], Heiko Reith[1], Gabi Schierning[1], Kornelius Nielsch[1], and Alexander Burkov[2] — [1]Leibniz institute for solid state and material science, Dresden, Germany — [2]Ioffe institute, St. Petersburg, Russia

Good thermoelectric materials need a high electrical conductivity and a low thermal conductivity. Common thermoelectric materials at room temperature are for example Bi2Te3 or Sb2Te3, which are toxic and rare materials. Promising alternatives are the silicides, because they are non-toxic and abundant. They also show a relatively high thermoelectric performance and are possible candidates for Weyl materials. Co1-xFexSi Samples were grown by Bridgeman method. Structure and chemical analysis of the samples were made by XRD, TEM and EDX. Afterwards we performed temperature and magnetic field dependent measurements on different silicide-compositions. Thermal conductivity, Seebeck-coefficient and electrical conductivity were measured with the thermal transport option of a Dynacool system by Quantum Design. In the structure analysis we identified the B20 crystal structure in our sample with a [111] orientation perpendicular to our measurement direction. In the magnetic field dependent measurements we analyse the difference between parallel and perpendicular applied magnetic fields in respect to the measurement direction. In parallel applied field we observed a negative magneto resistance with a maximum at 50K. For a perpendicular applied field we see a positive magneto resistance.

DS 16: 2D materials: Graphene and BN (joint session HL/DS)

Time: Tuesday 14:00–15:45 Location: A 151

DS 16.1 Tue 14:00 A 151

Field-effect proximity exchange coupling in bilayer graphene on ferromagnetic insulator — •Klaus Zollner, Martin Gmitra, and Jaroslav Fabian — Institute for Theoretical Physics, Regensburg, Germany

Graphene can be made magnetic by proximity effect through ferromagnetic substrates. We show, by realistic first-principles calculations, that bilayer graphene on $Cr_2X_2Te_6$, a family of ferromagnetic insulators that can be exfoliated in single layers (X = Si and Ge), experiences a layer dependent proximity exchange effect [1]. Due to short range of this proximity effect and the intrinsic layer dependent formation of low energy bands in bilayer graphene, only the valence band gets spin split. In addition, we apply realistic electric fields across the heterostructure, to tune the potential energy of the bilayers and find that we can switch electron and hole bands, along with the exchange splitting. With that we predict fully electrically tunable magnetism for transport carriers, which opens a vast field of proximity spintronics.

This work was supported by DFG SPP 1666, SFB 689, SFB 1277, and by the European Unions Horizon 2020 research and innovation programme under Grant agreement No. 696656.

[1] K. Zollner, M. Gmitra, and J. Fabian, arXiv:1710.08117 (2017).

DS 16.2 Tue 14:15 A 151

Spin-relaxation and Yu-Shiba-Rusinov states in Superconducting Graphene — •Denis Kochan — University of Regensburg, Regensburg, Germany

2D materials in a proximity of superconductor are expected to host a wide spectrum of different phenomena. In my talk I will focus on spin-relaxation in graphene proximitized by an s-wave superconductor. Adatom impurities can affect spin-relaxation via locally enhanced spin-orbit coupling (SOC) and local magnetic moments. I will discuss their impact on quasiparticle spin-relaxation with an attempt to disentangle contributions from the local SOC and local magnetic moments. Moreover, I will analyze a stability of the induced local magnetic moments and the emergence of Yu-Shiba-Rusinov (YSR) bound states in such proximity induced superconducting systems.

This research was supported by DFG SFB 1277 and GRK 1570 and by the European Union's Horizon 2020 research and innovation programme under Grant agreement No. 696656.

DS 16.3 Tue 14:30 A 151

Magnetic field-induced metal-insulator transition of graphene at filling factor ν=0 — •Sung Ju Hong, Christopher Belke, Johannes C. Rode, Benedikt Brechtken, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany

We have observed magnetic field-induced metal-insulator transition (MIT) at filling factor ν=0 of hexagonal boron nitride (h-BN) encapsulated single-layer graphene. The temperature dependent longitudinal resistance (R_{xx}) with ν=0 shows MIT at critical magnetic field, $B_c \approx 8$T below (above) which metallic (insulating) behavior occurs. In the metallic regime, the negative magnetoresistance appears, which can be explained by counter-propagating opposite-spin polarized edge state [1,2]. In the insulating regime, the divergence of the R_{xx} was obtained and the resistance showed thermal activation gap behavior. We attribute the MIT with ν=0 to the magnetic field-induced transition from spin polarized state to valley polarized state at B_c.

[1] Peng Wei *et al.*, Nature Mater. **15**, 711 (2016).
[2] Javier D. Sanchez-Yamagishi *et al.*, Nature Nanotech. **12**, 118 (2017).

DS 16.4 Tue 14:45 A 151

Graphene Nanoribbons on Hexagonal Boron Nitride: Deposition and Transport Characterization — Christian Kick[1], Andreas Lex[1], •Tobias Preis[1], Akimitsu Narita[2], Kenji Watanabe[3], Takashi Taniguchi[3], Klaus Müllen[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Regensburg, Germany — [2]Max Planck Institute of Polymer Research, Mainz, Germany — [3]National Institute for Materials Science, Tsukuba, Japan

We contacted cove-type graphene nanoribbons (cGNRs) of different widths (4 and 6 carbon dimers) with different metals (NiCr-Au and Pd) and measured their I-V-characteristics. The cGNRs were chemically synthesized and are solution processable in THF or chlorobenzene after sonification (see [1] for the synthesis). This solution was subsequently drop-cast onto exfoliated hexagonal boron nitride (hBN) on an SiO_2 wafer. With AFM we observe the formation of ordered cGNR domains that are aligned along the crystallographic axes of the hBN. With electron beam lithography and metalization, we successfully contacted the cGNRs with NiCr-Au and Pd contacts and measured their I-V-characteristics. The transport through the ribbons was dominated by the Schottky behavior of the contacts between the metal and the ribbon. We could not observe any gate dependence so far which could be due to screening effects of the metal contacts.

[1] A. Narita, *et al.*, Nature Chemistry **6**, 126 (2014).

DS 16.5 Tue 15:00 A 151

Plasmons and excitons in few layer graphenes — •Jorge Enrique Olivares Peña and Sam Shallcross — FAU Erlangen-Nürnberg

We present a general method for studying plasmons and excitons in low dimensional systems, based on (i) an operator equivalence method to establish a continuum $H(\mathbf{r}, \mathbf{p})$ Hamiltonian from a general underlying tight-binding method, and (ii) application of the bootstrap functional within the framework of time dependent density functional theory to study excitonic effects. We apply this method to the graphene twist bilayer, finding that the excitonic correction to the optical absorption spectrum is important in the small angle limit.

[1] S. Shallcros et al., arXiv 1607.00920 (2016)
[2] S. Shallcross et al. , Phys. Rev. B 93,035452 (2016)

DS 16.6 Tue 15:15 A 151

Towards gate-controlled photoluminescence of hexagonal boron nitride quantum emitters — •Alessio Scavuzzo[1], Christian Strelow[2], Marko Burghard[1], Alf Mews[2], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute of Physical Chemistry, University of Hamburg, Germany — [3]École Polytechnique Fédérale de Lausanne, Switzerland

In the past few years, quantum emission from defect states embedded in crystalline structures has attracted increasing interest due to its promising applications in future quantum information technologies. While the properties of color centers in large band-gap 3D semiconductors like diamond or 4H-SiC are well-established, more recently attention is directed toward quantum emission from 2D systems. Along these lines, hexagonal boron nitride (hBN) has recently emerged as a very attractive 2D platform to host robust, visible light single photon emitters. Here, we report our experiments that address the possibility to control the quantum emission from hBN monolayers through electrostatic gating. To this end, we use confocal microscopy to probe the lifetime and intensity of the light emission from hBN quantum emitters within hBN/graphene vertical heterostructures as a function of temperature and back gate voltage. Moreover, through complementary Raman mapping, we demonstrate the importance of the hBN and graphene layer thickness, as well as the quality of the interface between the layers.

DS 16.7 Tue 15:30 A 151

Quantum Light in 1D and 2D Curved Hexagonal Boron Nitride Systems — •Nathan Chejanovsky[1,2], Youngwook Kim[2], Andrea Zappe[1], Benjamin Stuhlhofer[2], Takashi Taniguchi[3], Kenji Watanabe[3], Durga Dasari[1,2], Amit Finkler[1], Jurgen H. Smet[2], and Jörg Wrachtrup[1,2] — [1]3rd Physics Institute, Universität Stuttgart, Pfafenwaldring 57, 70569, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569, Stuttgart, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

Low-dimensional wide bandgap semiconductors open a new playing field in quantum optics using sub-bandgap excitation. 2D hexagonal boron nitride (h-BN) has been reported to host single quantum emitters (QEs), linking QE density to perimeters. [1] We investigate a curvature and perimeter-abundant BN system - one-dimensional BN nanotubes (BNNTs).

I discuss our recent publication [2] demonstrating similarities between QEs in BNNT and h-BN for: Emission spectra, anti-bunching,

SEM imagery, curvature effects, boron-oxide emission and sensitivity to commercial solvents.

These findings open possibilities for precision engineering of QEs, puts h-BN under a similar umbrella of transition metal dichalcogenides QEs and provides a model explaining QEs spatial localization and formation using electron and ion irradiation and chemical etching.

[1] Chejanovsky, N. et al. Nano letters 2016, 16, 7037-7045. [2] Chejanovsky, N. et al. Scientific reports 2017, 7, 14758 (1-14)

DS 17: Poster Session I

Time: Tuesday 18:15–20:15 Location: Poster B

DS 17.1 Tue 18:15 Poster B

Coherent manipulation of a single electron surfing on a sound wave — Shintaro Takada[1,2], •Hermann Edlbauer[1], Arne Ludwig[3], Andreas D. Wieck[3], Tristan Meunier[1], and Christopher Bäuerle[1] — [1]Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38000, Grenoble, France — [2]National Institute of Advanced Industrial Science and Technology (AIST), National Metrology Institute of Japan (NMIJ), 1-1-1 Umezono, Tsukuba, Ibaraki, 305-8563, Japan — [3]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, 44780, Bochum, Germany

Surface acoustic waves (SAW) provide a promising platform to realize quantum optics experiments with electrons at the single particle level. Earlier experiments have shown SAW-assisted single electron transport between spatially separated quantum dots over a distance of 4 mm with an efficiency of about 92 % [1]. Here we go an important step further. We couple two quantum channels by a tunnel barrier along a region of 2 μm and demonstrate transport over a distance of 22 μm with extremely high efficiency above 99 %. Changing energy detuning in the coupling region we can partition the electron on-demand into the two paths. Lowering the barrier height we additionally observe tunnel oscillations of the probability that the electron ends up at the upper or the lower channel. This finding demonstrates coherent manipulation of the electron quantum state on the fly. Our results pave the way for the implementation of a solid state flying qubit having high relevance in fundamental research and quantum information technology.

[1] Hermelin et al., Nature 477, 435 (2011)

DS 17.2 Tue 18:15 Poster B

Silicon Acousto-Electronics: Requirements for Ultrahigh-Frequencies — •Robert Ukropec[1], Boris Vratzov[2], Daan Kooij[1], Paulo V. Santos[3], and Wilfred G. van der Wiel[1] — [1]NanoElectronics Group (NE), MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands. — [2]NT&D - Nanotechnology & Devices, Aachen, Germany. — [3]Department of Semiconductor Spectroscopy, Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany.

Acousto-electronic transport and phonon cavities generated by surface acoustic waves (SAWs) are playing a central role in the rapidly emerging field of quantum acoustics, a phonon analogue of quantum optics on a chip. To enter the quantum regime, both ultrahigh-frequency (UHF, >10 GHz) SAWs and suitable host materials are indispensable. So far, research in this field has mainly concentrated on GaAs-based substrates. We investigate silicon, which is attractive for its long spin lifetimes and thus, for the interconnectivity of qubits via SAWs generated by piezoelectric multilayers. Integration of UHF-SAW technology with these structures for carrier and spin transport is our motivation. UHFs are achieved via small SAW wavelength (down to 260 nm) transducers fabricated by nano-imprint lithography. We compare numerical simulations and experimental network analysis of piezoelectric multilayers on Si to evaluate these material systems for application in quantum acousto-electronic transport.

DS 17.3 Tue 18:15 Poster B

Coupled surface acoustic waves cavities — •André Luiz O. Bilobran[1], Mauricio M. de Lima Jr.[1], and Paulo V. Santos[2] — [1]University of Valencia - Institute of Materials Sciences, 46890 Paterna, Valencia (Spain) — [2]Paul-Drude-Institut für Festkrperelektronik, Hausvogteiplatz 57, D-10117 Berlin (Germany)

A few years ago it was demonstrated that fundamental effects of quantum-wave transport (Bloch oscillations, Wannier-Stark ladders and Landau-Zener tunneling) can be studied with surface acoustic waves (SAWs) propagating in 1D coupled acoustic cavities. Posteriorly, it was shown that the cavities - a periodic arrangement of metal stripes within a surface acoustic delay line on piezoelectric substrate - can be electrically tuned by controlling the potential of the cavities' electrodes. Changing from floating stripes, i. e., electrically isolated, to short circuited ones, the acoustic field changes due to the screening of the piezoelectric potential underneath the stripes. Here, we discuss the two dimensional finite element model that we have developed. The model describes fairly well the behavior of such devices without any adjustment parameters. In it, the mechanics and electrostatics models are coupled to simulate the piezoelectricity. Using a frequency domain study the eigenfrequencies can be predicted with an accuracy of less then 1%. The transmission around them, in dB, is estimated with an error smaller than 10% for the short circuited devices, whereas for the floating ones the accuracy decreases. Moreover we calculate the variation of parameters such as the stress, the strain and the displacement throughout the structures.

DS 17.4 Tue 18:15 Poster B

Generation of surface acoustic waves on doped semiconductor substrates — •Mingyun Yuan[1], Colin Hubert[1], Sander Rauwerdink[1], Abbes Tahraoui[1], Bob van Someren[2], Klaus Biermann[1], and Paulo Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Elf Software B.V., Rotterdam, Netherlands

We report on the electrical generation of surface acoustic waves (SAWs) on doped semiconductor substrates. This is implemented by using interdigital transducers (IDTs) placed on piezoelectric ZnO films sputtered onto evaporated thin metal layers. Two material systems are investigated, namely ZnO/Au/GaAs and ZnO/Ni/InP. The rf-field applied to the transducer is electrically screened by the highly conductive metal film underneath the ZnO film without any extra ohmic losses. As a result, absorption of the rf-field by the mobile carriers in the lossy doped region underneath the IDT is avoided, ensuring efficient SAW generation. We find that the growth temperature of the ZnO film on the metal layer affects its structure and, thus, the efficiency of SAW generation. With this technique, the SAW active layers can be placed close to doped layers, expanding the application range of SAWs in semiconductor devices.

DS 17.5 Tue 18:15 Poster B

Acoustic transport of charge carriers and electron spins in quantum wires — •Paul L. J. Helgers[1,2], Klaus Biermann[1], Haruki Sanada[2], Yoji Kunihashi[2], and Paulo V. Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik Berlin, Germany — [2]NTT Basic Research Laboratories, NTT Corporation, Atsugi, Japan

We investigate a concept for acoustically driven single-photon-sources (SPS), based on planar GaAs quantum wires (QWRs) embedded in an optical microcavity. The QWRs are fabricated by photolithography, wet chemical etching and anisotropic MBE overgrowth. In this concept, spin-polarized carriers are optically injected at one end of the quantum wire and then acoustically transported to a QD-like recombination center at the other QWR end where they recombine, emitting single photons. The one-dimensionality of the QWR reduces Dyakonov-Perel spin dephasing during acoustic transport, thereby correlating the excitation polarization with the emission polarization. The SPS properties are improved by a microcavity.

In this contribution, we observe line-edge-roughness (LER), leading to QWR width variations up to several tens of nm, which complicate acoustic transport. We show that LER is mainly caused by the photolithography process. Secondly, we observe charge transport in GaAs(113)A QWRs and in cavity-embedded GaAs(001) QWRs on lengths of several tens of microns. Furthermore, spin lifetimes in the GaAs(001) QWRs approach the nanosecond timescale, promising spin transport lengths of several microns. We will evaluate the potential of these structures to be used as efficient acoustically driven SPSs.

DS 17.6 Tue 18:15 Poster B

Solid-state magnetic traps and lattices — •Johannes Knörzer[1], Martin J. A. Schuetz[2], Géza Giedke[3,4], Hans

Huebl[5], Mathias Weiler[5], Peter Zoller[6,7], Mikhail D. Lukin[2], and J. Ignacio Cirac[1] — [1]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany — [2]Physics Department, Harvard University, Cambridge, MA 02318, USA — [3]Donostia International Physics Center, Paseo Manuel de Lardizabal 4, E-20018 San Sebastián, Spain — [4]Ikerbasque Foundation for Science, Maria Diaz de Haro 3, E-48013 Bilbao, Spain — [5]Walther-Meissner-Institut, Walther-Meißner-Str. 8, 85748 Garching, Germany — [6]Institute for Theoretical Physics, University of Innsbruck, A-6020 Innsbruck, Austria — [7]Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, A-6020 Innsbruck, Austria

We investigate platforms which realize AC Stark-shift induced traps and lattices for (pseudo-)spins in semiconductors. In close analogy to optical lattices, we discuss tunable magnetic lattices for probing quantum many-body phenomena and quantum simulation. Realistic parameters, imperfections and readout schemes are discussed along with a detailed case study for two implementations, one based on surface acoustic waves and another based on a resonating LC circuit.

DS 17.7 Tue 18:15 Poster B

Complex-Oxide Acousto-Electronics — •Yigitcan Uzun[1], Boris Vratzov[2], Alexander E. M. Smink[1], and Wilfred G. van der Wiel[1] — [1]NanoElectronics Group, MESA+ Institute for Nanotechnology, University of Twente, PO Box 217, 7500 AE Enschede, The Netherlands — [2]NT&D - Nanotechnology and Devices, Aachen, Germany

Surface acoustic waves (SAWs) are capable of capturing free charge carriers and transporting them along their propagation path, resulting in an acoustoelectric current. So far, acoustoelectric transport has been realized mainly in AlGaAs/GaAs based structures. Here, we intend to realize acoustoelectric transport in the two-dimensional electron system at the LaAlO3/SrTiO3 (LAO/STO) interface. This has been shown to have extraordinary low-temperature properties, such as a high carrier mobility, superconductivity and magnetism. Experiments were carried out in a Pb[ZrxTi1-x]O3(PZT)/LAO/STO tri-layer heterostructure. Initially, a 10 unit cell thick layer of LAO was grown on a TiO2-terminated STO substrate and was patterned in a Hall-bar shape in order to define the SAW path. A 200 nm thick top piezoelectric PZT layer was deposited. SAWs were generated by using interdigital transducers. The SAW resonance frequency was measured by S-parameters analysis and the dependency of the acoustoelectric current on the SAW power was analyzed.

DS 17.8 Tue 18:15 Poster B

Quantum optics with electrons using surface acoustic waves — •Hugo V. Lepage, Chris J. B. Ford, and Crispin H. W. Barnes — Cavendish Laboratory, Department of Physics, University of Cambridge, Cambridge CB3 0HE, United Kingdom

The time evolution of a quantum particle can be described by the time dependent Schrödinger equation (TDSE). An analytical solution to this problem can only be found in a few very simple cases and numerical solutions are hard in general. We use a GPU-accelerated code to parallelize the computation of the TDSE and obtain accurate simulations of a wave function evolving through an arbitrary dynamic underlying potential. The focus of these simulations is to investigate single electron transport driven by surface acoustic waves (SAWs). SAW-driven transport is particularly interesting since it adds a new level of confinement to the electrons, suppressing their dispersion. Through non-dispersive control of single electrons, we propose a framework to implement a positive-operator-valued measure (POVM) using experimentally realistic potentials.[1] Furthermore, we simulate the coherent transport of single electrons across a tunnel-coupled wire. Our simulation results are compared to experimental observations by a collaborating group at the CNRS in Grenoble, France. In this presentation, we provide insight into the various phenomena related to single electron transport and put forward experimentally realizable designs for future optics-like protocols. [1] Arvidsson-Shukur, D.R.M., Lepage, H.V., Owen, E.T., Ferrus, T. and Barnes, C.H.W., 2017. Protocol for fermionic positive-operator-valued measures. Physical Review A, 96(5), p.052305.

DS 17.9 Tue 18:15 Poster B

The Giant Atom Regime of Quantum Acoustics — •Gustav Andersson[1], Baladitya Suri[1], Lingzhen Guo[2], Thomas Aref[1], Göran Johansson[1], and Per Delsing[1] — [1]Chalmers University of Technology, Gothenburg, Sweden — [2]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

We investigate the dynamics of a superconducting transmon qubit interacting with surface acoustic waves (SAWs) on a piezoelectric substrate through interdigitial transducers. This "quantum acoustic" platform allows us to perform experiments analogous to quantum optics with a crucial difference - the artificial atom has characteristic dimensions much larger than the wavelength of the slow-propagating acoustic field. We engineered artificial atoms that couple to the propagating field at two distant points such that the time of flight of phonons between them introduces a significant, deterministic time delay. This allows us to probe the unexplored "giant atom" regime of quantum optics, with characteristic signatures of non-Markovianity. Phonons emitted into the acoustic channel by such a "giant atom" from one coupling point interact with the atom again through the other point, leading to revivals in the excited state population. A dispersively coupled microwave resonator allows us to read-out the excited state population of the qubit, thereby enabling us to perform its time-domain characterisation. We observe the non-exponential energy relaxation as well as the phonon scattering properties of giant atoms with a resonance frequency in the 2-2.5 GHz range.

DS 17.10 Tue 18:15 Poster B

Acoustically tuned dynamic wavelength division multiplexing — •Dominik D. Bühler[1], Antonio Crespo-Poveda[1], Klaus Biermann[2], Andrés Cantarero[1], Paulo V. Santos[2], and Mauricio M. de Lima[1] — [1]Materials Science Institute, University of Valencia, Spain — [2]Paul-Drude Institute for Solid State Electronics, Berlin, Germany

Phasar multiplexers based on arrayed waveguide grating (AWG) devices are key components in modern integrated photonic systems. Acoustically tuning these multiplexers enables robust, compact and fast responding devices improving on recently demonstrated technology. Different concepts will be presented in each of which a surface acoustic wave (SAW) is induced in such a way that its propagation direction coincides perpendicularly with the AWG. The WGs of this grating introduce dispersion and connect two multimode interference (MMI) couplers of distinct lengths that are employed as a power splitter and combiner, respectively. By tuning the SAW amplitude this setup allows us to alter the refractive index in each arm discretely and, thus, introduce specific phase shifts resulting in wavelength depended constructive interference at each of the outputs of the combiner MMI. This mechanism can be readily applied for wavelength routing and circuit switching in optical networking systems of essentially any material platform. The devices here are presented for operation at the telecommunication wavelengths around 1.55 μm, working on a (Al,Ga)As platform and tuned by a SAW in the low GHz range.

DS 17.11 Tue 18:15 Poster B

VO2-SnO2 nanocomposite films for smart windows applications — Alexandr Belenchuk[1], Oleg Shapoval[1], Sergiu Vatavu[2], Arcadi Chirita[2], and •Vasily Moshnyaga[3] — [1]IIEN, Academy of Sciences, Chisinau, Republic of Moldova — [2]Moldovan State University, Republic of Moldova — [3]Erstes Physikalisches Institut, Georg-August-Universität Göttingen, Germany

Vanadium dioxide, VO2, is a promising thermochromic material due to a drastic change of the infrared transmittance at the metal-insulator transition. However, a high transition temperature, Tmi=68C, and low transmittance impede industrial applications of VO2-based smart windows. To address these challenges, we employed a nanocomposite approach, which allows one to increase the transmittance and to generate a strain between nanocrystals to reduce Tmi. Nanocomposite VO2-SnO2 thin films were grown by a metalorganic aerosol deposition (MAD) technique on amorphous SiO2 substrates under reduced oxygen conditions. A single solution containing metalorganic precursors of vanadium and tin was used. Atomic-force (AFM) and scanning-electron (SEM) microscopy revealed dense films, composed of homogeneous nanocrystals with irregular shape. X-ray diffraction evidences a V1-xSnxO2 solid solution in spite of huge lattice mismatch between the oxides. A low temperature annealing [1] was used to achieve the VO2/SnO2 phase separation by means of a spinodal decomposition. Financial support from the STCU Project and DFG via SFB 1073 (TP A02) is acknowledged. [1] Zenji Hiroi et al., Chem. Mater. 25, 2202 (2013)

DS 17.12 Tue 18:15 Poster B

Depletion layer spectroscopy on (010) and (-201) β-Ga_2O_3 single crystals — •Holger von Wenckstern, Rainer Picken-

HAIN, and MARIUS GRUNDMANN — Universität Leipzig , Felix-Bloch-Institut für Festkörperphysik, Halbleiterphysik, Leipzig

The properties of β-Ga_2O_3 and the possibility of bulk crystal growth by e.g. edge-defined film-fed growth, float-zone and Czochralski method render the material interesting for high-power applications and deep-UV photo detection[1]. The performance of devices is typically limited by defects incorporated during growth and processing. We present a comprehensive investigation of unintentionally doped (-201)- and (010)-oriented β-Ga_2O_3 bulk single crystals grown by edge-defined film-fed growth (*Tamura coporation*) by thermal admittance spectroscopy TAS and deep-level transient spectroscopy (DLTS). For that coplanar Ohmic and Schottky barrier diodes were fabricated and characterized at room temperature by current-voltage measurements. Comparing the differently oriented crystals revealed differences in the appearance and concentration of deep-level defects and different effective mass-like donors in the freeze-out regime.

[1] H. von Wenckstern, Adv. Electron. Mater. **3**, 1600350 (2017).

DS 17.13 Tue 18:15 Poster B

Investigations of Ge-doped $(Al,Ga)_2O_3$ thin films — •A. WERNER, H. VON WENCKSTERN, and M. GRUNDMANN — Halbleiterphysik, Universität Leipzig, Leipzig, Germany

Since deep-ultraviolet photo-diodes find wide use in technical applications like flame detection, solar-blind materials like semiconducting Ga_2O_3 are of peculiar interest. Ga_2O_3 has a large bandgap of 4.4-4.9 eV which can be enlarged by alloying with Al_2O_3[1].

The investigated $(Al,Ga)_2O_3$ thin films were grown by pulsed laser deposition (PLD) on (00.1) Al_2O_3. We investigated the influence of the growth parameters such as growth temperature (T_g) and oxygen partial pressures ($p(O_2)$) on the structural, optical and electrical properties of the samples by X-ray diffraction, energy-dispersive X-ray spectroscopy, atomic force microscopy, transmission, and Hall effect measurements, respectively.

The thin films have $(\bar{2}01)$ orientation and the cation incorporation strongly depends on the deposition parameters. At a given T_g, the incorporation of Al is favored for lower $p(O_2)$ due to higher dissociation energy of the Al-O bond compared to the Ga-O bond. At a given $p(O_2)$, the incorporation of Al is favored for higher T_g due to desorption of gallium sub-oxides during growth[2]. Furthermore, we show the influence of Ge-doping on the conductivity.

[1] H. von Wenckstern, Adv. Electron. Mater 3, 1600350 (2017).
[2] P. Vogt and O. Bierwagen, APL Mater. 4, 086112 (2016).

DS 17.14 Tue 18:15 Poster B

Occurence of the ϵ-phase in $(In_xGa_{1-x})_2O_3$ and $(Ga_xAl_{1-x})_2O_3$ thin films — •A. WERNER[1], H. VON WENCKSTERN[1], C. STURM[1], D. SPLITH[1], V. PROZHEEVA[2], R. HOELLDOBLER[1], and M. GRUNDMANN[1] — [1]Halbleiterphysik, Universität Leipzig, Leipzig, Germany — [2]Department of Applied Physics, Aalto University, Espoo, Finland

The wide bandgap semiconductor Ga_2O_3 appears in five polymorphs of which only the so-called ϵ-phase has a high spontaneous polarization P along its c-axis[1]. Within heterostructures, a discontinuous change of P at the heterointerface occurs, resulting in charge accumulation. Therefore, stabilization of the ϵ-phase within the ternary alloys $(In,Ga)_2O_3$ or $(Ga,Al)_2O_3$ is required in order to utilize the two-dimensional charge carrier gases within electronic devices. We present studies of the occurrence of the ϵ-phase in ternary alloys of Ga_2O_3 with In_2O_3 and Al_2O_3. Samples with continuous composition spread[2] were grown by pulsed laser deposition on (00.1) Al_2O_3. As target segments we used Ga_2O_3/In_2O_3 or Ga_2O_3/Al_2O_3. Each segment was additionally doped with tin to facilitate the formation of the ϵ-phase[3]. Resulting thin films were investigated by means of X-ray diffraction, transmission, energy-dispersive X-ray spectroscopy, Raman spectroscopy, and atomic force microscopy. We observed a monotonic shift of the ϵ-reflexion in dependency of In-/Al-content; for example the (002)-reflex shifts to lower angles with increasing In-content.

[1] M. B. Maccioni *et al.*, Appl. Phys. Express 9, 04102 (2016).
[2] H. v. Wenckstern *et al.*, CrystEngComm 15, 10020 (2013).
[3] M. Kracht *et al.*, Phys. Rev. Applied 8, 054002 (2017).

DS 17.15 Tue 18:15 Poster B

Optical and Magnetic Properties of Spinel Type Ferrites in Relation to their Crystallographic Order — •VITALY ZVIAGIN[1], PAULA HUTH[2], CHRIS STURM[1], DANIEL SPEMANN[3], STEPHAN MÄNDL[3], JÖRG LENZNER[1], ANNETTE SETZER[1], JAN MEIJER[1], REINHARD DENECKE[2], PABLO ESQUINAZI[1], MARIUS GRUNDMANN[1], and RÜDIGER SCHMIDT-GRUND[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstr. 5, Germany — [2]Universität Leipzig, Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Linnéstr. 2, Leipzig — [3]Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, Leipzig

$ZnFe_2O_4$ (ZFO) and composite $Zn_xFe_{3-x}O_4$ thin films were fabricated on $SrTiO_3$ (100) and TiN/MgO (100) substrates by pulsed laser deposition. Assigned electronic transitions in the dielectric function show a clear dependence on temperature as well as pressure during deposition and annealing processes. A decrease in the octahedral Fe^{2+} site occupancy with an increase in Zn concentration in composite films was observed in the band to band transition as well as the valence specific elemental composition, determined by spectroscopic ellipsometry and analysis of Fe 3p and 2p XPS core levels, respectively. Change in the ferrimagnetic response and electronic structure was examined after annealing ZFO films in argon and oxygen atmospheres at different temperatures as well as after irradiation by Ne^+ ions with different fluences. Along with complementary methods such as Raman, AFM and SEM, we show the influence of crystallographic order on magnetic properties of normal, disordered and inverse spinel ferrite thin films.

DS 17.16 Tue 18:15 Poster B

Characterization of transport properties of thin β-GaO layers — •JOHANNES BOY[1], MARTIN HANDWERG[1], ROBIN AHRLING[1], RÜDIGER MITDANK[1], GÜNTER WAGNER[2], ZBIGNIEW GALAZKA[2], and SASKIA F. FISCHER[1] — [1]AG Neue Materialien, Humboldt-Universität zu Berlin, Institut für Physik, Newtonstrasse 15, D-12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, Max-Born-Strasse 2, D-12489 Berlin, Germany

Gallium oxide has been of great interest as a functional material for high power applications, due to its wide band gap and high breakthrough field. Knowledge about the transport properties of the material is a requirement for the design and production of gallium oxide based electric devices. In this work, homoepitaxially MOVPE-grown Si-doped β-GaO films have been investigated with regard to electric and thermoelectric transport over a wide temperature range. We have designed a measurement platform, which allows us to carry out van-der-Pauw-, Hall- and Seebeck-measurements on the same sample. The Seebeck coefficient S, conductivity σ, Hall carrier density n and Hall mobility μ have been measured in thin films, which have to be distinguished in terms of film thickness, doping concentration and mobility of the charge carrier. Seebeck coefficients in the range of a few hundreds μV/K have been measured at room temperature and below. The measurement of the Seebeck coefficient and Hall carrier density allows a discussion of the temperature-dependent Hall scattering factor r_{sc} in various β-GaO thin films.

DS 17.17 Tue 18:15 Poster B

Influence of Ga incorporation into bixbyite In_2O_3 thin films on the performance of Schottky barrier diodes thereon — •DANIEL SPLITH, STEFFEN LANZINGER, SOPHIE MÜLLER, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Leipzig, Germany

Oxide semiconductors like In_2O_3 are promising materials for a new generation of transparent electronic devices. Although first Schottky contacts on In_2O_3 were realized recently using a reactive sputtering process [1], rectification of such contacts remained poor. Incorporation of Mg, acting as an acceptor in In_2O_3, improves the rectification [2]. Further improvement can be expected from Ga incorporation into the bixbyite In_2O_3 phase, since In incorporation into the monoclinic β-Ga_2O_3 phase decreases the barrier height of Schottky contacts on β-Ga_2O_3 thin films significantly [3].

In this contribution we investigate the influence of Ga incorporation into the bixbyite In_2O_3 phase on the rectifying behavior of Schottky contacts. In_2O_3 thin films with and without Ga admixture were grown by pulsed laser deposition. Schottky contacts were realized by sputtering of Pt. In the IV-characteristics, a significantly smaller reverse current can be observed for the samples having a Ga admixture, leading to an improved rectification. Additionally, first thermal admittance spectroscopy measurements were performed on such thin films.

[1] H. von Wenckstern *et al.*, APL Mat. **2**(4), 046104 (2014)
[2] F. Schmidt *et al.*, Phys. Status Solidi B, **252**(10), 2304-2308 (2015)
[3] H. von Wenckstern *et al.*, ACS Comb. Sci. **17**(12), 710-715 (2015)

DS 17.18 Tue 18:15 Poster B

A pulsed laser deposition technique to control the composi-

tion of ternary thin films in growth direction demonstrated on the $(Al_x,Ga_{1-x})_2O_3$ alloy — •Max Kneisz, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Leipzig, Germany

In conventional pulsed laser deposition (PLD) a continuous variation of the composition of ternary thin films in growth direction is not possible since the number of discrete alloy combinations is limited by the amount of targets which can be mounted in the setup. We therefore propose a technique using only a single elliptically-segmented target with two regions of different composition. We control the Al/Ga ratio of the thin films by varying the radial position of the PLD laser spot on the target and thereby changing the ratio of the path lengths of the laser spot in the different regions. In analogy to our approach for lateral continuous composition spreads [1] (lateral CCS), we call this method vertical CCS. We will show that we are able to control the composition of $(Al_x,Ga_{1-x})_2O_3$ thin films in growth direction quasi continuously or stepwise. Therefore films with varying single Al-contents are grown using the new technique on c-sapphire substrates. The Al-content in the films is determined by transmission spectroscopy. The structural and optical quality is similar to films grown via conventional PLD.
[1] H. von Wenckstern *et al.*, CrystEngComm **15**, 10020 (2013)

DS 17.19 Tue 18:15 Poster B

Electrical properties of unipolar devices based on amorphous zinc oxynitride — •Anna Reinhardt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Semiconductor Physics Group

Amorphous zinc oxynitride (a-ZnON) was demonstrated to be a promising high-mobility semiconductor for low-temperature fabricated, high-performance thin-film transistors [1–3]. Up to now, only metal-insulator-semiconductor field-effect transistors based on a-ZnON were reported.

Here, we present our results on metal-semiconductor field-effect transistors (MESFETs) using reactively sputtered platinum gate-contacts to control the current flow in the sputter deposited a-ZnON channel. On/off ratios of 10^5 and saturation mobilities of about $50\,cm^2V^{-1}s^{-1}$ are achieved. Furthermore, the electrical properties of the Schottky gate diode were analyzed by means of temperature-dependent current-voltage measurements.

[1] Y. Ye *et al.*, J. Appl. Phys. 106, 074512 (2009)
[2] H.-S. Kim *et al.*, Sci. rep. 3, 1459 (2013)
[3] A. Reinhardt *et al.*, Phys. Status Solidi A 213 (7), 1767 (2016)

DS 17.20 Tue 18:15 Poster B

Influence of pre-growth conditions on the interface formation in $SrTiO_3$ homoepitaxial thin films grown with pulsed laser deposition (PLD) — •Laura Bogula, Toni Markurt, Martin Albrecht, and Jutta Schwarzkopf — Max-Born-Str. 2, 12489 Berlin, Germany

In this poster a systematic study on the pre-growth conditions of a model perovskite system, namely homoepitaxial $SrTiO_3$ thin films grown by pulsed laser deposition (PLD) will be presented. In order to understand the origin of its functional properties and the correlation to defects the interface between substrate and film is of utmost importance. Therefore, we investigated the influence of different pre-growth conditions like oxygen partial pressure and substrate temperature on the surface reconstruction and the resulting interface. On as prepared $SrTiO_3$ substrates we observed a $(\sqrt{13} \times \sqrt{13}) - R33.7°$ reconstruction causing a non-stoichiometric interface measured both with transmission electron microscopy and x-ray diffraction. However, with vacuum annealing the surface structure can be altered to more favourable reconstructions for homoepitaxial thin film growth.

DS 17.21 Tue 18:15 Poster B

Electrical charcterization of thin monocrystalline homoepitaxial β-Ga_2O_3 films — •Robin Ahrling[1], Johannes Boy[1], Martin Handwerg[1], Rüdiger Mitdank[1], Zbigniew Galazka[2], Günter Wagner[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, 12489 Germany

As a wide band gap semiconductor with a high breakthrough field, gallium oxide (Ga_2O_3) has shown to be a promising material for applications in high power electronics. However, it is not yet clear how its electrical properties may change with a variation of crystal thickness. These changes may be caused by a change in scattering mechanisms or an inhomogeneity in crystal growth.

Here, homoepitaxially MOVPE-grown monocrystalline Si-doped β-Ga_2O_3 films of thicknesses between 28 nm and 225 nm were electrically characterized in a temperature range from 300 K down to 10 K. Van-der-Pauw and Hall-measurements have been performed to determine conductivity, Hall density and carrier mobility in those films. It was found that above 150 nm thickness the films show a behavior similar to the bulk. Below 100 nm a drastic drop of the mobility with decreasing thickness was seen. The Bergmann model, based on surface scattering of electrons due to their wavelength, was used to describe this dependence and showed an overall good agreement with the data. An alternative explanation is inhomogeneity in the sample growth process. In any case, this reduction in mobility for thin films has to be considered for future applications in devices.

DS 17.22 Tue 18:15 Poster B

growth mode evolution during (100)-oriented β-ga2o3 homoepitaxy — •zongzhe cheng[1], michael hanke[1], zbigniew galazka[2], and achim trampert[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7 10117 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany

our work focuses on the analytics of (100)-oriented beta-Ga2O3 homoepitaxy as grown by MBE. In-situ reflection high-energy electron diffraction (RHEED) reveals sharp strike patterns that are indicative for a 2D layer-by-layer mode accompanied by a (1*1) surface reconstruction. The crystal structure of the thin film shows a high quality and matches coherently with the substrate underneath, as probed by in-situ synchrotron-based high resolution x-ray diffraction (HRXRD) and azimuthal RHEED maps. In contrast to the substrate, there is a high density of stacking faults and twin domains in the layers found by ex-situ transmission electron microscopy (TEM), which serve as a mark of the layers. The twins form from the coalescence of nucleated islands, which are elongated along b-direction. As monitored by the RHEED oscillations, the layer thickness can be controlled very precisely, therefore making it a good candidate for research and design of 2D electronics.

DS 17.23 Tue 18:15 Poster B

Resistive switching in memristive CBRAM devices — •Sven Dirkmann[1] and Thomas Mussenbrock[2] — [1]Ruhr-Universität Bochum, Lehrstuhl für Theoretische Elektrotechnik, 44780 Bochum, Germany — [2]BTU Cottbus-Senftenberg, Lehrstuhl für Theoretische Elektrotechnik, 03046 Cottbus, Germany

We report on resistive switching of memristive electrochemical metallization devices (CBRAM) using 3D kinetic Monte Carlo simulations describing the transport of ions through a solid state electrolyte of an Ag/TiOx/Pt thin layer system. The ion transport model is consistently coupled with solvers for the electric field and thermal diffusion. We show that the model is able to describe not only the formation of conducting filaments but also its dissolution. Furthermore, we calculate realistic current-voltage characteristics and resistive switching kinetics. Finally, we discuss in detail the influence of both the electric field and the local heat on the switching processes of the device. Furthermore, the reset process is discussed in detail.

This work is funded by the German Research Foundation DFG in the frame of Research Unit FOR2093.

DS 17.24 Tue 18:15 Poster B

Devices and Integrated Circuits Based on Amorphous Zinc-Tin-Oxide — •O. Lahr, S. Vogt, Z. Zhang, H. von Wenckstern, and M. Grundmann — Universität Leipzig, Semiconductor Physics Group, Leipzig, Germany

Currently there exists an increasing demand for low cost electronics and novel devices based on sustainable materials. Amorphous zinc-tin-oxide (ZTO) as a promising candidate paves the way for such technology since it only consists of abundant, non-toxic elements and can be deposited at room temperature with tunable charge carrier densities between 10^{16} cm^{-3} and 10^{19} cm^{-3} as well as mobilities up to 32 cm^2/Vs [1].

We present metal-semiconductor field effect transistors (MESFETs) and inverters based on amorphous n-type ZTO channels. The thin films were deposited at room temperature via long throw magnetron sputtering using a target with a 67 % ZnO and 33 % SnO_2 composition. On/Off ratios greater than 8 orders of magnitude are achieved for reactively sputtered Pt gate contacts with an 5-10 nm thick insulating i-ZTO layer in-between for rectification ratio enhancement [2]. Corresponding MESFET-based inverters show a peak gain maximum

(pgm) up to 330 at V_{DD} = 3 V, thus ZTO is a suitable candidate towards more advanced circuits as for instance ring oscillators [3].

[1] Bitter *et al.*, ACS Appl. Materials & Interfaces, **9**, 31, 2017.
[2] Schlupp *et al.*, Physica Status Solidi (a), **214**, 10, 2017.
[3] Klüpfel *et al.*, Advanced Electronic Materials, **2**, 7, 2016.

DS 17.25 Tue 18:15 Poster B

A Variable Gas Injection System for Rapid Precursor Testing in Focused Electron Beam Induced Deposition — •Robert Winkler[1,2], Georg Arnold[1,2], Juergen Sattelkow[1,2], Andrew Smith[3], and Harald Plank[1,2] — [1]Institute for Electron Microscopy and Nanoanalysis Graz University of Technology, 8010 Graz, Austria — [2]Graz Centre for Electron Microscopy, 8010 Graz, Austria — [3]Kleindiek Nanotechnik GmbH, Aspenhaustrasse 25, 72770 Reutlingen, Germany

Focused electron beam induced deposition (FEBID) is an additive, direct-write technology for the controlled on-demand fabrication of functional nano-structures on virtually any given material and surface morphology. Beside the strong current trend towards true 3D nano-fabrication with yet unpreceded flexibility, the material aspect is gaining increasing importance as the functionality finally decides about the applicability in research and development. From a chemical point of view, there was very strong progress during the last 3 years in the frame of the EU COST action CELINA, which brought essential insights and introduced new precursors. Those, however, need to be tested in an iterative fashion where technical flexibility is one of the highest demands. In this contribution we focus on a versatile and flexible gas injection system for rapid precursor testing of new materials. We also discuss how the system can be used for other exposure experiments such as purification or sensor applications. As we will show, the system provides unique advantages and an uncomplicated handling as essential element for further progress in the field of FEBID.

DS 17.26 Tue 18:15 Poster B

Investigation and utilization of catalytic processes in FEBIP techniques for nanofabrication — •Elif Bilgilisoy, Christian Preischl, Florian Vollnhals, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander University Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

In our group, we use and investigate Focused Electron Beam Induced Processing (FEBIP) techniques ultra-high vacuum (UHV) to fabricate arbitrary shaped nanostructures. Therefore, we use the highly focused electron beam of a scanning electron microscope in UHV to either directly modify adsorbed precursor molecules (electron beam induced deposition, EBID) or to locally modify the substrate such that it becomes active towards the decomposition of subsequently dosed precursor molecules (electron beam induced surface activation, EBISA) [1]. In the corresponding experiments with the precursors $Fe(CO)_5$ and $Co(CO)_3NO$ we observed diverse catalytic processes, like precursor decomposition at the pristine substrate, autocatalytic growth and decomposition on deposits of the other precursor. We will present and discuss the corresponding observations, e.g., the partially very different chemical sensitivities of the two precursors, the possibility to quench the catalytic activity of a surface by the preparation of organic layers and in particular how to exploit the findings for the improvement of FEBIP [2].

[1]H. Marbach, Appl. Phys. A 117 (2014), 987
[2]Drost et al., Small Methods, 1 (2017) 1700095

DS 17.27 Tue 18:15 Poster B

Evaluation of critical electron doses for surface activation in electron beam induced surface activation (EBISA) — •Florian Vollnhals, Christian Preischl, Martin Drost, Fan Tu, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen

The world of focussed electron beam induced processing encompasses not only electron beam induced deposition (EBID) and etching (EBIE), but also techniques like electron beam induced surface activation (EBISA).[1] In EBISA, an surface is locally modified by a electron beam such that it becomes active towards the decomposition of a subsequently dosed precursor, here $Fe(CO)_5$. The deposit can grow autocatalytically, i.e. via the local decomposition of further $Fe(CO)_5$ molecules, to form clean, polycrystalline iron deposits on the surface. Susceptible surfaces include oxides (TiO_2, SiO_2) as well as molecular layers (Porphyrins on various substrates).

In order to better understand the activation mechanisms and their dependence on the experimental parameters, we exploit the backscattering behavior of electrons commonly observed as BSE proximity effect to fabricate deposits and compare these to Monte-Carlo simulations. This allows to evaluate critical activation parameters and asses their implications for the EBISA process.

[1] Walz et al., Angew. Chem. Int. Ed. 49 (2010), 4669; Marbach, Appl. Phys. A 117 (2014), 987; Drost et al., Small Methods, 1 (2017) 1700095

DS 17.28 Tue 18:15 Poster B

Reduction and annihilation of wrinkles in graphene by He^+ ion bombardment at elevated temperatures — •Alexander Herman, Philipp Valerius, and Thomas Michely — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

Due to thermal mismatch of substrate and graphene, wrinkles form in CVD grown graphene upon cooling from the growth temperature to ambient. Wrinkles typically form a network with a characteristic lateral scale of micrometers. Wrinkles affect graphene's electrical and thermal properties through scattering processes in an unfavorable way. Therefore, methods to avoid wrinkle formation or to eliminate wrinkles are highly desirable.

Using a high CVD growth temperature of 1400°C for graphene on Ir(111) we force a large amount of wrinkles to result in the absence of any additional treatment. By additional low fluence, low energy noble gas ion irradiation at temperatures around the CVD growth temperature we show through scanning tunneling microscopy, that the height and length of the resulting wrinkles can be reduced until they are eventually completely eliminated. However, as side effects blisters and small vacancy clusters pinned to the moiré of graphene with Ir(111) show up.

DS 17.29 Tue 18:15 Poster B

Controllable p-doping of wafer-scale few-layer MoxNb1-xS2 — •Tien Tung Luong[1], Yen-Teng Ho[1], Peng Lu[2], Yung-Ching Chu[1], Chao An Jong[3], Edward Yi Chang[1], and Jason C.S. Woo[2] — [1]National Chiao Tung University, Hsinchu, China, Republic of (ROC) — [2]University of California, Los Angeles, Los Angeles, United States — [3]National Nano Device Laboratories, National Applied Research Laboratories, Hsinchu, China, Republic of (ROC)

Exfoliated monolayer MoS2 shows a great possibility FET for next generation due to the ultra-high carrier confinement. Nevertheless, exfoliation method is not suitable for practical applications on a large scale and disadvantages in controlling layer number and doping. 2D MoS2 can be used in many kinds of application fields, such as low power logic circuits, flexible electronics, sensors, memories and photovoltaic. etc. For integration circuit application, it is important to form p-type channels, Nb is the promising candidate for p-type dopant in MoS2. In this works, a very thin MoOx:Nb film was deposited on a commercial 2-inch sapphire wafer using a co-sputtering and then was sulfurized in H2S ambient at 750 oC to form few-layer MoxNb1-xS2. The effective mobility and effective hole concentration examined by Hall measurement and inferred from a field-effect measurement are strongly dependent both on the Nb power of co-sputtering and on the sulfurization conditions. Within some conditions, the effective mobility drastically increases as increasing the Nb incorporation and consequent the hole concentration in MoxNb1-xS2. The results present a feasible synthesis method for controllable p-doping of wafer-scale few-layer MoxNb1-xS2.

DS 17.30 Tue 18:15 Poster B

Utrafast dynamics in MoS2 probed by transient Raman spectroscopy — •Christoph Boguschewski, Jingyi Zhu, and Paul H.M. van Loosdrecht — II. Physikalisches Institut der Universität zu Köln

Mono-layer transition metal dichalcogenides (TMDs) form the most important materials platform for the emerging field of valleytronics. In order to further develop this field, it is crucial that one understands the dynamical aspects of valley excitations, including both population and polarization dynamics. Here we present a study of these dynamics in MoS2 using picosecond time resolved spontaneous Raman scattering. Apart from an insight into the phonon population dynamics, this technique yields a detailed insight in the population and polarization dynamics of valley excitations through the transient behavior of a doubly resonant Raman response in TMDs.

DS 17.31 Tue 18:15 Poster B

Epitaxially grown h-BN on Ir(111) under He ion irradia-

tion: A route to form one atom thick membranes with an ordered array of nanometer sized holes — •Philipp Valerius, Carsten Speckmann, Alexander Herman, and Thomas Michely — II. physikalisches Institut, Universität zu Köln, Germany

Chemical vapor deposition of borazine molecules on Ir(111) results in a well aligned monolayer of hexagonal boron nitride (h-BN) which forms an incommensurate moiré with (11.7x11.7) h-BN on (10.7x10.7) Ir unit cells. The large h-BN super cell consists of a flat physisorbed mesa with small chemisorbed valleys which form a 2D hexagonal lattice with a pitch of about 3 nm. Here we demonstrate that single vacancies created in the h-BN monolayer on Ir(111) by low fluence 500 eV He ion irradiation at elevated temperatures order to vacancy clusters that are located in the initial valley regions. Consequently, a 2D antidot lattice of small holes with diameters of 0.5-1 nm is formed. The vacancy cluster formation is traced back to single vacancy mobility and preferential bonding of vacancy cluster edges to Ir(111) in the valley regions. Moreover, similar irradiation experiments for an h-BN monolayer on Pt(111) show that our observations represent a general principle of irradiation induced antidot lattice formation, rather than a unique case. Possible uses of such nanomesh membranes based on low energy irradiation are outlined.

DS 17.32 Tue 18:15 Poster B

Local stacking order in few-layer graphene — Fabian Rudolf Geisenhof[1], •Felix Winterer[1], and Ralf Thomas Weitz[1,2] — [1]Physics of Nanosystems, Physics Department, Ludwig Maximilians Universität, München, Germany — [2]NanoSystems Initiative Munich (NIM) and Center for NanoScience (CeNS), München, Germany

The electronic bandstructure of few-layer graphene depends strongly on the local stacking order. For example, it was shown that in contrast to Bernal stacking, ABC stacking exhibits flat conduction bands. These flat bands could possibly lead to exchange-interaction driven novel states [1,2]. It is, therefore, essential to understand and characterize the local stacking order of few-layer graphene samples.

Here, we investigate the local stacking order of few-layer graphene using Atomic Force Microscopy, Raman Spectroscopy and SNOM Measurements. We discuss the surprising observation that wet processing can transform the local stacking from ABC to ABA stacking order and induce further stacking boundaries while others are straightened out.

[1] R.T. Weitz, M.T. Allen, B.E. Feldman, J. Martin, and A. Yacoby, Broken-symmetry states in doubly gated suspended bilayer graphene, Science 330, 812 (2010)

[2] Y. Nam, D.-K. Ki, M. Koshino, E. McCann and A.F Morpurgo, Interaction-induced insulating state in thick multilayer graphene, 2D Mater. 3 045014 (2016)

DS 17.33 Tue 18:15 Poster B

Magnetic-Field-Induced Rotation of Polarized Light Emission from Monolayer WS_2 — •Robert Schmidt[1], Ashish Arora[1], Gerd Plechinger[2], Philipp Nagler[2], Andrés Granados del Águila[3], Mariana V. Ballottin[3], Peter C. M. Christianen[3], Steffen Michaelis de Vasconcellos[1], Christian Schüller[2], Tobias Korn[2], and Rudolf Bratschitsch[1] — [1]Institute of Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany — [2]Department of Physics, University of Regensburg, 93040 Regensburg, Germany — [3]High Field Magnet Laboratory (HFML-EMFL), Radboud University, 6525 ED Nijmegen, The Netherlands

Atomically thin transition metal dichalcogenides (TMDCs) are potential building blocks of future applications in the field of "valleytronics". Valley polarization and valley coherence are two important physical mechanisms observed in monolayer TMDCs, such as MoS_2, WS_2, and WSe_2. We investigate the effect of valley coherence in a WS_2 monolayer by measuring the linear polarization of the photoluminescence from the A exciton in high magnetic fields. The magnetic field causes a valley Zeeman splitting of the K^+ and K^- valleys of 8 meV at 30 T. The splitting causes a rotation of the emission polarization with respect to the excitation, accompanied by a reduction of the polarization degree. Both of these phenomena are explained with a model based on two noninteracting coherent two-level systems. Our results light the way for manipulating the phase between the K^+ and K^- valley, which is important for future valleytronic devices.

DS 17.34 Tue 18:15 Poster B

2-Dimensional Atomic Crystals of Transition Metal Dichalcogenides — •Jakub Schusser[1,2], Zakariae El Youbi[1,3], Jan Minar[2], Cephise Cacho[3], Christine Richter[1], and Karol Hricovini[1] — [1]University of Cergy-Pontoise, Paris, France — [2]University of West-Bohemia, New technologies research centre, Plzen, Czech Republic — [3]CLF, RAL, Harwell Campus, Didcot, United Kingdom

Recent development in two-dimensional materials such as graphene, hexagonal boron nitride or transition metal dichalcogenides (TMDCs) has shown such material promising for several applications. TMDCs in particular, are a group of layered materials (e.g. NbSe2, MoS2, MoSe2 WS2, MoTe2) which, despite being structurally similar are particularly interesting due to their strong chemical stability, large flexibility, optical properties and the array of electronic properties ranging from semiconducting to metallic depending on their exact composition, geometry and thickness. Due to similarities such as band gap in a visible spectrum, TMDCs have previously been studied for photovoltaic applications.

We measured thin films (one and several monolayers) of MoSe2, MoS2 and MoTe2 using photoelectron spectroscopy (XPS, ARPES, SARPES). More specifically, the aim of our studies was to determine the changes in the electronic structure when depositing the films on different substrates and when the film thickness is increasing. We followed as well the evolution of the spin texture near the K, K* and M points of the surface Brillouin zone.

DS 17.35 Tue 18:15 Poster B

Spin and Charge Transport in Doped Graphene as a Tailored Carbon Allotrope — •Marie-Luise Braatz[1,2], Nils Richter[1,2], Alexander Tries[1,2,3], Axel Binder[4], Hai I. Wang[3], 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]Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany — [4]BASF SE, 67056 Ludwigshafen, Germany

Graphene is a remarkable material with numerous extraordinary properties, among them a high charge carrier mobility. However, it does not have a band gap, which is necessary for many applications. To modify graphene in this respect we employ chemical doping which has been shown to have an effect on the electronic structure [1]. Hence, we use heteroatom-doping, in particular nitrogen, to modify the structure as well as the electronic and magnetotransport properties. The amount of dopants is systematically varied so different dopant concentrations can be compared. The samples are then analyzed by Raman and electron microscopy to elucidate the changes in structure. Measuring the magnetoresistance at various temperatures and fields allows us to correlate the structure to the charge transport properties [2].

[1] H. Wang et al., ACS Catal. 2, 781 (2012)

[2] M. Rein et al., ACS Nano 9, 1360 (2015)

DS 17.36 Tue 18:15 Poster B

Defect enhanced carrier cooling dynamics in graphene — •Eduard Unger[1], Roland Kozubek[2], Stefan Weber[1], Mischa Bonn[1], Marika Schleberger[2], and Dmitry Turchinovich[1,2] — [1]Max-Planck-Institut für Polymerforschung, 55128 Mainz — [2]Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg

The present study deals with one of the main drawbacks that characterizes graphene namely the breakdown of THz conductivity for electric fields typical in the semiconductor industry. This results in undesirable limitations in its potential applications as a new material for the next generation of electronics. Our research aims to overcome this limitation by studying the influence of defects on the charge carrier dynamics. Specifically, in order to study the role of structural defects on the charge carrier cooling dynamics via optical pump - THz probe measurements, we introduce the defects into CVD graphene via Xenon irradiation. It comes out that irradiated graphene shows an increase in negative photoconductivity and enhanced charge carrier cooling. Furthermore, THz-TDS measurements confirmed an enhancement of THz conductivity for low defect concentrations. These findings provide a potential way to improve graphene high frequency performance.

DS 17.37 Tue 18:15 Poster B

Fully relativistic ab initio calculations based on the layer Korringa-Kohn-Rostoker method — •Andreas Held, Voicu Popescu, Jürgen Braun, and Hubert Ebert — Department Chemie, Ludwig-Maximilians-Universität München

Understanding the physics of systems with reduced dimensions (multilayer, 2d-materials, surfaces) is a crucial factor for the development of new electronic devices. For this purpose, a computationally ex-

tremely efficient and formally robust method, the layer Korringa-Kohn-Rostoker (LKKR) method, has been proposed by MacLaren and Pendry [1]. The scheme is hardly used in particular in its relativistic representation in dealing with the calculations for the electronic structure and transport properties. We included the LKKR scheme in our fully relativistic spin-polarized KKR code [2] that allows us to investigate the impact of relativistic effects like spin-orbit coupling onto layered systems. An implementation of the coherent potential approximation (CPA) allows the evaluation of disorder effect in alloys. With the so-called alloy-analogy [3] model finite temperatures can be treated with lattice vibrations and spin fluctuations.

[1] J.M. MacLaren *et al.*, *Phys. Rev. B* **40**, 12164 (1989); J.M. MacLaren *et al.*, *Comp. Phys. Comm.* **60**, 365 (1990). [2] H. Ebert *et al.*, *Rep. Prog. Phys.* **74**, 096501 (2011). [3] H. Ebert *et al.*, *Phys. Rev. B* **91**, 165132 (2015).

DS 17.38 Tue 18:15 Poster B

In-situ TEM investigation of NaCl decomposition encapsulated in graphene liquid cells — Fredrik Bräuer, •Tibor Lehnert, and Ute Kaiser — Electron Microscopy Group of Materials Science, University of Ulm, Ulm 89081, Germany

By in-situ transmission electron microscopy we investigate the decomposition process of encapsulated sodium chloride (NaCl) in a graphene liquid cell. We repeated the experiments more than 15 times and found that the actual decomposition process is always very similar. However, it was found out, that these crystals have extremely different stability times. That means the electron dose they can accept before the decomposition process starts deviates massively. This leads to the assumption, that the process is not only determined by the interaction of electron beam and ionic crystal. Due to our investigations a connection between the stability of NaCl and the chemical etching of the graphene layers could be established.

DS 17.39 Tue 18:15 Poster B

Structural ordering of molybdenum disulfide studied via reactive molecular dynamics simulations — •Paolo Nicolini[1], Rosario Capozza[2], and Tomas Polcar[1,3] — [1]Czech Technical University in Prague, Prague, Czech Republic — [2]Istituto Italiano di Tecnologia-IIT, Genova, Italy — [3]nCATS, University of Southampton, Southampton, United Kingdom

Molybdenum disulfide, the most studied member of the transition metal dichalcogenides family, has been used as a solid lubricant for several decades, showing extremely low friction coefficients[1] and stability to high temperature. Its lubricating properties are ascribed to the weak van der Waals interactions between sulfur atoms in the crystalline layered structure. Moreover MoS2, even when prepared in the amorphous state or made of randomly oriented domains, can undergo shear induced structural transitions to the more ordered layered state affecting its tribological properties[2]. Exploiting a classical force field[3] able to treat explicitly formation and breaking of bonds, we investigate by molecular dynamics simulations, the shear induced structural changes and possible layer formation in the amorphous molybdenum disulfide. The ordering process is studied in details, with particular regard to the estimation of the thermodynamic properties that govern the process itself. A connection with crystallization theories is finally found, conferring a predictive power to the achieved results.

[1] J.M. Martin et al., Phys. Rev. B, 48, 10583(R) (1993). [2] J. Moser, F. Lévy, Thin Solid Films, 228, 257 (1993). [3] T. Liang et al., Phys. Rev. B, 79, 245110 (2009).

DS 17.40 Tue 18:15 Poster B

X-ray absorption spectroscopy studies on transition metal dichalcogenide heterostructures — •Florian Rasch[1], Sage Bauers[2], Gavin Mitchson[2], Kyle Hite[2], Danielle Hamann[2], David Johnson[2], Javier Herrero-Martín[3], Manuel Valvidares[3], Bernd Büchner[1,4], 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 — [4]Department of Physics, TU Dresden, Dresden, Germany

Over the last years transition metal dichalcogenides (TMDs) have provided a wide playground to study their electronic properties in the crossover from 3D bulk to 2D monolayer structures. A novel way to study the effect of dimensionality on TMDs is given by a new class of materials, i.e. thin film heterostructures with chemical formula $(MSe)_m/(TSe2)_n$, where m layers of a monochalcogenide MSe (e.g. M = Pb, Sn) and n layers of a TMD (e.g. T = Nb, V) are altenrately stacked. In these materials the dimensionalities m and n as well as the constituents M and T can be precisely controlled, allowing for systematic studies of the electronic properties as a function of m, n, M and T. Here, we want to introduce these materials and their trends in electrical properties upon tuning the dimensionality and exchanging the constituents. We will discuss details of the electronic structure of $(MSe)_1/(NbSe_2)_1$ (M = Bi, Sn, Pb) by combining results of x-ray absorption spectroscopy with preliminary bandstructure calculations.

DS 17.41 Tue 18:15 Poster B

Revisiting graphene oxide chemistry via spatially-resolved electron energy loss spectroscopy — •Alberto Zobelli[1], Anna Tararan[1], Ana Benito[2], Wolfgang Maser[2], and Odile Stéphan[1] — [1]Laboratoire de Physique des Solides, University of Paris-Sud, CNRS, Orsay, France — [2]Instituto de Carboquímica ICB-CSIC, Zaragoza, Spain

The type and distribution of oxygen functional groups in graphene oxide (GO) and reduced graphene oxide (RGO) remain still a subject of great debate. Local analytic techniques are required to access the chemistry of these materials at a nanometric scale. Electron energy loss spectroscopy in a scanning transmission electron microscope can provide the suitable resolution, but GO and RGO are extremely sensitive to electron irradiation. In this work we employ an optimized experimental setup to reduce electron illumination below damage limit. GO oxygen maps obtained at a few nanometers scale show separated domains with different oxidation levels. The C/O ratio varies from about 4:1 to 1:1, the latter corresponding to a complete functionalization of the graphene flakes. In RGO the residual oxygen concentrates mostly in regions few tens of nanometers wide. Specific energy-loss near-edge structures are observed for different oxidation levels. By combining these findings with first-principles simulations we propose a model for the highly oxidized domains where graphene is fully functionalized by hydroxyl groups forming a 2D-sp3 carbon network analogous to that of graphane.

DS 17.42 Tue 18:15 Poster B

Surface-assisted synthesis of 0-, 1-, and 2-dimensional structures — •Katayoun Gharagozloo-Hubmann, Niclas Sven Mueller, Christian Lotze, Katharina J. Franke, and Stephanie Reich — Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

The on-surface synthesis of graphene nanoribbons based on halogenated unsaturated hydrocarbons is an already known and often used concept.[1] Molecular precursors were designed that led to the synthesis of ribbons with different symmetry and width.[2]

We propose a novel concept for the on-surface synthesis of 0-, 1-, or 2-dimensional structures. We suggest to select the target precursor from commercially available molecules and use the template substrates for the growth of graphene substructures. We already demonstrated the growth of 2D graphene, when using extended metal substrates.[3] This concept not only provides access to the various graphene substructures, but also impressively demonstrates the use of weak molecular interactions for the production of more complex structures via covalent coupling.

[1] Cai, JM; Ruffieux, P; Jaafar, R; Bieri, M; Braun, T; NATURE 2010, 466, 7305, 470.

[2] Ruffieux, P; Wang, S; Yang, B; Sanchez-Sanchez, C; Liu, J; NATURE 2016, 531, 7595, 489.

[3]Gharagozloo-Hubmann, K; Müller, NS; Giersig, M; Lotze, C; Franke, KJ; Reich, S; J. Phys. Chem. C 2016, 120 (18), 9821.

DS 17.43 Tue 18:15 Poster B

A biosynthetic pathway reconstituted within compartmentalized vesicles — •Akanksha Moga — Max Planck Institute of colloids and Interfaces, Potsdam, Germany

Cells are complex chemical systems composed of distinct compartments that function in a systematic manner. Compartmentalization of the cell is considered as a key step in the direction of eukaryotic evolution that accommodates multiple bio-chemical reactions. These compartments establish physical boundaries for biological processes that enable the cell to carry out different metabolic activities at the same time. In the discipline of bottom-up synthetic biology, lipid vesicles serve as an artificial cell but there is need to compartmentalize the processes within these vesicles. Here, we aim to mimic a cell by developing compartmentalized Giant Unilamellar Vesicles (cGUVs), as an artificial cell model.To illustrate the role of compartments, we study a

multi-compartment enzymatic pathway, biosynthesis of molybdenum co-factor (Moco). Moco biosynthesis is highly conserved and ubiquitous pathway that takes place in a typical eukaryotic mitochondrion. The reactions involves cascade of protein/enzymatic reactions but protein encapsulation is not always supported by conventional lipid vesicles generation techniques. Therefore, we have employed an emulsion based phase transfer method to not only produce cGUVs but also to encapsulate specific substrates. Our preliminary results have shown promise with reproducibility of stable GUVs encapsulating various compounds and enzyme from Moco biosynthesis.

DS 17.44 Tue 18:15 Poster B

Antiferromagnetic interfaces in ferromagnetic perovskite heterostructures — •Vitaly Bruchmann-Bamberg and Vasily Moshnyaga — I. Physik. Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The magnetism in strongly correlated oxide perovskites, e.g. manganites $La_{0.7}Sr_{0.3}MnO_3$ (LSMO), is well-known to be governed by indirect super- or double-exchange mechanism via oxygen p-states. A ferromagnetic (FM) or an antiferromagnetic (AFM) ground state evolves, depending on the configuration and occupancy of d-orbitals. An unusual AFM coupling at the interface between two FM perovskites, i.e. a metallic LSMO ($T_{C,LSMO}$=350 K) and an insulating double perovskite La_2CoMnO_6 (LMCO) ($T_{C,LMCO}$=230 K), was observed. The LSMO/LMCO heterostructures were grown on (100)- and (111)-oriented $SrTiO_3$ substrates by metalorganic aerosol deposition technique. The interfacial AFM coupling appears for $T<T_{C,LMCO}$=230 K and is maximal in (001)-oriented heterostructures. The role of termination layers at LSMO/LMCO interfaces on the exchange mechanisms is discussed within Goodenough-Kanamori-Anderson rules of magnetic couplings.

DS 17.45 Tue 18:15 Poster B

Ni_xO thin films - impact of composition x on optical parameters — •Martin Becker, Fabian Michel, Angelika Polity, and Peter J. Klar — Institute for Exp. Physics I and Center for Materials Research (LaMa), Justus Liebig University Giessen, Germany

Ni_xO thin films were grown on single crystal sapphire substrates of various orientation by ion beam sputtering of a Ni metal target in a mixed argon and oxygen atmosphere. Epitaxial growth was verified by X-ray diffraction measurements on all substrates. Surface morphology and surface roughness were explored via atomic force microscopy. Consequential, Ni_xO films on *c*-plane and *a*-plane sapphire were found to be best suited to serve as antiferromagnetic pinning layers.
For thin films grown on *c*-plane sapphire the composition of the film was varied systematically by changing the ratio of inert gas (Ar) and reactive gas (O_2). The information of chemical bonding was investigated via X-ray photoelectron spectroscopy. Optical characterization yielded a strong dependence of the refractive index and the optical band gap of Ni_xO on composition x, although the samples were very similar relating to their structure. The dependence of the refractive index of Ni_xO on composition x contributes substantially to the broad span of values reported for Ni_xO in literature.

DS 17.46 Tue 18:15 Poster B

Electrical conductivity measurements of ultrathin ferrite films on MgO(001) — •Tobias Pollenske, Jari Rodewald, Tobias Pohlmann, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

The semiconducting and ferrimagnetic behavior make ultrathin epitaxial ferrite films like $NiFe_2O_4$ or $CoFe_2O_4$ promising candidates in the field of spintronics. Due to their spin dependent tunneling barrier they are well-suited to be used as spin filters. Here, the resistance of the films is a crucial property for the formation of suitable tunneling barriers and thus for the performance as a spin filter.

Hence, in this work a measurement setup is taken into operation to investigate the temperature dependent conductivity of ultrathin ferrite films. First, different types of contacts in van-der-Pauw geometry are tested in order to optimize the performance of the measurement setup. Furthermore, ultrathin $Ni_xFe_{3-x}O_4$ films on MgO(001) with different stoichiometries ($0 \leq x \leq 2$) are prepared via reactive molecular beam epitaxy (RMBE) and their conductivity is analyzed with respect to the different cation ratios.

DS 17.47 Tue 18:15 Poster B

Electrical Permittivity Determination of ScAlN Thin Films — •Niclas Feil[1], Nicolas Kurz[2], Mohammad Fazel Parsapourkolour[3], and Oliver Ambacher[1] — [1]Laboratory for Power Electronics, INATECH-Department of Sustainable Systems Engineering, University of Freiburg, Emmy-Noetherstr. 2, 79110 Freiburg, Germany — [2]Laboratory for Compound Semiconductor Microsystems, IMTEK-Department of Microsystems Engineering, University of Freiburg, Georges-Koehler-Allee 103, Germany — [3]Electroceramic Thin Films Group, EPFL, Laussane, Switzerland

Wurtzite scandium-aluminiumnitride ($Sc_xAl_{1-x}N$) is a material with outstanding properties. For instance, 400 % increase of the piezoelectric strain constant d_{33} for $Sc_{0.43}Al_{0.57}N$ compared to AlN was reported. This results in a substantially enhanced electromechanical coupling, which is needed for future high frequency piezoacoustic filter devices for the upcoming 5G mobile radio standard. All tensor components are needed for the design of these devices. However, dielectric tensor components are still missing. In this work, the missing ϵ_{11} component of the dielectric tensor for $Sc_xAl_{1-x}N$ is determined experimentally for the first time. We developed a method for the determination of the basal permittivity component ϵ_{11}. It is based on the electrical capacitance measurement of interdigital test structures and finite element model optimization. The developed approach was validated with c-axis oriented sapphire substrates and AlN thin films. We observe that the $\frac{\epsilon_{11}}{\epsilon_{33}}$ ratio of $Sc_{0.15}Al_{0.95}N$ and AlN are different which highlights the change in anisotropic properties.

DS 17.48 Tue 18:15 Poster B

Quantitative disentanglement of fully controllable coherent and incoherent laser-induced surface deformations by time-resolved x-ray reflectivity — •Marc Herzog[1], Mathias Sander[1], Jan-Etienne Pudell[1], Matias Bargheer[1,2], Roman Bauer[3], Valentin Besse[4], Vasily Temnov[4,5], and Peter Gaal[3] — [1]Institut für Physik und Astronomie, Universität Potsdam, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [3]Institut für Festkörper- und Nanostrukturphysik, Universität Hamburg, Germany — [4]IMMM CNRS 6283, Université du Maine, 72085 Le Mans cedex, France — [5]CNRS UMR 8635, Université Paris-Sacley, 78035 Versailles cedex, France

High-frequency surface acoustic waves (SAWs) are not only present in any mobile phone, they are a powerful tool for fundamental research, e.g., to investigate the coupling of the lattice to other degrees of freedom in solids. SAWs with specific wavevectors can be generated by transient grating (TG) excitation using ultrashort laser pulses. In absorbing media, however, most of the optical excitation energy is deposited as incoherent, thermal strain. By using time-resolved x-ray reflectivity, we measure and decompose the absolute amplitudes of these transient coherent and incoherent periodic surface distortions which is very challenging using all-optical experiments. Moreover, we refine the TG technique to get full spatiotemporal coherent control of both coherent and incoherent excitations individually in order to suppress or enhance whatever is of primary interest.

DS 17.49 Tue 18:15 Poster B

Partial Least Square Regression of AES depth profiles and UV-visible spectroscopy for determining oxide layer thicknesses on technical copper — •Jan Stiedl[1,2,3], Simon Green[3], Thomas Chassé[2], and Karsten Rebner[1] — [1]Reutlingen University, Alteburgstrasse 150, 72762 Reutlingen, Germany — [2]University of Tuebingen, Auf der Morgenstelle 18, 72076 Tuebingen, Germany — [3]Robert Bosch GmbH, Postfach 1342, 72703 Reutlingen, Germany

In research as in industry, copper is a very commonly used raw material. Due to its electrical properties, copper is used both in battery development and in the development of control units for automotive and non-automotive applications. To ensure the electrical properties and the adhesion of material used in the contacting and packaging technology, the surface of the copper must not be covered by uncontrolled growth of oxide layers. In order to assess this, photoelectron spectroscopy, such as XPS or AES is used. However, these methods are not sufficient for satisfactory statistics and cover-age of production batches. For this purpose, an UV-visible spectroscopy measurement system was developed, which can qualitatively and quantitatively characterize the surface with a Partial Least Square regression (PLS) model in the range of 0 - 50 nm. Superimposed absorption and interference spectra are used to determine oxide layers. PLS is used as a data evaluation tool to establish a regression between the UV-Visible spectra and AES depth profiles. The accuracy of the regression is about 5 %. Already known methods cannot be used in these cases, mostly due to the high roughness of the technical copper surfaces.

DS 17.50 Tue 18:15 Poster B

Infrared Mueller Ellipsometry of Thin Films — •Andreas Furchner, Cordula Walder, and Karsten Hinrichs — Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Schwarzschildstraße 8, 12489 Berlin, Germany

Non-isotropic thin films can be characterized by their Mueller matrix (MM), a 4x4 matrix that describes the sample's optical properties upon interaction with polarized light. Besides anisotropy and structure, Mueller matrices in the infrared region provide information on, for example, film chemistry, composition, and molecular interactions. However, laboratory thin-film MM measurements in the infrared are inherently difficult, in part because of source prepolarization, non-ideal polarizers, and low optical throughput.

We developed a powerful IR Mueller ellipsometer with high optical throughput that enables sensitive MM measurements of thin films below 100 nm. The measurement scheme can be restricted to a subset of defined polarizer settings, allowing one to extract quadruples of Mueller matrix elements within a few 10 seconds to minutes. Tandem polarizers gurantee a sufficiently high degree of polarization necessary to accurately measure block-offdiagonal MM elements, while optional retarders provide access the fourth row or column of the Mueller matrix. Both normalized and absolute Mueller matrices can be obtained.

We demonstate Mueller matrix measurements of thin polymer films and, in cooperation with HZB Berlin, of trapezoidal SiO2 gratings, the offdiagonal MM elements of which are highly sensitive towards structure and orientation.

DS 17.51 Tue 18:15 Poster B

Molecular Beam Deposition of thin YbzFeSb3 films on (001) oriented KCl — •Felix Timmermann — Universität Augsburg, Augsburg, Germany

Increasing interest in the development of alternative energy sources led to an extended research in the field of thermoelectricity. For a good efficiency of thermoelectric generators, there is a need of materials with special transport properties. The goal is to find compounds with a large Seebeck coefficient α, good electrical conductivity σ and low thermal conductivity κ. Skutterudites, such as FeSb3, are materials that meet those criteria well. The insertion of filler atoms like Yb increases the thermal stability and has the potential to increase to improve the thermoelectric properties further.

In this work the materials iron, antimony and ytterbium were thermally evaporated and deposited on heated (001) oriented KCl-substrates by molecular beam epitaxy in order to achieve epitaxial growth of thin YbzFeSb3 films. It could be shown that there is a strong dependence of the growth rate of antimony to the iron flux and the substrate temperature. Furthermore a drastic increase of the growth rates of iron and antimony with increasing ytterbium flux was observed. Structural characterization was carried out in situ by Reflection High-Energy Electron Diffraction and ex situ by X-Ray Diffraction and Transmission Electron Microscopy.

DS 17.52 Tue 18:15 Poster B

Investigation of the Density of States of Phase Change Materials by Tunneling Spectroscopy — •Lisa Metzner[1], Dominik Gholami Bajestani[1], Henrik Padberg[1], Tobias Schäfer[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA - FIT, RWTH Aachen University, Germany

Due to their unique physical properties, phase change materials (PCM) are promising candidates for future data storage applications. By applying electrical or laser pulses, they can be switched reversibly between an amorphous and a crystalline state on a nanosecond timescale. These states are characterized by a large optical and electrical contrast, which is utilized for rewritable optical data storage and phase change RAM applications. Furthermore, the resistivity can be tuned over several orders of magnitude by disorder control, which allows for possible multilevel memory devices in the future. In order to fully understand the electronic properties of those materials, the density of states (DOS), especially in the vicinity of the Fermi level, is a crucial quantity. This contribution presents the method of tunneling spectroscopy, which allows the determination of the DOS around the Fermi energy with a resolution of up to 0.2 meV, complementing to photoelectron spectroscopy which is typically limited by a resolution of around 0.1 eV. The measurements were performed using tunnel junctions, produced by in-situ sputter deposition in order to prevent the PCM from surface contamination. Besides the introduction of the procedure, tunneling spectra of PCMs with a varying degree of disorder are presented.

DS 17.53 Tue 18:15 Poster B

Structural Characterisation of Crystalline Lead-Antimony-Telluride Alloys — •Alexander Rochotzki[1], Johannes Reindl[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA - FIT, RWTH Aachen University, 52056 Aachen, Germany

The material class of chalcogenides has great potential for practical applications, ranging from optical and electrical data storage to thermoelectrics. For the latter, materials on the tie line between PbTe and Sb_2Te_3 are interesting candidates. In the past, the group of Shelimova et al. has already investigated such compounds in their thermodynamic stable hexagonal phase with respect to structure and possible thermoelectric applications [1].

In the hexagonal phase of $(PbTe)_x(Sb_2Te_3)_{1-x}$, the intrinsic vacancies form layers, similar to the isoelectronic phase-change materials on the tie line between GeTe and Sb_2Te_3, which additionally exhibit a metastable cubic phase, not yet seen in $(PbTe)_x(Sb_2Te_3)_{1-x}$. In this work we aim to synthesise the metastable cubic phase of PbSbTe while characterising and optimising the structural properties of the compounds fabricated.

[1] Shelimova, L.E. et al., *Inorganic Materials*, Vol. 40, 1440 (2004)

DS 17.54 Tue 18:15 Poster B

Two-dimensional growth of three-dimensionally bonded GeTe — •Isom Hilmi, Andriy Lotnyk, Jürgen Gerlach, Philipp Schumacher, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e.V., 04318, Leipzig, Germany

In this work, epitaxial thin films of three-dimensionally (3D)-bonded GeTe are grown on a two dimensionally (2D)-bonded ultra-thin Sb2Te3 seeding layer on Si(111) by pulsed laser deposition. The GeTe films are grown in trigonal phase with epitaxial relationships of GeTe(0001) || Sb2Te3(0001) || Si(111) and GeTe[11-20] || Sb2Te3[11-20] || Si[-110]. The use of a seeding layer is shown to extend the epitaxial window towards lower temperature regimes up to 145 °C. Additionally, the surface quality of the GeTe films is also significantly improved. Local structure investigation of the epitaxial films reveals the presence of a superposition of twinned domains, which is assumed to be an intrinsic feature of these thin films. This work paves a way to improve epitaxial growth and film quality of 3D-bonded alloys by the use of 2D-bonded seeding layer.

DS 17.55 Tue 18:15 Poster B

Structural changes in epitaxial Ge2Sb2Te5 thin films with highly ordered vacancy layers upon ns-laser irradiation — •Mario Behrens, Andriy Lotnyk, Jan Griebel, Jürgen Gerlach, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e.V., Permoserstr. 15, 04318, Leipzig, Deutschland

Chalcogenide phase-change materials can be rapidly switched between their amorphous and crystalline phase by being exposed to electrical or optical pulses. Since both phases differ greatly in their reflectivity and conductivity, these materials can be employed for non-volatile optical and electrical data storage based on the phase-change storage mechanism. In this study, ns-laser pulse induced phase transformations of the most prominent chalcogenide phase-change material Ge2Sb2Te5 (GST225), epitaxially grown on Si(111) substrates by pulsed laser deposition, are investigated. X-ray diffraction and aberration-corrected high-resolution scanning transmission electron microscopy of the as-deposited films revealed the formation of cubic GST225 phase with ordered vacancy layers. By applying ns UV-laser pulses the GST225 films were reversibly switched between their crystalline and amorphous state, resulting in a reflectivity contrast of up to 22 %. Within the recrystallization process the amorphous thin films were transformed into a crystalline GST225 phase with disordered vacancies. The influence of laser parameters on the phase changes is discussed.

DS 17.56 Tue 18:15 Poster B

Thermoelectric performance of multilayers of Sb_2Te_3 thin films and Pt nanoparticles — •Darius Pohl, Heiko Reith, Frank Schmidt, Gabi Schierning, Kornelius Nilesch, and Bernd Rellinghaus — IFW Dresden

Three material properties (Seebeck coefficient, electrical and thermal conductivity) define the efficiency of a thermoelectric material stated as figure of merit ZT. Introducing additional interfaces in the material is considered as an effective means to further improve the perfor-

mance of thermoelectric devices. This is generally attributed to either a change of the local electronic density of states or to a significant increase of phonon scattering at interfaces and defects. In the present study, we investigate the thermoelectric properties of discontinuous thin film multilayers of alternating Sb_2Te_3 thin films and Pt nanoparticles. Both, the thin films and the Pt nanoparticle are prepared by RF and DC magnetron sputtering, respectively. The thermoelectric performance of the likewise prepared $[(Sb_2Te_3)|Pt-nP's]_N$ samples is correlated with the details of the local structure and chemical composition as provided by (HR)-TEM, EDXS and EELS investigations.

DS 17.57 Tue 18:15 Poster B

Highly conductive thin-films based on solution-processed silver nanoparticles for spray-on antennas — •Marco Bobinger[1], Michael Haider[1], Andreas Albrecht[1], Yash Goliya[1], Johannes Russer[1], Markus Becherer[1], and Paolo Lugli[2] — [1]Department of Electrical and Computer Engineering, Technical University of Munich, Munich, Germany — [2]Free University of Bozen-Bolzano, Bozen-Bolzano, Italy

Antennas are commonly deposited to rigid substrates using a physical vapour deposition process that requires high vacuum and eventually also high temperatures. Solution-processed inks that are based on e.g. metal nanowires or -particles have recently attracted a high research and commercial interest attributed to scalable synthesis protocols and readily available deposition techniques under ambient conditions.

In this contribution, we report on the fabrication and characterization of conductive thin-films based on spray-coated silver nanoparticles. In order to enhance the conductivity of the sub 250 nm thick films, different sintering techniques such as thermal annealing and high intensity light pulse sintering were investigated under ambient conditions. After sintering, films with a thickness around 130 nm and a resistivity around 64 nOhm*m, which is only around a factor of 4.8 higher than the value reported for bulk silver, were produced. The drastic reduction in resistance from almost non-conductive can be ascribed to the coalescence of the 50 nm particles to a percolating silver film. Furthermore, the highly conductive films were tested for spray-on antennas on rigid and flexible substrate using an original coplanar design.

DS 17.58 Tue 18:15 Poster B

Memsensors: emerging properties for neuromorphic engineering — •Alexander Vahl[1], Jürgen Carstensen[2], Sören Kaps[2], Thomas Strunskus[1], Oleg Lupan[2], Rainer Adelung[2], and Franz Faupel[1] — [1]Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Multicomponent Materials, Kaiserstr. 2, 24143, Kiel, Germany — [2]Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Functional Nano Materials, Kaiserstr. 2, 24143 Kiel, Germany

In biological neuronal systems such as the human brain, adaptation is very important for efficient use of neuronal capabilities and learning. In this work we present a concept to translate adaptation into neuromorphic engineering at the example of memsensors. Memsensors are a class of two terminal devices that combine the basic features of memristive devices (pinched hysteresis) and sensors (change in electrical resistivity depending on an external stimulus). Apart from their inherited properties, memsensors have the capability to adapt to the external stimulus as well as a strongly stimulus dependent I-V characteristic. The electrical behavior of a general memsensor was modelled by a three component equivalent circuit, based on two memristive elements in series and in parallel to a sensitive element respectively.

DS 17.59 Tue 18:15 Poster B

Resistive Switching Behavior of Polycrystalline PCMO Thin Films with AlOx Tunnel Oxide — •Alexander Gutsche[1], Christoph Bäumer[1], Rainer Waser[1,2], and Regina Dittmann[1] — [1]Peter Gruenberg Institut, Forschungszentrum Juelich GmbH, Germany — [2]Institut fuer Werkstoffe der Elektrotechnik (IWE-2), RWTH Aachen, Germany

Redox based memory is a promising candidate for nonvolatile memory to replace flash memory and can be used as basis for novel neuromorphic circuits. Most of the employed systems show filamentary switching, which causes a high variability in resistivity induced by the stochastic filament formation process. Another type of resistive switching is interface type switching, which occurs for example in hetero structures consisting out of a tunnel barrier (AlOx) and a mixed-valence manganite (PCMO). Interface type switching suffers less from resistivity variability, because of the area scaling, i.e., the resistance value is inversely proportional to the surface area. In addition it is possible to adapt the memory device current to a given circuit requirement. Here we will present the switching characteristics of polycrystalline PCMO thin films grown on Pt substrates with an Al tunnel barrier, taking into account the influence of the growth temperature on the pulsed laser deposited PCMO film. The investigation of the formation step of the AlOx tunnel barrier shows a strong dependence of the initial state of the memory device, what can also be seen in the formation voltage, which is influenced by the initial state. Also we will present measurements of the area scalability of the memory cell.

DS 17.60 Tue 18:15 Poster B

Flexible Co-based Heusler alloy/muscovite heteroepitaxy — •Yi-Cheng Chen[1,2], Min Yen[2], Anastasios Markou[1], Benedikt Ernst[1], Claudia Felser[1], and Ying-Hao Chu[2] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]National Chiao Tung University, Taiwan

Co-based ferromagnetic Heusler compounds show high spin polarization combined with high Curie temperature of ≈ 700 K. In this study, we demonstrate the epitaxy of Co_2MnGa Heusler alloy on flexible muscovite substrate, which paves a way toward flexible spintronic devices. The epitaxial Co_2MnGa Heusler film on muscovite substrate was prepared by magnetron sputtering. Muscovite is chosen as a flexible substrate for Heusler alloy since its melting point meets growth condition for epitaxy. The epitaxy was characterized by X-ray diffraction and the epitaxial relationship between the substrate and the film was found to be [110] Mica||[1 -1 0]Co2MnGa. The bending affects the magnetization and the transport properties of the thin films. The saturation magnetization is increased by 7.6 percent under bending condition. The demonstration of Co_2MnGa/muscovite heteroepitaxy provides a new perspective on developing devices with a huge potential for flexible spintronic.

DS 17.61 Tue 18:15 Poster B

Large-scale spray deposition of carbon nanotube-based thin-film devices — •Florin-Cristian Loghin[1], Aniello Falco[2], Marco Bobinger[1], Alaa Abdellah[1], Markus Becherer[1], Paolo Lugli[2], and Almudena Rivadeneyra[1] — [1]Institute for Nanoelectronics-Technische Universität München, Munich, Germany — [2]Free University of Bozen-Bolzano, Bozen-Bolzano, Italy

Due to their remarkable electrical and mechanical characteristics, Carbon nanotubes (CNTs) are ideal candidates for a wide range of applications. The possibility to fabricate CNT thin-films via solution processing techniques has enabled the way to low-cost CNT thin-film devices including thin-film transistors (TFTs) and circuits, thermal and chemical sensors as well as transparent conductive films (TCFs). In this contribution, we report on a spray deposition technique, which can produce uniform, reproducible thin-films suitable for a wide range of applications. The use of non-invasive solvents (DI-H2O) as well as low processing temperatures (<65°C) permits for the process to be easily integrated into existing technology platforms. Furthermore, the resolution down to 10 CNTs/um2 per deposited layer allows for precise device engineering. In order to better display this technology, proof of concept devices were fabricated and characterized, including TFTs, chemical sensors and TCFs.

DS 17.62 Tue 18:15 Poster B

Pulsed Laser Deposition of $PbZr_{0.52}Ti_{0.48}O_3$ thin films on stainless steel — •Juliette Cardoletti, Aldin Radetinac, Philipp Komissinskiy, and Lambert Alff — Technische Universität Darmstadt, Institute of Materials Science, Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany

With the acute need for miniaturisation of devices and components, the use of bending tongues (cantilevers or wider beams) based on piezoelectric ceramics is increasing. Up to date most devices are created by gluing piezoelectric elements onto metallic structures with epoxy.

Some papers present a new solution by depositing a $PbZr_{0.52}Ti_{0.48}O_3$ (PZT) thin film by sol-gel on nickel foils using HfO_2 and $LaNiO_3$ (LNO) as buffer layers [1].

This work aims to deposit PZT and LNO thin films on stainless steel by Pulsed Laser Deposition (PLD). Using a physical vapour deposition method potentially allows for a better process control and is better applicable to microelectromechanical systems (MEMS).

[1] H.G. Yeo and S. Trolier-McKinstry, J. Appl. Phys. 116, 014105 (2014).

DS 17.63 Tue 18:15 Poster B

Distinct Emission Characteristics of Nano-Sized Metal-Organic Hybrid Structures — •Maximilian Rödel[1], Verena Kolb[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

Nano-sized organic-metal hybrid structures offer unique and attractive optical properties for example, in lighting applications like organic LEDs. Moreover, by means of shadow-nanosphere-lithography we are able to fabricate these structures in hexagonally ordered arrays [1]. In this contribution, we report on laterally structured zinc-phthalocyanine (ZnPc) films in close proximity to nanostrucured gold or silver facettes and their resulting optical excitations posessing a coupled exciton plasmon character. Besides demonstrating a remarkable increase in light-outcoupling and quantifying the geometrical and plasmonic contributions, we investigate the occurrence and spectral signature of collective modes generated via plasmon-mediated interaction between the neighbouring discrete ZnPc nanovolumes.

[1] V. Kolb, J. Pflaum, Opt. Express 25 (2017) 6678

DS 17.64 Tue 18:15 Poster B

Interactions at the interface of TMPcs and graphene covered metal surfaces: Influence of fluorination and intercalation — •David Balle, Peter Grüninger, Reimer Karstens, Hilmar Adler, Thomas Chassé, and Heiko Peisert — Institute of Physical and Theoretical Chemistry, Auf der Morgenstelle 18, 72076 Tuebingen, University of Tuebingen, Germany

Recent years have seen increasing research efforts in the field of transition metal phthalocyanines (TMPc) due to their special electronic, optical and magnetic properties making them potential suitable candidates for organo-electronic applications.

To manipulate interface interactions, which can drastically alter said properties, Graphene buffer layers offer a valuable tool. On Ni(111), a strongly bound and coupled Graphene layer behaves vastly different in regards to its buffer properties than an uncoupled, intercalated layer on the same substrate. The degree of coupling and interaction between the Graphene layer and the substrate is subject to the intercalating element, though, providing a method to finely tune the coupling by carefully choosing the intercalant, like Fe, Cu or Ge. Other electronic parameters of the TMPc, such as substitution of the terminal hydrogen atoms with fluorine, also play a crucial role if an interface interaction persists through the buffer layer like in the case of $CoPcF_{16}$ while the corresponding interaction is blocked for CoPc on intercalated Graphene on Ni(111) [1]. Investigations were carried out using mainly X-ray absorption and photoemission spectroscopies (XAS, PES).

[1] Balle et al., J. Phys. Chem. C 2017, 121, 18564-18574

DS 17.65 Tue 18:15 Poster B

Kelvin-Probe Force Microscopy and Conductive-AFM Studies of the Contact Formation with 1-(Pyridin-2-yl)-3-(quinolin-2-yl)imidazo[1,5-a]quinoline in Layered Structures — •Clemens Geis[1], Eric Yanchenko[1], Georg Albrecht[1], Jasmin Martha Herr[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, JLU Giessen, Germany — [2]Institute of Organic Chemistry, JLU Giessen, Germany

1-(Pyridin-2-yl)-3-(quinolin-2-yl)imidazo[1,5-a]quinoline was investigated as a model compound of a new class of organic semiconductors which receives increased interest for applications in material science, mainly regarding blue organic light emitting diodes (OLED). In order to construct electronic devices, a proper alignment of the energy levels of contact materials and emitters is mandatory for an efficient charge carrier injection. In this work the contact potential differences of emitters, anode and cathode materials are investigated by Kelvin-probe force microscopy (KPFM). A layered sample design allowed to measure all potential differences in a single device. A Fermi level close to the occupied orbitals of the organic layer was determined showing the dominance of hole conduction. Current-voltage characteristics of test devices confirmed appropriate contact formation by current onsets at low voltages. These results are compared to first measurements at 1,3-disubstituted imidazo[1,5-a]pyridines and -quinolines to establish a systematic optimization.

DS 17.66 Tue 18:15 Poster B

Initial Growth of DNTT Thin Films on Ag(111) — •Daniel Bischof, Maximilian Dreher, Andrea Huttner, Felix Widdascheck, Tobias Breuer, and Gregor Witte — FB Physik Phillips-Universität Marburg 35032 Marburg, Germany

The high charge carrier mobility of the novel organic semiconductor (OSC) dinaphthothienothiophene (DNTT) has created large interest in this compound in view of potential efficient devices. Since device characteristics are largely governed by interfaces to metallic electrodes, the structure and coupling at metal surfaces is of fundamental interest. Here, we combined STM and NEXAFS to investigate the initial stage of DNTT film growth on Ag(111) substrates. While initially a relaxed monolayer of flat-lying molecules is formed, at large coverage a compressed monolayer forms, where molecules exhibit a herringbone arrangement. Interestingly, multilayer films reveal a temporal dewetting, yielding the formation of discrete islands surrounded by regions with the relaxed monolayer.

DS 17.67 Tue 18:15 Poster B

Gas adsorption on self-assembled monolayers — •Christian Albers, Susanne Dogan, Michael Paulus, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund

The influence of gases on hydrophobic surfaces especially on self-assembled monolayers (SAM) is in focus of the recent research [1, 2]. An X-ray reflectivity study on the adsorption behaviour of different organic gases on long alkyl chains (Octadecyltrichlorosilane (OTS) $SiCl_3C_{18}H_{37}$) is presented. Silicon wafers were exposed to piranhia solution to get a hydrophilic interface and then treated with OTS-solution in order to induce SAM formation on the surface [3]. Subsequently, they were exposed to dense gas phases near the condensation pressure of isobutane, perfluorobutane and octafluoropropane. The results show, that the SAM are not penetrated by the gas molecules. Even at pressures close to the condensation pressures of the used gases there is no change in the SAM structures.

[1] L. Böwer et al. J. Phys. Chem. 15 (2011), S. 8235-18238.
[2] F. Giebel et al. Coll. Surf. A 504 (2016), S 126-130.
[3] M. Mezger et al. Proc. Natl. Acad. Sci. U.S.A. 103 (2006), S. 18401.

DS 17.68 Tue 18:15 Poster B

Infrared Spectroscopic Study on Phosphonic Acid Modification of Nickel Oxide — •Valentina Rohnacher[1,2], Sabina Hillebrandt[1,2], Florian Ullrich[2,3], Sebastian Hietzschold[2,4], Sebastian Beck[1,2], and Annemarie Pucci[1,2] — [1]Kirchhoff Institut für Physik, Uni Heidelberg — [2]Innovationlab GmbH, Heidelberg — [3]TU Darmstadt — [4]TU Braunschweig

Solution-processed nickel oxide (sNiO) thin films have shown promising characteristics as hole transport material in organic photovoltaic cells (OPVs) leading to a better interfacial compatibility between the transparent conductive oxide electrode and the organic semiconductor layer. In this study, sNiO thin films have been modified by a dipolar self-assembled monolayer (SAM) of 4-cyanophenylphosphonic acid (CYNOPPA) to gain full control of the surface properties. Infrared vibrational spectroscopy gives insight into the composition of the investigated material and can be used for monitoring orientation of characteristic vibrations or functional groups. Together with photoelectron spectroscopy, contact angle measurements and OPV device characteristics, a deeper understanding of the structure-function relationship of the modified sNiO have been achieved. The results reveal that hydroxide species of the sNiO films play a crucial role for the chemisorption of SAMs on sNiO. Besides the increased work function and improved wettability, the sNiO surface has been successfully passivated by chemisorption of CYNOPPA.

DS 17.69 Tue 18:15 Poster B

Growth Kinetics-Controlled Morphology of DNTT Thin Films on KCl (001) — •Darius Günder, Andrea Huttner, Tobias Breuer, and Gregor Witte — FB Physik, Philipps-Universität Marburg

The novel organic semiconductor dinaphthothienothiophene (DNTT) has recently gained interest for molecular electronic devices due to its high charge carrier mobility [1]. While the main focus here is typically on transistor characteristics, the microstructure and morphology of the organic semiconductor films are usually less well known. In previous work, a substrate mediated control of the molecular orientation as well as notable dewetting was observed for DNTT [2]. In the present study, we report on the coexistence of two different film morphologies on KCl (001) substrates. Using atomic force microscopy (AFM) we show that by variation of the kinetic growth parameters such as substrate temperature and evaporation rate the amount of both structures can be precisely tuned. Complementary X-Ray diffraction (XRD) measure-

ments reveal different molecular orientations in these two morphologies. Interestingly, both structures grow epitaxially on the KCl (001) surfaces in different discrete azimuthal orientations as observed from statistical analysis of AFM data and inplane XRD scans.

[1] Xie et al., Advanced Materials 25, 3478 (2013)
[2] Breuer et al., ACS Applied Materials & Interfaces 9, 8384 (2017)

DS 17.70 Tue 18:15 Poster B

FePc and $FePcF_{16}$ on Rutile: Influence of the defects and the crystal orientation on the interaction — •Reimer Karstens, David Balle, Axel Belser, Thomas Chassé, and Heiko Peisert — Institute of Physical and Theoretical Chemistry, Auf der Morgenstelle 18, 72076 Tuebingen, University of Tuebingen, Germany

Nowadays, organic semiconductor electronics are extensively investigated due to their electronic, magnetic, optical properties and their possible applications. Transition metal phthalocyanines (e.g. FePc) on rutile surfaces represent an important model system for organic semiconductor-oxide interfaces. Moreover, such interfaces are of high interest for applications, like dye-sensitized solar-cells. Our research focus lies on the influence of three parameters on the interface interaction: vacancies, crystal orientation and changed electronic properties by fluorination of the phthalocyanine molecule. Reconstructed rutile single crystal surfaces (TiO_2 (100)-(1 × 3) and TiO_2 (110)-(1 × 1)) are used, where the defect concentration is controlled by the oxygen amount during the annealing. The orientation of the phthalocyanine molecules and the interface interaction were investigated by photoemission and x-ray absorption spectroscopy. The interaction involves in particular the nitrogen atoms of the phthalocyanine. Clear differences are observed in the interaction for different TMPc molecules and defect concentrations.

DS 17.71 Tue 18:15 Poster B

Hexacene - Thin film studies on Au(110) with x-ray spectroscopies — •Peter Grüninger[1,2], David Balle[1], Reimer Karstens[1], Heiko Peisert[1] und Holger F. Bettinger[2] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany — [2]Institute of Organic Chemistry, University of Tübingen, Germany

Acenes are an important class of polycyclic aromatic hydrocarbons. However molecules larger than pentacene, a well-known material for organic electronics, are difficult to handle due to their low solubility and high reactivity. Here, we focus on the synthesis and thin film properties of the six-ringed hexacene. Although hexacene could be isolated in the bulk many years ago, the preparation of well-defined thin films remains a challenge. After synthesis of hexacene via modified Meerwein-Ponndorf-Verley reduction of hexacene-6,15-quinone, we successfully evaporated hexacene on Au(110) for the first time. We studied the electronic properties and the molecular orientation using x-ray absorption and photoemission spectroscopy (XAS, PES). The occupied and unoccupied structure is compared to pentacene. The orientation of hexacene in the monolayer range was almost flat lying, whereas larger tilt angles to the surface were found in thin films.

DS 17.72 Tue 18:15 Poster B

Controlling the work function of metals by means of phthalocyanine thin films — •Felix Widdascheck, Alrun Hauke, and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7, D-35032 Marburg, Germany

Efficient charge transfer at the interface between organic semiconductors and the respective device electrodes is of key importance for the advancement of organic electronics. It depends crucially on the energy level alignment and the reduction of potential injection barriers at such interfaces. A promising approach to effectively tune work functions and therefore optimize interface energetics are monolayers of flat lying molecules as contact primers. Compared to self-assembled monolayers they promise lower contact resistance due to shorter tunneling distances. Due to their high flexibility and flat absorption geometry phthalocyanines are an ideal model system to identify important parameters for this process. The presented study combines STM and Kelvin Probe measurements to compare the effect of highly ordered thin films of different phthalocyanines on the work function of metals and their possible use as contact primers. An additional focus is the importance of structural order and the influence of adsorbed film thickness.

DS 17.73 Tue 18:15 Poster B

Planar and porous polypyrrole/silicon hybrid material systems — •Pirmin Lakner[1], Manuel Brinker[2], Andreas Stierle[1], Patrick Huber[2], and Thomas Keller[1] — [1]DESY Deutsches Elektronen-Synchrotron Hamburg, Nanolab — [2]TU Hamburg-Harburg, Institut für Werkstoffphysik und Werkstofftechnologie

The investigation of interfaces in two-dimensional planar systems plays an elementary role in the investigation of porous hybrid materials, since it allows effects in more complex geometries to be attributed to their underlying causes. For the analysis of polypyrrole/silicon hybrid material systems, an electrochemical cell has been developed that enables the in-situ and nanometer-accurate investigation of the electropolymerization of pyrrole on planar silicon crystals using X-ray reflectometry. At the same time, electron density profiles and characteristic potential curves are recorded and layer heterogeneity is measured using SEM and AFM. The electrochemical cell enables the investigation of the voltage-induced swelling behaviour of polypyrrole, which opens up possible applications of porous polypyrrole/silicon hybrid material systems as actuators or sensors and optimizes them with regard to mechanical and electrical properties.

DS 17.74 Tue 18:15 Poster B

Materials Science of ALD Fresnel Zone Plates — •Umut T. Sanli[1], Chengge Jiao[2], Margarita Baluktsian[1], Kersten Hahn[3], Yi Wang[3], Vesna Srot[3], Gunther Richter[1], Iuliia Bykova[1], Markus Weigand[1], Gisela Schütz[1], and Kahraman Keskinbora[1] — [1]MPI for Intelligent Systems, Stuttgart — [2]FEI, Eindhoven — [3]MPI for Solid State Research, Stuttgart

X-ray microscopy is a very strong tool to investigate matter providing high penetration depths combined with structural, chemical and magnetic contrast. One of the most widely used X-ray optics is the Fresnel zone plate (FZP), particularly for ultrahigh resolution X-ray microscopy. A FZP is an alternating set of transparent and opaque concentric rings and its resolution is given by the width of its outermost zone. Currently, the direct imaging resolutions using FZPs have saturated to about 10 nm (in half-pitch). For lower values, wave-coupling effects dominate with a significant penalty to the diffraction efficiencies. One promising solution is to tilt the zones to the Bragg angle, which is a significant fabrication challenge. Hereby the material properties, which require a more stringent quality, are of critical importance since the zones must have a low roughness both radially and longitudinally and the interfaces must be chemically extremely smooth. Furthermore, the microstructure and morphology must be controlled to avoid diffuse scattering. Here we present a new fabrication route for FZP arrays with zones tilted to the Bragg angle by a combination of FIB pre-structuring and subsequent ALD. We demonstrate the quality of these optics and discuss their potential for sub-10 nm resolutions.

DS 17.75 Tue 18:15 Poster B

Investigation of the influence of molecular and atomic nitrogen ion species during thin film growth — •Michael Mensing, Philipp Schumacher, Jürgen W. Gerlach, and Bernd Rauschenbach — Leibniz Institute of Surface Engineering (IOM), Leipzig, Germany

Ion beam assisted deposition enables the control of thin film properties by changing the ion beam parameters such as the ion kinetic energy or the ion flux. However, as a consequence of the utilization of typical ion sources, the ion beam consists of a blend of multiple ion species at distinct ion kinetic energy distributions. In this work, an energy and mass selected ion beam is created and utilized to deposit epitaxial GaN nanofilms on $Al_2O_3(1\bar{1}02)$ at elevated temperatures of up to 700°C. This well established material system is used to independently investigate the influence of hyperthermal molecular and atomic nitrogen ions on the resulting film properties during the initial stages of the film growth. In addition, ion energies and material fluxes are varied. The resulting films are characterized by *in situ* RHEED, *in vacuo* AES and AFM, XRD as well as XRR.

DS 17.76 Tue 18:15 Poster B

Deposit Transition Metal or Metal Oxides Thin film on Silicon Wafer by Atomic Layer Deposition (ALD) for High Efficient Photoelectrochemical Water Splitting — •Haojie Zhang[1], Alexander Sprafke[1], Stefan L. Schweizer[1], Wouterg A. Maijenburg[2], and Ralf Wehrspohn[1,3] — [1]Institute of Physic, Martin-Luther-University Halle-Wittenberg, Heinrich-Damerow-Strasse 4, 06120 Halle, Germany. — [2]Center for Innovation Competence (ZIK) "SiLi-nano", Martin Luther University Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Straße 3, 06120 Halle, Germany. — [3]Fraunhofer Institute for Microstructure of Materials and

Systems, IMWS, Walter-Hülse-Straße 1, 06120 Halle, Germany.

Photoelectrochemical water splitting is advanced by the development of the highly efficient catalysts that promote the performance of the water splitting, while also maintaining the excellent stability for integration with the photoactive semiconductor as the light absorber. Here, we demonstrate the deposition of Ni, Co and/or their oxides thin films on the silicon wafer by the plasma enhanced atomic layer deposition (ALD). The deposited thin film with the uniform properties and simultaneously provide excellent water splitting performance. Furthermore, the combined silicon, as a light absorber also been protected effectively by the deposited thin film to perform a highly efficient light absorb. The combined device provides an excellent performance for the photoelectrochemical water splitting contributed by the synergy effect of high activity deposited thin film and semiconductor.

DS 17.77 Tue 18:15 Poster B

Electrochemical Deposition of Compact or Porous ZnO Thin Films on Metallic or Non-Metallic 3D-Microstructures — •Dominik Damtew, Martina Stumpp, and Derck Schlettwein — IAP, JLU Giessen, Germany

Semiconducting thin films of ZnO are of interest as electrode materials, e.g. in dye-sensitized solar cells, chemical sensors. Compared to physical gas-phase methods like thermal evaporation or sputtering, electrochemical deposition of thin films is more cost effective, less harmful to the environment and allows deposition onto complex-shaped objects and into blind holes. Our study is focused on the electrochemical deposition of ZnO out of aqueous zinc nitrate or zinc chloride baths at 70 $°C$ onto metallic and non-metallic wires, nets and 3D foams. Aside from the deposition of thin compact ZnO films, hybrid ZnO/dye (EosinY) films were deposited to produce porous films following dissolution of EosinY. Depositions were carried out both by galvanodynamic and by potentiostatic methods. The films were characterized by laser and scanning electron microscopy. Applying short (galvanodynamic) pulses of 10 ms of a constant current density of around 7.5 - 35 mA/cm^2 allowed deposition of very homogenous compact ZnO films on different materials and structures. Porous films could be deposited with pore sizes of 1 - 20 nm. The galvanodynamic method proved as perfectly suited to deposit in deeper regions of the 3D structures, while potentiostatic deposition led to film growth preferably on outer regions and to less homogenous films.

DS 17.78 Tue 18:15 Poster B

Chemical Solution Deposition of Poly(methyl methacrylate) thin films via dielectric barrier discharge — •Fan Guo[1,2], Lisa Wurlitzer[1,2], Wolfgang Maus-Friedrichs[1,2], and Sebastian Dahle[1,2] — [1]Clausthal Centre of Material Technology, 38678 Clausthal-Zellerfeld, Germany — [2]Institute of Energy Research and Physical Technologies, 38678 Clausthal-Zellerfeld, Germany

Plasma-enhanced chemical vapour deposition (PECVD) is an effective method to synthesise Poly(methyl methacrylate)(PMMA) thin films. Normally, the monomer methyl methacrylate (MMA), used as a precursor, is plasma polymerized in the gas phase. In this work, a new way to synthesize PMMA thin films from the liquid phase of MMA via a dielectric barrier discharge (DBD) is presented. The idea of this plasma-enhanced chemical solution deposition (PECSD) is based on radical initiation at the interface with a liquid phase of MMA by a non-thermal plasma. With this method, no vacuum condition or carrier gas streams are needed as opposed to the common PECVD technique. The deposited films were characterized with attenuated total reflection (ATR) infrared spectroscopy, differential scanning calorimetry (DSC) and gel permeation chromatography (GPC).

DS 17.79 Tue 18:15 Poster B

Plasma-assisted atomic layer deposition of Cobalt — •Mihir Dass[1], Sara Azimi[1], Haojie Zhang[2], Bodo Fuhrmann[3], and Stuart Parkin[1] — [1]Max Planck Institute of Microstructure Physics — [2]Fraunhofer Institute for Microstructure of Materials and Systems — [3]Martin Luther University Halle-Wittenberg

Atomic layer deposition (ALD) is a vapor phase technique capable of producing thin films of a variety of materials. Based on sequential, self-limiting reactions, ALD offers exceptional conformality on three-dimensional and patterned structures, thickness control at nearly monolayer level, and tunable film composition. With these advantages, ALD has emerged as a powerful tool for many industrial and research applications. Although some materials like certain metal oxides (Aluminium Oxide and Zinc Oxide) have received tremendous attention, deposition of pure metals is still in its infancy. We have shown plasma-assisted ALD deposition of Cobalt and are developing new processes for deposition on various substrates (unpublished data). We assess the deposition quality through XPS, AFM, XRD and TEM. Successful deposition of such stacks will open up possibilities to include new materials and develop novel electronic and spintronic devices.

DS 17.80 Tue 18:15 Poster B

Zone-Casting as a fully scalable deposition technique for high quality perovskite films — •Daniel Heimfarth, Simon Ternes, and Yana Vaynzof — Center for Advanced Materials, Heidelberg

With the performance of hybrid organometal-halide perovskite solar cells improving rapidly over the last several years, the future integration of this technology into industrial applications becomes a relevant topic. Specifically, common fabrication processes used in a laboratory setting, such as spin-coating, need to be replaced by scalable techniques, while maintaining excellent photovoltaic performance.

We investigate the suitability of zone-casting(also known as bar-casting), a meniscus-assisted deposition method for the fabrication of high quality perovskite films for photovoltaic applications. The method offers a large parameter space for investigation, including among others the substrate and solution temperatures as well as the deposition speed. We demonstrate that by tuning these parameters we are able to obtain a variety of perovskite films with different microstructures. A combination of high deposition speed and moderate substrate temperature results in uniform layers with large crystalline domains (200 μm) advantageous for perovskite photovoltaics. We demonstrate that the technique can be utilized for the large area fabrication of functional photovoltaic devices, with initial studies showing promising results with regards to the device power conversion efficiencies.

DS 17.81 Tue 18:15 Poster B

Optical ellipsometry used for real-time monitoring of atomic layer epitaxy — •Fryderyk Lyzwa[1,2], Premysl Marsik[2], Vladimir Roddatis[3], Christian Bernhard[2], Markus Jungbauer[1], and Vasily Moshnyaga[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]University of Fribourg, Department of Physics and Fribourg Center for Nanomaterials, Chemin du Musée 3, 1700 Fribourg, Switzerland — [3]Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Nanoscience and modern material physics are based on the growth and study of thin films with thicknesses spreading down to one atomic layer. The monitoring process itself is of great importance in order to confirm the successful film growth and to gain information on the electronic properties, defect formation, interfacial reconstructions etc. already during the growth. In this study, Ruddlesden-Popper thin films of SrO(SrTiO3)n=4 were grown by means of metalorganic aerosol deposition in the atomic layer epitaxy mode on SrTiO3(100), LSAT(100) and DyScO3(110) substrates. An optical ellipsometry setup was used to monitor the deposition of single atomic layers with subatomic sensitivity. The measured time dependences of ellipsometric angles, Δ(t) and Ψ(t), were described by using a simple optical model, considering the sequence of atomic layers SrO and TiO2 with corresponding bulk refractive indices. As a result, valuable online information on the growth process, the film structure and defects were obtained.

DS 18: Optical Analysis of Thin Films (Reflection, Ellipsometry, Raman, IR-DUV Spectroscopy, ...): Session I

Time: Wednesday 9:30–13:00 Location: H 0111

Invited Talk DS 18.1 Wed 9:30 H 0111

Infrared nanopolarimetric analysis of structure and anisotropy of thin films — •Karsten Hinrichs and Timur Shaykhutdinov — Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Schwarzschildstr. 8, 12489 Berlin, Germany

IR spectroscopic techniques can deliver simultaneously high chemical and structural contrast, be coupled with optical models and numerical calculations and typically are non-destructive and label-free. In this contribution recent progress and perspectives in IR spectroscopic nanopolarimetric analysis (30 nm resolution) using an extended version of a photothermal IR nanoscopy (AFM-IR) technique are presented. In particular, several highly sensitive polarization dependent nanoscale studies of anisotropic thin film materials, as polymer, protein and polaritonic films as well as supramolecular aggregates are discussed.[1-4]

[1] T. Shaykhutdinov et al, Supramolecular Orientation in Anisotropic Assemblies by Infrared Nanopolarimetry, ACS Macro Lett. 2017. 6: 598-602.

[2] K. Hinrichs et al, Electrochemical Modification of Large Area Graphene and Characterization by Vibrational Spectroscopy, in K. Wandelt (ed.), Encyclopedia of Interfacial Chemistry, Elsevier (2018).

[3] T. Shaykhutdinov et al, Mid-infrared nanospectroscopy of Berreman mode and epsilon-near-zero local field confinement in thin films, Opt. Mater. Express 2017. 7: 3706-3714.

[4] F. Rösicke et al, Functionalization of any substrate using covalently modified large area CVD graphene, Chem. Comm. 2017. 53: 9308-9311.

15 min. break.

DS 18.2 Wed 10:15 H 0111

Investigation on the electric-field-induced switching effect of copper-tetrathianoquinodimethane by polarized Raman spectroscopy — •Yanlong Xing[1], Eugen Speiser[1], Petra S. Dittrich[2], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e. V, 12489 Berlin, Germany — [2]Department of Biosystems Science and Engineering, ETH Zurich, CH-4058, Basel, Switzerland

Copper-tetrathianoquinodimethane (Cu-TCNQ) is a kind of important material due to its electric-field-induced reversible switching characteristics in conductivity. However, there is still inconsistency in reported studies regarding the switching effect: one proposed mechanism is the phase/composition changes (from phase II to phase I or between charged and neutral TCNQ molecules); the other mechanism is the Schottky contact between Al electrodes and Cu-TCNQ. To clarify this issue, we performed polarized Raman measurement on Cu-TCNQ crystals upon applying electric field by using a microdevice with Pt electrodes.

The rotational polarized Raman spectra showed the different crytal structures of the two phases of Cu-TCNQ (I and II). When applying an electric field to Cu-TCNQ wire (phase I), only after a threshold voltage, electron transfer between TCNQ0 and TCNQ- could be observed by the Raman signal of TCNQ0. A quantitative study on the Raman intensity and conductivity of Cu-TCNQ was under investigation, as well as the crystal structure changes of Cu-TCNQ.

DS 18.3 Wed 10:30 H 0111

Infrared spectroscopic ellipsometry of trapezoidal SiO2 columns and protein coated lamellar gratings — •Cordula Walder[1], Andreas Furchner[1], Matthias Zellmeier[2], Jörg Rappich[2], Helge Ketelsen[3], and Karsten Hinrichs[1] — [1]Leibniz Institut für Analytische Wissenschaften ISAS e.V., Schwarzschildstraße 8, 12489 Berlin — [2]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekuléstraße 5, 12489 Berlin — [3]SENTECH Instruments GmbH, Schwarzschildstraße 2, 12489 Berlin

The in-situ ellipsometric characterization of structured surfaces is interesting for applications like light management in solar cells, biotemplates and biosensors. In this work we aim to enhance the understanding of the results for periodic micrometer-sized structures in the infrared spectral regime where the vibrational fingerprints of the investigated materials become visible. Two-dimensional SiO2 trapezoidal columns on silicon with periods from 10 to 20 um in both lateral directions were characterized. The infrared Müllermatrix spectra of these samples were modelled by RCWA for different azimuth angles of sample rotation. Simulations show that the off-diagonal Müllermatrix elements can be particularly sensitive to changes of the lengths of the trapezoids and the azimuth angle. As an example for a structured biohybrid interface SiO2 line gratings on silicon wafers were coated with monolayers of human serum albumin (HSA protein). Analysis of the ellipsometric spectra delivered structural properties as well as the vibrational bands of the nanometer-thin protein layer.

DS 18.4 Wed 10:45 H 0111

Raman spectroscopy study of lattice and electron dynamics in a $SrIrO_3$ film — •Kaushik Sen, Kai Kleindienst, Dirk Fuchs, Karsten Wolf, Rolf Heid, and Matthieu Le Tacon — Institute for Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany

$SrIrO_3$ has been proposed as a candidate to realize the so-called 'topological insulator' phase due to its strong spin-orbit coupling (0.4 eV) and electron-electron correlations (0.5 eV). The narrow bands and their extreme sensitivity to the rotations of IrO_6-octahedra place the compound close to a metal-insulator transition. This has motivated us to investigate the lattice dynamics of these systems, which potentially plays an important role in conductivity. We report the lattice and electron dynamics in a 60 nm thick $SrIrO_3$ film using Raman scattering experiments as a function of temperature and light polarizations. With confocal Raman spectroscopy, we measured the temperature dependence of phonons modes with A_g and B_{2g} symmetries. Corresponding atomic displacements are assigned with the help of first-principle lattice dynamics calculations. Finally, an electronic continuum could directly be evident. We particularly focus our attention on the anomalous temperature dependence of the frequency of the B_{2g} phonon around 390 cm^{-1} (arises from the rotation of IrO_6-octahedra, which is out-of-phase along the direction of c-axis). This indicates an anomalous phonon hardening below 50 K, which deviates from the expected anharmonic phonon decay. It further displays a strong Fano asymmetry attesting the coupling of this mode to the underlying continuum.

DS 18.5 Wed 11:00 H 0111

Polarization dependent photoluminescence and Raman spectroscopy of single III-nitride nanowires — •Maximilian Ries[1,2], Pascal Hille[3], Jörg Schörmann[3], Eugen Speiser[2], Martin Eickhoff[3,4], and Norbert Esser[1,2] — [1]School of Analytical Sciences Adlershof (SALSA), Albert-Einstein-Strasse 5-9, 12489 Berlin — [2]Leibniz Institut für Analytische Wissenschaften - ISAS e.V., Schwarzschildstrasse 8, 12489 Berlin — [3]Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen — [4]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee NW1, 28359 Bremen

Modern LEDs are frequently made of III-nitride structures, with applications ranging from lightning, optoelectronics to life sciences and health care. To allow excellent performance, complex heterostructures and nanostructures must be fabricated with high precision. Recently, III-nitride nanowires have been employed in sensor devices due to their high surface-to-volume ratio, tunable optical properties and the possibility for surface functionalization. These devices are usually based on arrays of vertically aligned nanowires grown along the c-axis. To suppress ensemble effects and understand the impact of parameters such as alloy composition and morphology on optical properties, we performed polarization dependent measurements of photoluminescence and Raman spectroscopy on single III-nitride nanowires. Combined with transmission and scanning electron microscopy experiments we investigated the nature of defect luminescence and alloy inhomogeneity.

DS 18.6 Wed 11:15 H 0111

In-situ Monitoring of Lateral Hydrogen Diffusion in Amorphous and Polycrystalline Tungsten Trioxide Thin Films — •Simon Burkhardt[1,2], Matthias T. Elm[1,2,3], Bernhard Lani-

Wayda[4], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Center for Materials Research (LaMa), Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Gießen, Germany — [4]Mathematical Institute, Arndtstrasse 2, 35392 Gießen, Germany

Tungsten trioxide (WO_3) thin films show remarkable changes of their optical properties upon reversible ion insertion making them essential components in electrochromic devices. The development of such devices demands a fundamental understanding of charge carrier transport in WO_3. In-situ transmission spectroscopy during locally confined electrochemical hydrogen insertion is used to investigate the lateral diffusion of hydrogen inside amorphous and polycrystalline WO_3 thin films. The absorbance of WO_3 thin films is resolved spatially and temporally at a wavelength of (637 ± 15) nm. The results reveal concentration-dependent diffusion processes in both, amorphous and polycrystalline WO_3. By comparing experimental data with numerical simulations, the dependence of the diffusion coefficient on the hydrogen concentration is investigated. Although amorphous WO_3 thin films are known for their faster coloration kinetics, the diffusivity of hydrogen in polycrystalline WO_3 is found to exceed the diffusivity of hydrogen in amorphous WO_3.

15 min. break.

DS 18.7 Wed 11:45 H 0111

A condensed Krypton conversion electron source with ellipsometry monitoring for the KATRIN experiment — •Stephan Dyba for the KATRIN-Collaboration — Institut für Kernphysik, WWU Münster

The KATRIN (**KA**rlsruhe **TRI**tium **N**eutrino) experiment will perform an ultra-precise measurement of the endpoint region of the energy spectrum of electrons from tritium β-decay to determine the neutrino mass with a sensitivity of 0.2 eV (90% C.L.). To achieve the required accuracy, the kinetic energy of the decay electrons is measured using a MAC-E filter type spectrometer. To characterize the transmission properties of the KATRIN main spectrometer a movable calibration source has been constructed, using mono-energetic conversion electrons from the decay of the ^{83m}Kr isomer as a natural standard. For this purpose the radioactive krypton atoms from a ^{83}Rb generator are frozen onto a HOPG substrate at a temperature below 30 K. This **C**ondensed **Kr**ypton **S**ource (CKrS) uses sub-monolayer film thicknesses to provide decay electrons with a narrow line width and stable line position. The substrate is prepared by heating and laser ablation. The substrate with the sub-monolayer ^{83m}Kr and condensing residual gas are monitored using PCSA type ellipsometry, where analyzer and the light detector are directly mounted near to the substrate under ultra-high vacuum in the cold environment. The whole system is movable to allow to freely position the source within the magnetic fluxtube of the experiment.

This project is supported by BMBF, contract number 05A11PM2.

DS 18.8 Wed 12:00 H 0111

Electron capture by Sn polaron in Kesterite solar cells — •Sunghyun Kim[1], Ji-Sang Park[1], and Aron Walsh[1,2] — [1]Thomas Young Centre and Department of Materials, Imperial College London, London, United Kingdom — [2]Department of Materials Science and Engineering, Yonsei University, Seoul, Republic of Korea

The kesterite mineral, such as Cu2ZnSnS4 (CZTS), has attracted much attention as a replacement of the commercial Cu(In,Ga)S2 light absorber, consisting of only earth-abundant elements, and thus has the potential to support a Terawatt photovoltaic industry. Non-radiative carrier recombination is the likely origin of large open-circuit voltage deficit which is the primary bottleneck for achieving efficient kesterite solar cells. We have performed first-principles calculations within the framework of density functional theory to search for killer recombination centers in CZTS. The sulfur vacancy in CZTS is electrically benign not producing any donor levels in the band gap. However, we find that the sulfur vacancy can act as an efficient non-radiative site with the aid of an intermediate state involving Sn polaron formation. We point out that trap-assisted recombination does not necessarily accompany a charge transition level deep in the band gap of a semiconductor.

DS 18.9 Wed 12:15 H 0111

Electroreflectance and photoluminescence of Cu2(Zn1-x,Cdx)SnS4 thin film solar cells — •Segiu Levcenco[1], Shreyash Hadke[2], Lydia Helena Wong[2], and Thomas Unold[1] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner Platz 1, 14109 Berlin, Germany — [2]Energy Research Institute @ NTU Nanyang Technological University 637553, Singapore

Although Cu2(Zn1-x,Cdx)SnS4 (CZCTS)- absorber layers have demonstrated efficiency of 11.5% in thin film solar cells devices their optical and defect properties are not investigated sufficiently. For instance, the band gap in these materials is often derived from the external quantum efficiency measurements and different reports have provided band gaps that vary for similar compositions of CZCTS. In this work we employ the electroreflectance (ER) and photoluminescence (PL) techniques for characterizing CZCTS devices. The effects of Cd content and Cu/(Zn+Sn) cations ratio on the electronic transitions are investigated. In the near band edge region the ER spectra provide distinct derivative like structures corresponding to transitions near the critical points of the dielectric function, which are used to evaluate the band gap transition energies. In addition, a defect recombination with transition energy in the range of 1.1-1.3 eV has been resolved in PL spectra.

DS 18.10 Wed 12:30 H 0111

Two-Dimensional Optical Transport Measurements in $CuInGaSe_2$ by Highly Spatially, Spectrally, and Time Resolved Cathodoluminescence Microscopy — •Mathias Müller[1], Torsten Hölscher[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 inhomegenieties, highly spatially, spectrally, and time resolved cathodoluminescence (CL) measurements have been performed on polycrystalline $CuInGaSe_2$ (CIGSe) with varying Cu/III-ratios (CGI: 0.8 and 0.87). For this purpose, one-dimensional and two-dimensional optical transport measurements are compared, and performed to determine lateral carrier diffusion lengths. The samples are etched with bromine-methanol to smoothen the surface for further processing. 220 nm thick Ti masks of different shapes are applied via photolithography. One-dimensional measurements are carried out in CL-linescans perpendicular to the mask's edge. In a second step for the two-dimensional measurements, the sample is excited by the pulsed e-beam in the center of circular apertures in the Ti-mask with diameters ranging from 2.5 μm to 50 μm. Both methods lead to concurrent low temperature ($T = 5$ K) diffusion lengths of ca. 20 μm. Furthermore, a strong spatial dependence of the carrier lifetime is revealed with lifetimes ranging from 17 ns to 50 ns over only a few μm.

DS 18.11 Wed 12:45 H 0111

Investigating the exitonic interactions by polarization-resolved spectro-microscopy of a textured squaraine thin film — •Dominik Höweling[1], Luca Beverina[2], Christoph Lienau[1], Martin Silies[1], and Manuela Schiek[1] — [1]Institute of Physics, University of Oldenburg, Germany — [2]University of Milano-Bicocca, Milano, Italy

Small conjugated molecules like squaraines are a promising alternative to semiconducting polymers in the field of organic photovoltaics. Understanding the exitonic interaction of these molecules enables us to tailor devices for specific applications. In this study we use a home-built linear polarization-resolved spectro-microscope to investigate the molecular packing of crystalline nHSQ nanostructures. A characteristic "double-hump" signature in the absorption spectrum of nHSQ has been ascribed to the excitation of an intermolecular charge transfer band [1]. Our optical measurements show the excitation of these peaks at different angles. When comparing these angles with the known out-of-plane crystallographic orientation [2] we can predict the in-plane orientation of the nHSQ molecules. [1] Zheng et al. Sol. Energy Mater Sol. Cells 157, 366 (2014) [2] Brück et al. PCCP 16, 1067 (2014)

DS 19: Lithography I: Focused Electron Beam Induced Processing: 3D Nano-Printing for Material Science (Focussed Session): Morning Session (joint session DS/KFM)

Considering 3D printing using fused-deposition modeling or higher-resolution variants with lasers applicable to polymers and metals, an analogous approach exists on the nanometer scale. With the aid of focused electron beam-induced deposition (FEBID) it is possible to create solid-state structures on the nanoscale. However, in contradistinction to large-scale 3D printing of simple plastic or metallic structures, FEBID is able to directly provide nano-materials with a wealth of interesting electronic, optical and magnetic properties. Due to this, focused electron beam-induced deposition has experienced a rapid expansion in the breadth of its application fields over the last 10 years. FEBID uses precursor gases which, being adsorbed on a surface, are dissociated in the focussed electron beam to form the deposit. Intensive research has pushed the capabilities of FEBID in two important areas. It is now possible to obtain fully metallic nanostructures of Fe, Co and FeCo-alloys and also of Au and Pt. In addition, very recently the simulation-guided nano-manufacturing of 3D structures has matured to such a degree that even complex 3D objects can now be fabricated under controlled conditions. The focused session will address these new developments spanning the range from the fundamentals of electron-precursor interaction, covering aspects of the rational design of optimized precursors, and showing recent work on superconducting, magnetic and plasmonically active materials, both in 2D and 3D.

Organized by

Name: Prof. Dr. Michael Huth, Institution: Physikalisches Institut, Goethe-Universität, City: Frankfurt am Main, Country: Germany, Email: michael.huth@physik.uni-frankfurt.de, Telephone number: +49-69-798-47235

Name: Ass. Prof. Dr. Harald Plank, Institution: Institut für Elektronenmikroskopie und Nanoanalytik, TU Graz, City: Graz, Country: Austria, Email: harald.plank@felmi-zfe.at, Telephone number: +43-316-873-8821

Name: Dr. Ivo Utke, Institution: EMPA, Swiss Laboratories for Materials Science and Technology, City: Thun, Country: Switzerland, Email: Ivo.Utke@empa.ch, Telephone number: +41-58-765-6257

Time: Wednesday 9:30–13:00 Location: H 2032

Invited Talk DS 19.1 Wed 9:30 H 2032

3D direct-write nanofabrication using an electron beam — •Jason Fowlkes[1], Robert Winkler[2,3], Eva Mutunga[4], Brett Lewis[5], Harald Plank[2,3], and Philip Rack[5] — [1]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — [2]Institute for Electron Microscopy and Nanoanalysis, Graz University of Technology, 8010 Graz, Austria — [3]Graz Centre for Electron Microscopy, 8010 Graz, Austria — [4]Bredesen Center for Interdisciplinary Research, The University of Tennessee, Knoxville, 37996, USA — [5]Department of Materials Science and Engineering, The University of Tennessee, Knoxville, 37996, USA

The deposition of 3D nanomaterials with precise geometry and function constitutes a major goal of nanoscience. Currently, the preeminent method for nanoprinting is focused electron beam-induced deposition(FEBID). During FEBID, the electron beam is scanned along a surface inducing the fragmentation and deposition of absorbed precursor molecules. Until recently, the suite of 3D objects that could be deposited was limited by the trial and-error nature of experiments and poor material quality. Our team has taken significant steps toward overcoming both roadblocks, the former being the focus of the current presentation. A FEBID CAD program will be presented that makes it possible to deposit complex, 3D nanoscale mesh style objects spanning micrometer length scales. A FEBID simulation will also be discussed. The simulation to CAD to experiment process flow will be demonstrated for the case of tailoring mesh object nanowire cross-sections.

Invited Talk DS 19.2 Wed 10:00 H 2032

Nanosuperconductivity with Focused Particle Beam Induced Deposition structures — •Rosa Córdoba[1,2], Javier Sesé[2,3], and José María De Teresa[1,2,3] — [1]Instituto de Ciencia de Materiales de Aragón (ICMA), CSIC - Universidad de Zaragoza, Spain — [2]Departamento de Física de la Materia Condensada, Universidad de Zaragoza, 50009 Zaragoza, Spain — [3]Laboratorio de Microscopías Avanzadas (LMA), Instituto de Nanociencia de Aragón (INA), Universidad de Zaragoza, Spain

In this contribution, we will show an inclusive scenario of Focused Particle Beam Induced Deposition (FEBID/FIBID) to grow nanosuperconductors and nanomagnets by using as a primary beam, heavy ions (Ga+ FIBID), light ions (He+ FIBID) and electrons (FEBID). First, Ga+ FIBID nanosuperconductors will be introduced, which include the mechanical properties of three-dimensional (3D) nanowires [1], the non-local vortex transport in sub-50 nm nanowires [2] and the magnetotransport properties of sub-10 nm superconducting nanowires [3]. Second, He+ FIBID nanotubes will be presented, highlighting their specific growth method, superconducting properties and microstructure [4]. Finally, FEBID 3D magnets will be shown, which are integrated in a hybrid (superconductor/ferromagnet) system [5,6]. [1]Córdoba et al., Nanotechnology 28-44 445301 (2017). [2]Córdoba et al., manuscript submitted to Applied Physics Letters. [3]Córdoba et al., manuscript in preparation. [4]Córdoba et al., manuscript submitted to Nano Letters. [5]Córdoba et al., Nanotechnology 27 355301 (2016). [6]Rouco et al., Sci. Rep. 7 5663 (2017).

Invited Talk DS 19.3 Wed 10:30 H 2032

Chemistry for ELectron-Induced NAnofabrication — •Petra Swiderek — University of Bremen, Institute for Applied and Physical Chemistry, Bremen, Germany

The European COST Action CELINA (Chemistry for ELectron- Induced NAnofabrication [1]) has, from 2013 to 2017, created a research network that aims at advancing focused electron beam induced deposition (FEBID) processes. It has done so by stimulating collaborative research that unravels the chemical reactions that are fundamental to FEBID, develops novel and improved precursor molecules, and tests their performance in the actual FEBID process. CELINA has thus assembled under its roof groups with expertise in electron-driven chemistry, precursor synthesis, and experts in FEBID from both academia and industry. This multidisciplinary effort is needed because of the many different physical and chemical aspects involved in the formation and processing of FEBID deposits as well as in their applications.

This contribution gives an overview of CELINA*s research program and highlights some of its results. Furthermore, it will discuss the different types of chemical processes inherent in FEBID and how they can be investigated using a combination of gas phase mass spectrometry and surface science experiments. Understanding and controlling each of these different chemistries poses significant challenges but is the key to ultimate deposit purity, spatial resolution, and deposition speed.

References: [1] http://celina.uni-bremen.de/celina

Invited Talk DS 19.4 Wed 11:00 H 2032

The direct electron beam writing of plasmonic nanostructures — •Katja Höflich — Helmholtz Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D – 14109 Berlin, Germany

Future IT systems will rely on photons instead of electrons. The potentially huge bandwidth of photons and their extremely small switching times render light indispensable for telecommunication and for information processing. The use of plasmonic nanostructures constitutes a promising approach for nanoscale optical devices since their minimum geometric features are not restricted by the diffraction limit.

The technique of electron beam induced deposition (EBID) has the potential to evolve as a novel route for the fabrication of complex plasmonic devices. EBID nanostructures are grown by the local dissociation of precursor molecules in the focus of an electron beam. While the focused electrons account for minimum structural features, the direct writing provides access to three dimensions in a single step.

A major challenge lies at depositing pure materials. It can be addressed by testing novel precursor compounds, oxidation-based purification or by using EBID nanostructures as a scaffold to be coated with the metal of choice. Recent examples of EBID-based plasmonic nanostructures include silver and gold helices with a strong dichroism in the visible range as well as silver nanostructures based on a novel carboxylate precursor.

15 min. break.

DS 19.5 Wed 11:45 H 2032

Direct printing of 3D nano-structures via focused electron beam induced deposition: Pattern generation — •Lukas Keller and Michael Huth — Institute of Physics, Goethe University, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

Fabrication of three-dimensional (3D) nano-architectures by focused electron beam induced deposition (FEBID) has matured to a level that highly complex and functional deposits are becoming available for nanomagnetics and plasmonics. The main issue of generating a desired 3D nano-structure is the control of the electron beam in the x-y-plane. However, the generation of suitable pattern files that define the electron beam deflection at any time during the deposition and reliably map the desired target 3D structure from a purely geometrical description to a shape-conforming 3D deposit is non trivial. Here we present our implementation of a pattern file generator that handles proximity effects, corrects for height-dependent precursor coverage and avoids shadowing effects regarding the directed component of the precursor flux. Several examples of successful 3D nano-fabrication using different precursors are presented that attest the effectiveness of the implementation.

DS 19.6 Wed 12:00 H 2032

Direct-Write Fabrication of Electric and Thermal High-Resolution Nano-Probes on Self-Sensing AFM Cantilever — •Juergen Sattelkkow[1,2], Johannes Froech[1,2], Robert Winkler[1,2], Christian Schwalb[3], Ernest Fantner[3], Vlado Stavrov[4], and Harald Plank[1,2] — [1]Institute of Electron Microscopy and Nanoanalysis, Graz University of Technology, Graz, Austria — [2]Graz Centre for Electron Microscopy, Graz, Austria — [3]GETec Microscopy Inc. & SCL Sensor.Tech. Fabrication Inc., Vienna, Austria — [4]AMGT, Botevgrad, Bulgaria

Atomic Force Microscopy (AFM) has evolved into an essential part in research and development due to its quantitative 3D surface characterization capabilities on the spatial nanoscale together with the possibility to access laterally resolved magnetic, chemical, mechanical, optical, electric or thermal properties of the sample surface. In this contribution, we demonstrate the direct-write fabrication of 3D nano-probes via focused electron beam induced deposition (FEBID) together with its respective AFM application. For conductive-AFM, Pt-C nano-pillars are initially fabricated by FEBID and then chemically transferred into pure Pt via gas assisted post-growth purification. For thermal nano-probes we use platinums temperature dependent, electric properties as transducing element together with FEBIDs 3D fabrication capabilities to realize free-standing nano-bridges. We demonstrate the reversible, quantitative temperature response together with fast response times of less than 30 ms/K. Finally, we show scanning thermal microscopy measurements, revealing thermal surface gradients on the nanoscale.

DS 19.7 Wed 12:15 H 2032

High-Fidelity 3D-Nanoprinting via Focused Electron Beams: Growth Fundamentals — •Robert Winkler[1,2], Brett Lewis[3,4], Jason Fowlkes[3,4], Philip Rack[3,4], and Harald Plank[1,2] — [1]Institute for Electron Microscopy and Nanoanalysis Graz University of Technology, 8010 Graz, Austria — [2]Graz Centre for Electron Microscopy, 8010 Graz, Austria — [3]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — [4]Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee 37996, USA

3D-printing of functional structures has emerged to an important technology in research and development, although it becomes very challenging when aiming on nano-sized geometries. Among the very few direct-write techniques on that scale, Focused Electron Beam Induced Deposition (FEBID) has been demonstrated to be a promising candidate as it allows the fabrication of functional, freestanding 3D nano-architectures on almost any substrate, enabling novel applications. Predictable, reliable and reproducible fabrication, however, often suffered due to the numerous process parameter and their mutual relationships. In this contribution, we comprehensively discuss the complex interplay between most process parameters and successfully trace back their implications to the precursor working regime. Beside the fundamental aspect of our findings, we separate dominant parameters from those with minor implications. By that, we are able to explain unwanted deviations during 3D growth and derive certain rules for precise, predictable and reproducible 3D-nanofabrication via FEBID.

DS 19.8 Wed 12:30 H 2032

Mechanical Properties of 3D Nano-Architectures Fabricated via Focused Electron Beam Induced Deposition — Johannes Froech[1,2], Juergen Sattelkow[1,2], Robert Winkler[1,2], Christian Schwalb[3], Ernest Fantner[3], and •Harald Plank[1,2] — [1]Institute for Electron Microscopy and Nanoanalysis Graz University of Technology, 8010 Graz, Austria — [2]Graz Centre for Electron Microscopy, 8010 Graz, Austria — [3]GETec Microscopy Inc. & SCL Sensor.Tech. Fabrication Inc., 1220 Vienna, Austria

With the recent introduction of controlled 3D nano-printing via focused electron beam induced deposition, an entirely new range of applications such as nano-optics, -mechanics, or -electronics comes within reach whose fabrication is extremely challenging or even impossible with alternative techniques. In this contribution, we focus on mechanical properties of freestanding, Pt based 3D nano-architectures for atomic force microscopy (AFM) based application as high-resolution thermal nano-probes. A combined approach of finite element simulation, AFM based force spectroscopy and real-time imaging via scanning electron microscopy is used to identify and compensate highly unwanted peculiarities. In more detail, we discuss an unexpectedly strong influence of non-straight side branches as well as the consequences of fabrication mismatches on the lowest nanoscale, leading to non-linear mechanical behaviour and morphological twisting, respectively. The combined outcome of our findings demonstrate the high demands on nanoscale accuracy during 3D nano-printing to exploit the full potential in terms of predictable mechanical properties.

DS 19.9 Wed 12:45 H 2032

Correlative in-situ characterization of 3D nanostructures by combining SEM and AFM — •Christian Schwalb[1], Marcel Winhold[1], Pinar Frank[1], Stefan Hummel[1], Roland Sachser[2], Michael Huth[2], Jürgen Sattelkow[3], and Harald Plank[3] — [1]GETec Microscopy GmbH, Vienna, Austria — [2]Physikalisches Institut, Goethe University Frankfurt, Germany — [3]FELMI, Graz, Austria

Focused electron-beam-induced processing represents one of the most flexible approaches for functional nanostructure fabrication. During and after the growth process, e.g., electrical in-situ measurements as well as energy-dispersive X-ray spectroscopy are commonly employed to characterize electrical and chemical properties of fabricated structures. However, one major drawback is the lack of further in-situ analysis tools which grants access to real 3D topographic information, laterally resolved conductance maps, local magnetic or mechanical properties. We present a novel AFM that allows correlative in-situ analysis by combining the full SEM and AFM capability. The AFM measurement takes place in the field of view of the electron beam and thus allows for non-destructive and non-contaminating analyses of FEBID structures directly after fabrication. We make use of novel self-sensing cantilevers that are equipped with different specialized tips fabricated by 3D nano-printing of sharp purified metallic or magnetic tips. We present correlative in-situ conductive, magnetic and mechanical analysis of 3D nanostructures using these novel cantilever tips and discuss future applications.

DS 20: 2D materials: Chalcogenides I (joint session HL/DS)

Time: Wednesday 9:30–13:15 Location: A 151

DS 20.1 Wed 9:30 A 151

Theory of Strain-Induced Confinement in Transition Metal Dichalcogenide Monolayers — •Matthew Brooks and Guido Burkard — Universität Konstanz, Konstanz

Recent experimental studies of out-of-plane straining geometries of transition metal dichalchogenide (TMD) monolayers have demonstrated sufficient band gap renormalisation for device application such as single photon emitters. Here, a simple continuum-mechanical plate-theory approach is used to estimate the topography of TMD monolayers layered atop nanopillar arrays. From such geometries, the induced conduction band potential and band gap renormalisation is given, demonstrating a potential shape that is independent of the height of deforming nanopillar. Additional, with a semi-classical WKB approximation, the expected leakage of the strain potential may be estimated as a function of the height of the deforming nanopillar. This straight forward approach is in accordance with experiment, supporting recent findings suggesting that nanopillar height improves linewidth of the single photon emitters observed at the tip of the pillar, yet has no discernible influence over the wavelengths of the emitted photons.

DS 20.2 Wed 9:45 A 151

the role of dark exciton states in magneto-exciton valley depolarisation mechanisms In monolayer transition metal dichcalcogenides — •Alexander Pearce and Guido Burkard — Universität Konstanz, Konstanz, Germany

We present a theoretical study of the valley magneto-exciton relaxation dynamics in monolayer transition metal dichcalcogenides (TMDs) using a kinetic equation approach. The TMDs are direct band gap semiconductors with strong light-matter coupling which produce optical responses dominated by tightly bound excitons. The combination of the lattice symmetry and strong spin-orbit interaction gives rise to a rich selection rules allowing for optical control of the excitons valley polarisation. Experiments have shown that due to spin-orbit interactions there are spin forbidden transitions which lead to dark exciton states, and these states are found to possess long lifetimes due to their non-radiative decay and play a role in the depolarisation dynamics of the TMDs. Using a kinetic equation approach we investigate the interplay of the exchange interaction, a perpendicular magnetic field and the dark state scattering the time evolution of the exciton valley polarisation. We find that the influence of the dark states leads to longer valley relaxation times. We also explore the effect of an in-plane magnetic, which acts to "brighten" the dark states, which leads to an even greater increase in the valley relaxation time.

DS 20.3 Wed 10:00 A 151

Strain on molybdenum disulfide sheets with defects from first principles — •Mohammad Bahmani[1], Mahdi Faghihnasiri[2], and Thomas Frauenheim[1] — [1]BCCMS, Physics Department, Bremen University, Bremen, Germany — [2]Physics Department, Shahrood University of Technology, Shahrood, Iran

Single layer of transition metal dichalcogenides(TMDCs) are under intense investigations since the discovery of unique characteristics of 2D and Vann der Waals layered materials. They are predicted to be the most promising structure for various future nanoscale devices. They have also novel applications in spintronic and optoelectronic.

As a result of thermal equilibrium and the kinetics of processing, all real materials contain structural defects which show significant effects on their electrical, optical, vibrational, magnetic, and chemical properties. Besides, mechanical strain has very much influence on the electronic properties of 2D materials, particularly TMDCs. For example, 0.5% biaxial strain force direct band gap in molybdenum disulfide(MoS2) to become indirect since it breaks the crystalline symmetry.

Therefore, I study different types of point defects such as single and double sulfur(S), single molybdenum(Mo) vacancies, and removing a Mo with its three upper S neighbors. I also substitute a Mo vacancy with one and two S atoms. Furthermore, as the second aim of this study, I showed the modification of defect states under uniaxial and biaxial compression and tensile strain. For the case of one S vacancy, this moves shallow states into the valance band and importantly breaks the degeneracy of degenerate states.

DS 20.4 Wed 10:15 A 151

Optical absorption of a mechanically strained WSe_2 monolayer — •Iris Niehues[1], Robert Schmidt[1], Robert Schneider[1], Matthias Drüppel[2], Torsten Deilmann[2], Michael Rohlfing[2], Steffen Michaelis de Vasconcellos[1], Andres Castellanos-Gomez[3], and Rudolf Bratschitsch[1] — [1]Physikalisches Insitut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [3]Materials Science Factory, Instituto de Ciencia de los Materials de Madrid (ICMM-CSIC), E- 28049 Madrid

Atomically thin layers of transition metal dichalcogenides represent a new class of materials. Strain engineering allows to tune their fundamental optical transitions. We apply reversible uniaxial tensile strain of up to 1.4% to a WSe_2 monolayer. At increasing and decreasing tensile strain levels absorption spectra are recorded, and the strain-dependent energy shifts of the exciton resonances are measured[1]. Gauge factors of $-54\,\mathrm{meV/\%}$, $-50\,\mathrm{meV/\%}$, $+1\ \mathrm{meV/\%}$, and $-22\,\mathrm{meV/\%}$ are derived for the A, B, C, and D exciton, respectively. A comparison with ab initio GW-BSE calculations shows an excellent agreement with the measured data.

[1] R. Schmidt, I. Niehues, R. Schneider, M. Drüppel, T. Deilmann, M. Rohlfing, S. Michaelis de Vasconcellos, A. Castellanos-Gomez, and R. Bratschitsch, Reversible uniaxial strain tuning in atomically thin WSe_2 in: 2D Materials 3, 021011 (2016)

DS 20.5 Wed 10:30 A 151

Tunable electron-phonon interaction in MoS2 — •Max Bommert[1], Bastian Miller[1,2], Alexander Holleitner[1,2], and Ursula Wurstbauer[1,2] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 Munich, Germany

Transition metal dichalcogenides such as MoS2 are of current interest for optoelectronic application, as well as for studying fundamental aspects of light-matter interaction and excitonic properties in strictly two-dimensional semiconductors. We explore the impact of the charge carrier density on the electron phonon interaction by non-resonant and resonant Raman spectroscopy. We utilize MoS2 field effect structures with solid electrolyte and liquid ion gates, enabling a change of the 2D electron density by more than two orders of magnitude [1]. We report unusual polarization and charge carrier dependent behavior in resonant Raman spectra that points towards strong electron-phonon coupling in MoS2 and the importance of excitonic phenomena [2]. Alongside we investigate temperature dependent phase transitions through changes in transport and optical properties.

[1] Miller et al., APL 106, 122103 (2015)
[2] Miller, Bommert et al. (2018)

DS 20.6 Wed 10:45 A 151

Theory of Exciton-Exciton Interactions in Monolayer Transition Metal Dichalcogenides — •Florian Katsch, Malte Selig, Alexander Carmele, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik von Halbleitern, Technische Universität Berlin, 10623 Berlin, Germany

Due to the strong Coulomb interaction in monolayers of transition metal dichalcogenides (TMDs), the optical properties are governed by tightly bound electron-hole pairs in the vicinity of the band edge. In order to allow for efficient modeling, a theoretical description in a two particle exciton basis based on the unit-operator method [1] is introduced. The formalism incorporates TMD-typical Coulomb inter- and intravalley interactions up to three correlated excitons. The developed theory is applied to access the exciton dynamics [2,3] in the so-called coherent limit as well as exciton-phonon interactions [4]. The derived TMD Bloch equations contribute to the understanding of recent pump-probe experiments observing an immediate signal in the unpumped valley [5,6].

[1] A. L. Ivanov and H. Haug, *Physical Review B* **48**, 1490 (1993).
[2] V. M. Axt and A. Stahl, *Zeitschrift für Physik B Condensed Matter* **93**, 2 (1994).
[3] M. Lindberg et. al., *Physical Review B* **50**, 18060 (1994).
[4] M. Selig et. al., *Nature communications* **7**, 13279 (2016).

[5] C. Mai et. al., *Nano letters* **14**, 202 (2013).
[6] R. Schmidt et. at., *Nano letters* **16**, 2945 (2016).

DS 20.7 Wed 11:00 A 151

Optical spectra and bound excitons in MoTe2 from monolayer to bulk by many-body perturbation theory — •Saeideh Edalati-Boostan, Caterina Cocchi, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Among the transition-metal dichalcogenides, MoTe2 plays a relevant role as a good candidate for light-emitting devices. In the framework of GW and the Bethe-Salpeter equation as implemented in the exciting code [1], we study optical excitations in this material as a function of dimensionality, going from mono- and bilayers to the bulk. The role of spin-orbit coupling is assessed in band structures and optical spectra with respect to the number of layers. The calculated absorption spectra are characterized by a few bound excitons in the visible region with binding energies of the order of a hundred meV [2]. Bound electron-hole pairs, which are known to be both inter- and intra-layer in bulk MoTe2 [2], are analyzed in view of quantum confinement effects. This understanding is essential to eventually use this material in van der Waals heterostructures.

[1] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, and C. Draxl, JPCM 26, 36 (2014); D. Nabok, A. Gulans, and C. Draxl, PRB 94, 035118 (2016); S. Sagmeister, and C. Draxl, PCCP 11, 4451 (2009)

[2] A. Arora, M. Drüppel, R. Schmidt, T. Deilmann, R. Schneider, M. R. Molas, Ph. Marauhn, S. M. de Vasconcellos, M. Potemski, M. Rohlfing, and R. Bratschitsch, Nat Commun. 8, 639 (2017)

15 min. break.

DS 20.8 Wed 11:30 A 151

Thermal annealing effects on optical properties of 2D MoS_2 — •Oleg Gridenco, Kathrin Sebald, Christian Tessarek, Martin Eickhoff, and Jürgen Gutowski — Institute of Solid State Physics, University of Bremen, Germany

Mechanically exfoliated monolayers obtained by using natural crystals and deposited by a polymer transfer process on substrates suffer from residues on the surface which are hard to be removed. The residues as well as absorbed O_2 and H_2O at the surface of a monolayer are known to modify the optical and electrical properties resulting in a quenching of the photoluminescence (PL) and a reduction of the carrier mobility. We present a systematic thermal annealing study conducted by heating and laser annealing in order to remove such residues. The results show that the PL energy is blue-shifted and the PL intensity is enhanced by a factor of 1.8 after a thermal annealing cycle. The blue-shift points to a reduction of the trion contribution and a relative increase of free-exciton recombination. In addition, the overall PL enhancement can be related to a decrease of non-radiative recombination processes. A similar behaviour of the PL is observed after MoS_2 monolayers were exposed to UV laser irradiation for several seconds. The study provides a low-cost, large scale and effective route to enhance the PL efficiency which is important for the device performance.

DS 20.9 Wed 11:45 A 151

Spatiotemporal dynamics of the carrier capture into localized states in a TMDC monolayer — •Roberto Rosati, Frank Lengers, Doris E. Reiter, and Tilmann Kuhn — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Monolayers of transition metal dichalcogenides (TMDC) have attracted wide attention due to their interesting optical and electronic properties. Local strain distributions lead to the formation of embedded 0D confinement potentials which can be exploited, e.g., as single photon sources [1]. In such hybrid 2D-0D systems, the bound states of the 0D potential may be populated through carrier capture by emission of optical phonons. Such capture processes are known to generate non-trivial spatiotemporal dynamics in hybrid 1D-0D systems [2]. In this work we study the capture of a wave packet in a MoSe2 monolayer into localized states. We find interesting spatio-temporal dynamics of the trapped charge distribution associated with the capture into specific superposition states, which can be controlled by the propagation direction of the wave packet. To calculate the dynamics we use a recently introduced Lindblad single-particle approach, which allows us to deal with the dimensionality-related computational demands and, at the same time, catches the most relevant features of the carrier capture, in particular its locality [3].

[1] Kern et al., Adv. Mater., **28**, 7101-7105 (2016)
[2] Glanemann et al., Phys. Rev. B **72**, 045354 (2005)
[3] Rosati et al., Phys. Rev. B **95**, 165302 (2017)

DS 20.10 Wed 12:00 A 151

Strong Anisotropic Spin-Orbit Interaction Induced in Graphene by Monolayer WS2 — •Taro Wakamura[1], Francesco Reale[2], Pawel Palczynski[2], Cecilia Mattevi[2], Sophie Guéron[1], and Hélène Bouchiat[1] — [1]Laboratoire de Physique des Solides, Université Paris-Sud, Orsay, France — [2]Department of Materials, Imperial College London, London, United Kingdom

We demonstrate strong anisotropic spin-orbit interaction in graphene induced by monolayer WS2. Direct comparison between graphene/monolayer WS2 and graphene/bulk WS2 system in magnetotransport measurements reveals that monolayer transition metal dichalcogenide can induce much stronger SOI than bulk. Detailed theoretical analysis of the weak-antilocalization curves gives an estimated spin-orbit energy (Eso) more than 10 meV. The dominant z to -z symmetric spin-orbit interaction demonstrates strong valley-Zeeman spin-orbit interaction induced in graphene, consistent with the recent theoretical study. Dramatic increase of resistance around the Dirac point with decreasing temperature suggests the existence of the spin-orbit gap at the Dirac point.

DS 20.11 Wed 12:15 A 151

Electronic and optical properties of group-IV transition metal dichalcogenides monolayers and their heterostructures — •Ka Wai Lau, Caterina Cocchi, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

The interest in transition-metal dichalcogenides (TMDs) monolayers as promising materials for opto-electronics has rapidly increased in the last few years [1]. The majority of studies has been devoted so far to group-VI TMDs, with MoS2 and WS2 as the most relevant examples of this material class [1]. Here, we study monolayers of group-IV TMDs focusing on ZrS2 and HfS2. We investigate their electronic and optical properties in the framework of many-body perturbation theory (GW and the Bethe-Salpeter equation) as implemented in the all-electron full-potential code exciting [2]. The optical response of these systems is characterized by intense peaks in the visible region due to tightly-bound excitons with binding energies of the order of hundreds of meV. The degeneracy of the hole state at the Γ point with different dispersion along the M-Γ-K direction and the strong spin-orbit coupling in the valence band leads to several distinct excitonic states around Γ. Finally we study van-der-Waals heterostructures obtained by combining ZrS2 and HfS2 monolayers in view of understanding how different stacking patterns influence band alignment and optical excitations.

[1] K. F. Mak and J. Shan, Nat. Photon. 10, 216 (2016)
[2] A. Gulans et al., J. Phys.: Condens. Matter 26, 363202 (2014)

DS 20.12 Wed 12:30 A 151

Persistent photoconductivity in monolayer MoS_2 field effect transistors after UV irradiation — •Antony George[1], Mikhail Fistul[2,3], Uwe Hübner[4], Nirul Masurkar[5], David Kaiser[1], Christof Neumann[1], Andreas Winter[1], Arava Leela Mohana Reddy[5], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, 07743 Jena, Germany — [2]Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Daejeon 34051, Republic of Korea — [3]Russian Quantum Center, National University of Science and Technology "MISIS", 119049 Moscow, Russia — [4]Leibniz Institute of Photonic Technology, 07745 Jena, Germany — [5]Department of Mechanical Engineering, Wayne State University, 48202 Detroit, USA

We demonstrate long living photo-excited charge carriers in monolayer MoS_2 field effect transistors (FET) after UV irradiation. After irradiation, the FETs were found to be remaining in a high conductivity state at room temperature (RT) for a long time (ca. 30 days). We investigated the origin of the persistent photoconductivity (PPC) combining RT and low-temperature transport measurements with theoretical modeling. At low temperatures, a great enhancement of photo-induced conductivity with applied gate voltage was observed. We ascribe this to the UV irradiation of MoS_2, which results in inter-band transitions and the creation of a large number of electron-hole pairs, which are quickly spatially separated due to local variations of the band structure. Under such conditions, the recombination time drastically increases and

induces the PPC effect.

DS 20.13 Wed 12:45 A 151

Highly polarized excitons in atomically thin and bulk-like 1T'-ReSe$_2$ — •A. Arora[1], J. Noky[2], M. Drüppel[2], B. Jariwala[3], T. Deilmann[4], R. Schneider[1], R. Schmidt[1], O. Del Pozo-Zamudio[1], T. Stiehm[1], A. Bhattacharya[3], P. Krüger[2], S. Michaelis de Vasconcellos[1], M. Rohlfing[2], and R. Bratschitsch[1] — [1]Institute of Physics, University of Münster, Wilhelm-Klemm-Strasse 10, 48149 Münster, Germany — [2]Institute of Solid State Theory, University of Münster, D-48149 Münster, Germany — [3]Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai 400005, India — [4]Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Using low-temperature polarized optical absorption and photoluminescence spectroscopy, supported by GW-BSE ab initio calculations, we investigate excitons in the van der Waals semiconductor 1T'-ReSe$_2$ [1]. A red shift of the excitonic transition energy is observed when the crystal thickness is reduced from bulk towards a monolayer. The excitons exhibit a strong polarization anisotropy within the plane of the crystal, with dipole vectors pointing towards different crystal directions. This polarization behavior persists from bulk to monolayer thickness. We find that the excitons are strongly confined within the individual crystal layers, even for the bulklike case. We find a direct band gap in 1T'-ReSe$_2$ in our calculations, regardless of the crystal thickness. Our results pave the way for polarization-sensitive applications using two-dimensional semiconductors. [1] A. Arora et al., Nano Lett. 17, 3202-3207 (2017).

DS 20.14 Wed 13:00 A 151

The Influence of the environment on monolayer tungsten diselenide photoluminescence — •Lorenz Maximilian Schneider[1], Sina Lippert[1], Jan Kuhnert[1], Obafunso Ajayi[2], Dylan Renaud[1], Young Duck Kim[2,3], Wolfram Heimbrodt[1], James C. Hone[2], and Arash Rahimi-Iman[1] — [1]Department of Physics and Material Sciences Center, Philipps-Universität Marburg, 35032 Marburg , Germany — [2]Department of Mechanical Engineering, Columbia University, 10027 New York, USA — [3]Department of Physics and Center for Humanities and Sciences, Kyung Hee University, 02447 Seoul, Republic of Korea

In recent years, two-dimensional (2D) semiconductors have drawn a lot of attention due to their special properties. Since transition metal dichalgogenides (TMDs) are a potential candidate for opto-electronic applications in the visible range, they are of major interest and subject of many studies. Recent investigations have shown that encapsulating monolayers with hBN can improve signal quality greatly compared to flakes grown or exfoliated on common substrates. Here, we present a systematic study of the effects, that such encapsulation of monolayers with mainly hBN can have on the 2D material's optical properties using WSe_2. Besides the already known narrowing of the PL-linewidth, remarkable differences are found in the time evolution. hBN supported and encapsulated samples show a significantly stronger exciton-exciton annihilation as the reference samples on bare substrate. Furthermore, we show that this effect is also obtained if the heterostructure consists of two TMDs.

DS 21: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials IV (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Wednesday 10:30–13:00 Location: HL 001

Invited Talk DS 21.1 Wed 10:30 HL 001

Correlating electrons via adiabatic connection approach: a general formalism, approximations, and applications — •Katarzyna Pernal — Institute of Physics, Lodz University of Technology, Poland

Electronic systems are usually described by assuming a model Hamiltonian, which only partially recovers electron correlation effects. To assure a quantitative description one faces a problem of recovering the missing part of the correlation. Over years different methods have been developed, most of them originating from the perturbation theory.

In my talk I will present another, fairly general, approach based on the adiabatic connection formalism. The idea itself is not novel although it has not been considered as a way of adding electron correlation for multireference models. Until recently it has not been realized that by combining the adiabatic connection (AC) with the extended random phase approximation one obtains a general tool capable of accounting for dynamical electron correlation for a broad class of multireference wavefunctions, applicable even to systems including strongly correlated electrons. It will be shown that the AC-based approximation yields excellent results when applied to multireference models, exceeding in accuracy second-order perturbation-theory-based methods.

DS 21.2 Wed 11:00 HL 001

Density functional theory of electron transfer beyond the Born-Oppenheimer approximation: case study of LiF — •Chen Li[1], Ryan Requist[1], and Eberhard. K. U. Gross[1,2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel

We demonstrate that beyond Born-Oppenheimer (BO) effects can be accurately and seamlessly incorporated within a density functional framework. In alkali halides like LiF, there is an abrupt change in the ground state electronic distribution due to an electron transfer at a critical bond length $R = R_c$. We find that nonadiabatic electron-nuclear coupling produces a sizable elongation of the critical R_c by 0.5 Bohr, an effect which is very accurately captured by a simple and rigorously-derived nuclear mass-dependent correction to the exchange-correlation potential in density functional theory. Since this nonadiabatic term depends on gradients of the nuclear wave function and conditional electronic density, $\nabla_R \chi(R)$ and $\nabla_R n(r, R)$, it couples the Kohn-Sham equations at neighboring R points. Motivated by an observed localization of nonadiabatic effects in nuclear configuration space, we propose an approximation that reduces the search for nonadiabatic density functionals to the search for a single function. This work is a step towards bringing density functional theory beyond the limitations of the BO approximation.

DS 21.3 Wed 11:15 HL 001

Ground-State Quantum-Electrodynamical Density-Functional Theory — •Michael Ruggenthaler — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

In this talk I present a density-functional reformulation of correlated matter-photon problems subject to general external electromagnetic fields and charge currents [1]. I first show that for static minimally-coupled matter-photon systems an external electromagnetic field is equivalent to an external charge current. I employ this to show that scalar external potentials and transversal external charge currents are in a one-to-one correspondence to the expectation values of the charge density and the vector-potential of the correlated matter-photon ground state. This allows to establish a Maxwell-Kohn-Sham approach, where in conjunction with the usual single-particle Kohn-Sham equations a classical Maxwell equation has to be solved in order to capture the correlation induced by the transversal photon field. In the magnetic mean-field limit this reduces to a current-density-functional theory that does not suffer from non-uniqueness problems and if furthermore the magnetic field is zero recovers standard density-functional theory.

[1] "Ground-State Quantum-Electrodynamical Density-Functional Theory", M. Ruggenthaler, arXiv:1509.01417 (2017).

DS 21.4 Wed 11:30 HL 001

Design of auxiliary systems for observables: the dynamic structure factor and the electron addition and removal spectra — Marco Vanzini, Martin Panholzer, Lucia Reining, and •Matteo Gatti — LSI, CNRS, Ecole Polytechnique, Palaiseau, France

Density functional theory tells us that the external potential, and therefore all observables, are functionals of the ground state density. The exact functionals, however, are not known, and one has to find approximations. To obtain the density, Kohn and Sham have proposed the idea to use an "auxiliary system". Much research effort goes into finding better and better Kohn Sham potentials for the density and the total ground state energy. In order to access also observables other than the density, we have proposed to generalize the Kohn-Sham idea of an auxiliary system [1], and to design a "connector" that allows us to profit from calculations done in a model system [2,3]. We have recently shown that this is a successful strategy for the dynamic structure factor [2] and for the one-body spectral function of simple metals, semiconductors and insulators [3]. [1] M. Gatti, V. Olevano, L. Reining, and I. V. Tokatly, Phys. Rev. Lett. 99, 057401 (2007) [2] M. Panholzer, M. Gatti, and L. Reining, arXiv:1708.02992 [3] M. Vanzini, L. Reining, and M. Gatti, arXiv:1708.02450

DS 21.5 Wed 11:45 HL 001

Exact exchange energy of the ferromagnetic electron gas with dipolar interactions — •Camilla Pellegrini, Tristan Mueller, Kay Dewhurst, Sangeeta Sharma, and Eberhard K. U. Gross — Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We propose a density functional treatment of the magnetic dipole-dipole interaction as a spin-spin correction to the Coulomb force in the Breit-Pauli Hamiltonian. Within this microscopic approach, the Hartree-like term for the dipolar coupling corresponds to the classical magnetostatic energy currently implemented in micromagnetic calculations. In addition, we have derived quantum corrections by evaluating analytically the exact exchange energy (Fock term) for the homogeneous electron gas, within the linear response to a noncollinear magnetic field. We expect our functional to open the path towards a full ab initio description of inhomogeneous magnetic structures at the nanoscale, with applications to domain-wall operated spintronic devices.

DS 21.6 Wed 12:00 HL 001

Precise total-energy calculations at a significantly reduced cost — •Rudolf Zeller — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In density-functional calculations, the total-energy functional is stationary with respect to the density, the Kohn-Sham orbitals and the Kohn-Sham effective potential. This means that approximations for these quantities only lead to total-energy errors of second order provided that the total-energy functional is evaluated accurately without further uncontrolled approximations.

Unfortunately, usually the Kohn-Sham orbitals and thus the kinetic part of the total energy are evaluated by using a projection of the potential into a finite subspace of basis functions. This approximation damages the stationarity of the total energy as a functional of the potential.

A technique will be discussed which can relieve this deficiency so that a considerably smaller subspace of basis functions can be used for a precise evaluation of the kinetic part of the total energy. The advantage will be illustrated for the particular example of angular projection potentials as they are used in the full-potential Korringa-Kohn-Rostoker Green function method.

DS 21.7 Wed 12:15 HL 001

Approach to Orbital-free DFT with Englert-Schwinger model — •Jouko Lehtomäki and Olga Lopez-Acevedo — COMP Centre of Excellence, Department of Applied Physics, Aalto University, Finland

We briefly present the Englert and Schwinger (ES) model in comparison with other approaches to orbital-free DFT. Essential failure of many kinetic energy density functionals is that they can not describe the most tightly bound core electrons in a satisfactory manner. Englert-Schwinger model allows treating these problematic electrons with more accurate single-particle wavefunctions while still obtaining the self-consistent orbital-free solution to the electronic problem.

Specifically, we detail how the ES model compares to the more known Thomas-Fermi-Dirac-Weizsäcker model self-consistently in atoms. We look at the total energy and few geometric properties. We show qualitative improvement in Pauli potential, which shows unphysical singularities near nucleus when the most tightly bound electrons are not treated correctly. We present how augmentation of the model with Kohn-Sham orbitals allows us to explore all-electron solution to the OFDFT problem and how this paves way for an orbital-free DFT method which does not need pseudopotentials.

DS 21.8 Wed 12:30 HL 001

The Kerker Preconditioner for FLAPW Methods with Charge Density Mixing — •Miriam Hinzen, Edoardo Di Napoli, Daniel Wortmann, and Stefan Blügel — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In metallic systems of larger size the self-consistent field convergence of electronic structure calculations is often slowed down substantially due to charge sloshing: close to the Fermi level, little change in energy can cause large fluctuations in charge density. Mathematically speaking, the problem is ill-conditioned. For plane-wave methods the Kerker preconditioner effectively solved this problem, but for many other electronic structure methods, in particular all-electron methods as the FLAPW or KKR methods, a real-space formulation would be needed. We developed a formulation of the Kerker preconditioner for FLAPW methods with charge density mixing, implemented in `FLEUR` [1]. Numerical experiments show an enormous reduction of the number of iterations needed for convergence; even more importantly, the SCF convergence has become independent of the system size.
[1] www.flapw.de

DS 21.9 Wed 12:45 HL 001

Effect of spin on the generalized Pauli constraints in Reduced Density Matrix Functional Theory — •Nicole Helbig[1], Iris Theophilou[2], and Nektarios N. Lathiotakis[3] — [1]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vass. Constantinou 48, GR-11635 Athens, Greece

Reduced Density Matrix Functional Theory is a method that relies on the 1-1 correspondence between the many-body ground-state wave function and the first order reduced density matrix (1RDM) and uses the latter as its fundamental variable. Enforcing the generalized Pauli constraints during the energy minimization ensures that the 1RDM corresponds to a fermionic pure state. We demonstrate that these constraints are modified for open-shell systems if the spin degrees of freedom are taken into account. From the generalized Pauli constraints we also derive properties of the exact occupation numbers and natural orbitals which ensure that the 1RDM corresponds to an eigenstate of the total spin.

DS 22: Optical Analysis of Thin Films (Reflection, Ellipsometry, Raman, IR-DUV Spectroscopy, ...): Session II

Time: Wednesday 15:00–15:45 Location: H 0111

DS 22.1 Wed 15:00 H 0111

Giant Circular Dichroism of Enantiopure Prolinol-Derived Squaraine J-Aggregate Thin Films probed by Mueller Matrix Spectroscopy — •Manuela Schiek[1], Matthias Schulz[2], Jennifer Zablocki[2], Oliya S. Abdullaeva[1], Arne Lützen[2], Frank Balzer[3], and Oriol Arteaga[4] — [1]University of Oldenburg, D. — [2]University of Bonn, D — [3]University of Southern Denmark, Sonderborg, DK — [4]University of Barcelona, ES

We have achieved sizable ex-chiral-pool synthesis of enantiopure prolinol functionalized squaraine small molecular compounds with opposite handedness. The aggregation into intrinsically circular dichroic, molecular J-aggregates with quasimetallic reflection is controlled by thermal annealing. By Mueller matrix spectroscopy [1] we show an extraordinary high but true circular dichroism in spincasted thin films spectrally located at 780 nm. The ellipticity well reaches a value of 500 mdeg/nm and an intensive dissymmetry factor of 0.75, respectively, and is evenly distributed over the complete thin film area. So far, these values have no documented rival among intrinsic supramolecular circular dichroism, and thereby are revolutionary for the development of organic based chiral photonics and spintronics. [1] O. Arteaga, B. Kahr, Opt. Lett. 38 (2013) 1134.

DS 22.2 Wed 15:15 H 0111

Temperature dependent dielectric function of CuI — •Evgeny Krüger, Vitaly Zviagin, Chang Yang, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstr. 5, Leipzig

We present optical and structural properties of CuI thin films deposited by sputtering at temperatures varying from 55°C to 310°C on c-sapphire substrate. Scanning electron microscopy scans reveal a smooth surface morphology for films grown at temperatures above 160°C and large thickness inhomogeneity for films grown at lower temperatures. X-ray diffraction reveals good crystal quality for growth temperatures above 200 °C. The dielectric function (DF) was determined in a wide spectral range between (0.5 – 8.5) eV and for temperatures from 10 K to 300 K. The main features in the DF were assigned to exciton-related optical transitions at various critical points in the Brilluoin zone, revealing non-monotonic temperature dependence of the energy as well as strong screening for excitons related to higher critical points.

DS 22.3 Wed 15:30 H 0111

Interface states revealed by DFT calculation of reflectance anisotropy spectroscopy: GaP on Si(001) — •Charles Patterson and Pankaj Kumar — School of Physics, Trinity College Dublin, Dublin 2, Ireland

States localized at crystalline interfaces between dielectrics can be probed using optical reflectance anisotropy when the light is incident from the side of the material with the larger band gap. We present first-principles calculations of the anisotropy of the GaP/Si(001) interface [1] and compare them to the interface part of the anisotropy derived from measurements on several GaP thin films on Si(001) with different thickness [2]. The calculations show excellent agreement with experiment only for a gapped interface with a P layer in contact with Si. Interfaces are gapped only when the underlying Si is doped owing to excess electrons in the dimer layer at the GaP surface. Optical excitations from two states localized in several Si layers adjacent to the interface result in the observed anisotropy of the interface. A combination of theory and optical anisotropy experiment can therefore reveal localized electronic states and the atomic structure at buried interfaces.

[1] P. Kumar and C. H. Patterson, Phys. Rev. Lett. 118 237403 (2017) [2] O. Supplie et al., Phys. Rev. B 86, 035308 (2012)

DS 23: Lithography II: Focused Electron Beam Induced Processing: 3D Nano-Printing for Material Science (Focussed Session): Afternoon Session (joint session DS/KFM)

Considering 3D printing using fused-deposition modeling or higher-resolution variants with lasers applicable to polymers and metals, an analogous approach exists on the nanometer scale. With the aid of focused electron beam-induced deposition (FEBID) it is possible to create solid-state structures on the nanoscale. However, in contradistinction to large-scale 3D printing of simple plastic or metallic structures, FEBID is able to directly provide nano-materials with a wealth of interesting electronic, optical and magnetic properties. Due to this, focused electron beam-induced deposition has experienced a rapid expansion in the breadth of its application fields over the last 10 years. FEBID uses precursor gases which, being adsorbed on a surface, are dissociated in the focussed electron beam to form the deposit. Intensive research has pushed the capabilities of FEBID in two important areas. It is now possible to obtain fully metallic nanostructures of Fe, Co and FeCo-alloys and also of Au and Pt. In addition, very recently the simulation-guided nano-manufacturing of 3D structures has matured to such a degree that even complex 3D objects can now be fabricated under controlled conditions. The focused session will address these new developments spanning the range from the fundamentals of electron-precursor interaction, covering aspects of the rational design of optimized precursors, and showing recent work on superconducting, magnetic and plasmonically active materials, both in 2D and 3D.

Organized by

Name: Prof. Dr. Michael Huth, Institution: Physikalisches Institut, Goethe-Universität, City: Frankfurt am Main, Country: Germany, Email: michael.huth@physik.uni-frankfurt.de, Telephone number: +49-69-798-47235

Name: Ass. Prof. Dr. Harald Plank, Institution: Institut für Elektronenmikroskopie und Nanoanalytik, TU Graz, City: Graz, Country: Austria, Email: harald.plank@felmi-zfe.at, Telephone number: +43-316-873-8821

Name: Dr. Ivo Utke, Institution: EMPA, Swiss Laboratories for Materials Science and Technology, City: Thun, Country: Switzerland, Email: Ivo.Utke@empa.ch, Telephone number: +41-58-765-6257

Time: Wednesday 15:00–18:00 Location: H 2032

DS 23.1 Wed 15:00 H 2032

FEBIP on Metal-Organic Frameworks — •Christian Preischl[1], Elif Bilgilisoy[1], Florian Vollnhals[1], Kai Ahlenhof[2], Petra Swiderek[2], Hartmut Gliemann[3], Christof Wöll[3], and Hubertus Marbach[1] — [1]Physik. Chemie II, FAU Erlangen — [2]IAPC, Universität Bremen — [3]Institut f. funktionelle Grenzflächen, KIT

We report the fabrication of nanostructures down to single digit nanometer scale on metal-organic frameworks (MOFs) by FEBIP. Next to EBID[1], our second technique is Electron Beam Induced Surface Activation (EBISA). In EBISA the surface is locally activated by an electron beam and the subsequently dosed precursor is catalytically decomposed at the activated sites and forms a deposit.[2] Both approaches were investigated with $Fe(CO)_5$ and $Co(CO)_3NO$ on HKUST-1 and Cu-oxalate which is somewhat similar to HKUST-1 but the benzylic part in the organic linker is missing compared to the latter. Both samples were grown in a layer-by-layer method.[3][4] We demonstrate that both precursors are suitable for EBID on both samples, whereas EBISA works only with $Fe(CO)_5$ on the HKUST-1. We will compare the corresponding results and discuss especially the high potential of MOFs as substrates for novel FEBIP processes towards the fabrication 3D materials.

[1] W. van Dorp, C.W. Hagen, J. Appl. Phys. 104 (2008), 081301 [2] H. Marbach, Appl. Phys. A 117 (2014), 987; Drost et al., Small Methods 1 (2017), 1700095 [3] O. Shekhah et al., Angew. Chem. Int. Ed. 48 (2009), 5038 [4] I. Schrader et al., Langmuir 30 (2014), 11945

DS 23.2 Wed 15:15 H 2032

Focused Electron Beam Induced Deposition with halogenated organometallic Ru compounds — •Jakub Jurczyk[1,2], Christopher Brewer[3], Olivia Hawkins[3], Czeslaw Kapusta[2], Lisa McElwee-White[3], and Ivo Utke[1] — [1]Empa - Swiss Federal Laboratories for Materials Science and Technology,Thun, Switzerland — [2]AGH University of Science and Technology in Krakow, Kraków, Poland — [3]University of Florida, Gainesville, USA

Focused Electron Beam Induced Deposition (FEBID) studies of potential organometallic halogenated ruthenium precursors were performed. By now the best Ru FEBID result was achieved using bis(ethylcyclopentyldienyl) ruthenium(II) [1] giving a C:Ru ratio of 9:1 (10 at.% Ru) in as deposited material. Recent gas phase [2] and surface science studies [3] selected halogenated organometallic compounds as potential FEBID precursors. In this contribution we present three of them: n-allyl-Ru(CO)3Cl, n-allyl-Ru(CO)3Br, n-allyl-Ru(CO)3I. The deposit metal content was investigated as function of growth regimes and writing strategies for vertical and planar structures. First promising results of up to 20 at.% of Ru in as deposited material were achieved. Electrical properties of as deposited and annealed nanowires will be presented.

[1] J.H. Noh et al., App. Phys. A, 117, (2014), 1705-1713 [2] R. M. Thorman et al., Phys. Chem. Chem. Phys, 19, (2017), 13264-13271 [3] Spencer et al., J. Phys. Chem. C, 119, (2015), 15349-15359

DS 23.3 Wed 15:30 H 2032

Electron-induced reactions of surface-grown metal organic layers — •Kai Ahlenhoff and Petra Swiderek — University of Bremen, Institute for Applied and Physical Chemistry, Bremen, Germany

Metal-containing coordination materials grown on surfaces using layer-by-layer self-assembly processes are advantageous for focused electron beam deposition (FEBID) processes for several reasons. First, multilayer materials can serve as precursors which enable high processing speed due to their large surface density [1]. Also, an adlayer on a substrate used in a regular FEBID process relying on volatile precursors can suppress secondary electron emission from the underlying solid and thus lead to more precisely defined deposit shapes [2]. Third, the layer may be activated by an electron beam to provide a template for area-selective autocatalytic deposit growth in an EBISA process [2].

Despite these advantages, little is known about the electron-induced reactions in such materials and the resulting products. Therefore, this contribution presents studies on electron-induced desorption (ESD) from and post-irradiation reflection absorption infrared spectroscopy (RAIRS) of several surface grown metal-organic coordination polymers such as copper(II)oxalate [3] and HKUST-1 [4] but also including novel FEBID precursors.

References: [1] M. Bresin et al. Nanotechnol. 24 (2013) 035301. [2] M. Drost et al., SMALL Methods 1 (2017) 1700095. [3] K. Rückriem et al., Beilstein J. Nanotechnol. 7 (2016) 852. [4] B.W. Jacobs et al., Nanotechnol. 22 (2011) 375601.

DS 23.4 Wed 15:45 H 2032

Tuning and in-situ monitoring the hall resistance of ferromagnetic FEBID structures — •Roland Sachser and Michael Huth — Physikalisches Institut, Goethe-University, Frankfurt am Main, Germany

$HFeCo_3(CO)_{12}$ is an excellent FEBID precursor, which allows the deposition of magnetic and metallic CoFe alloy nanostructures. In contrast, the widely used $(CH_3)_3CH_3C_5H_4Pt$ standard precursor results in insulating deposits, consisting of Pt nanograins embedded in a carbonaceous matrix. In this contribution we will present measurements on samples prepared via co-deposition of both precursors. Varying the deposition conditions, the metal content of the deposits, and thus, the resistivity and the Hall resistance of the samples can be tuned. Furthermore, the co-deposited samples are sensitive to post-growth electron beam irradiation, which influences its electrical transport properties, as it is already known for normal FEBID deposits obtained by the Pt-precursor. We will show in-situ measurements of the Hall resistance directly inside the SEM by using the magnetic field provided by the immersion lens of the instrument. Further characterization is done via temperature-dependent electrical and magnetotransport measurements.

DS 23.5 Wed 16:00 H 2032

Purified and crystalline three-dimensional electron-beam-induced deposits: the successful case of cobalt — Javier Pablo-Navarro[1], César Magén[1,2], and •José María De Teresa[1,2] — [1]Laboratorio de Microscopías Avanzadas (LMA) - Instituto de Nanociencia de Aragón (INA), Universidad de Zaragoza, 50018 Zaragoza, Spain. — [2]Instituto de Ciencia de Materiales de Aragón (ICMA), Universidad de Zaragoza-CSIC, 50009 Zaragoza, Spain.

Purified and crystalline 3D cobalt nanowires of diameter below 90 nm have been fabricated by ex-situ high-vacuum annealing at 600 Celsius degrees after FEBID growth. While increasing the metallic content of the nanowires up to 95 atomic percent, the thermal annealing process induces the recrystallization of the pseudo-amorphous as-grown structure into bulk-like, hcp and fcc crystallites with lateral sizes comparable to the width of the nanowire. The net magnetization increases 80 percent with respect to as-grown values, close to the bulk cobalt value. This achievement opens new pathways for applications of this synthetic method in the fabrication of either individual or arrays of 3D high-purity and crystalline cobalt nanowires for high-density memory and logic devices, nanosensors and actuators, and could be a viable method to obtain other pure and crystalline 3D materials by FEBID.

DS 23.6 Wed 16:15 H 2032

Exploring new copper complexes for FEBID — •Luisa Berger[1], Katarzyna Madajska[2], Nils Boysen[3], Iwona Barbara Szymánska[2], Anjana Devi[3], and Ivo Utke[1] — [1]Empa - Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland — [2]Nicolaus Copernicus University, Torun, Poland — [3]Ruhr-Universität Bochum, Germany

Focused electron beam induced deposition (FEBID) is a well-established maskless direct write method for nanostructures [1]. The deposition of pure copper with FEBID has not been achieved so far and metal contents typically reached 13-25 at.% [2]. By exploring novel copper precursor classes - fluorinated copper carboxylates ([Cu2(u-O2CC2F5)4], [Cu2(EtNH2)2(u-O2CC2F5)4]) and a fluorine-free β-diketonate (Cu(tbaoac)2) - we intend to achieve the deposition of high purity structures. The latter was employed in FEBID recently [3] while carboxylates were reported as CVD precursors [4]. The influence of varying deposition parameters on appearance and composition was investigated. First interesting results lead to copper contents of 25 at.%.

[1] I. Utke, A. Gölzhäuser, Angew. Chem. Int. Ed. 49 (2010), 9328.

[2] A. Luisier et al., Journal of The Electrochemical Society, 151 (2004) C535.

[3] C. Haverkamp, K. Höflich et al., Beilstein Journal of Nanotechnology 2017 (in review)

[4] P. Piszczek, I. B. Szymańska, Chem. Vap. Deposition, 19 (2013) 251.

15 min. break.

DS 23.7 Wed 16:45 H 2032

Dedicated AS-ALD micro-reactor for FEBID nano-templates — •Peter Gruszka, Giorgia Di Prima, Roland Sachser, and

Michael Huth — Goethe Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

In recent years, conventional methods of nano-structuring are slowly reaching their lower limits. A novel bottom-up approach emerged[1], which combines focused electron beam induced deposition(FEBID) and area-selective atomic layer deposition(AS-ALD). FEBID is a serial, bottom-up and direct-write technique yielding structures with superior lateral resolution (< 10 nm), but with poor material quality. In contrast, ALD and especially AS-ALD are parallel and bottom-up approaches with exceptional thickness control resulting in high purity sub-nano films.

We successfully performed the combined FEBID-ALD process in our Nova 600 Dual Beam scanning electron microscope.[2] The ALD experiments were conducted on purified platinum FEBID-nanostructures[3] which were monitored via in-situ conductance measurements. For further investigation and optimization, we built a dedicated AS-ALD micro-reactor.

[1] Mackus, et al., J. Appl. Phys 107 (2010), 116102
[2] Di Prima, et al., Nano Futures 1(2) (2017), 25005
[3] Sachser, et al., ACS Appl. Mater. Interfaces 6 (2014), 15868

DS 23.8 Wed 17:00 H 2032

Fabrication of multi-component nanostructures by FEBID — •Fabrizio Porrati[1], Roland Sachser[1], Sven Barth[2], Gian Carlo Gazzadi[3], Stefano Frabboni[3], Christian Gspan[4], Harald Plank[4], Andreas Terfort[5], and Michael Huth[1] — [1]Goethe-Universität, Institut of Physics, Frankfurt am Main, Germany — [2]TU Vienna, Institute of Materials Chemistry, Wien, Austria — [3]University of Modena and Reggio Emilia, FIM Department, Modena, Italy — [4]TU Graz, Institute for Electron Microscopy and Nanoanalysis, Graz, Austria — [5]Goethe-Universität,Institute for Inorganic and Analytical Chemistry, Frankfurt am Main, Germany

The fabrication of multi-component polycrystalline or granular metals by FEBID represents a challenging research approach for the design of novel nanostructured materials. Currently, there are three different approaches for the fabrication of multi-component FEBID nanostructures: 1. deposition by single source heteronuclear precursors; 2. codeposition using two different precursors; 3. intermixing of multilayer nanostructures fabricated with different precursors by low-energy electron irradiation. These fabrication approaches allow the fabrication of a large number of tunable alloy nanostructured and intermetallic compounds. In this contribution, we present some examples of binary and ternary nanostructures fabricated by following these routes. In particular, we report on the fabrication, the structural characterization and magnetotransport measurements of CoFe alloys and Co2FeSi Heusler compounds.

DS 23.9 Wed 17:15 H 2032

Ac response of nano-granular metals prepared via FEBID — •Marc Hanefeld and Michael Huth — Physikalisches Institut, Goethe Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

Granular metals are of great interest for material sciences due to their diverse electronic transport properties and can generally be described as metallic nanoparticles surrounded by a dielectric amorphous matrix. They show promising possibilities for applications in different sensing mechanisms [1] and pose a topic of ongoing research concerning their response to a time-dependant ac stimulus [2].

Focused Electron Beam Induced Deposition (FEBID) is a versatile technique to create nano-granular metals comprising a variety of elements and a high tunability of the samples properties. Additionally, electron irradiation is the perfect tool to tune important conduction parameters like the inter-grain coupling strength and the volume fraction of the crystallites compared to the surrounding matrix, ultimately influencing the conductance regime of the deposits. In our group we have a wide knowledge about Pt(C)-FEBID deposits and the effect of electron irradiation upon them, as well as their dc electronic transport properties [1]. We will present first measurements on the ac response of such deposits and show the capabilities of FEBID to create an ideal model environment for an in depth analysis of the ac conduction characteristics of granular metals depending on their properties.

[1] Huth, et al., Microelect. Eng. 2017. doi:10.1016/j.mee.2017.10.012.
[2] Bakkali, et al., Sci. Rep. 2016;6:29676. doi:10.1038/srep29676.

DS 23.10 Wed 17:30 H 2032

Energy collection from green-house infra-red emission using nanogranular compoundmaterials — •Koops Hans Wilfried Peter — HaWilKo GmbH , Ober-Ramstadt, Germany

According to a 10 years average measurement of NASA of the earth's energy household, the sun sends 340,4 W/m^2 direct to the earth, but only 163,3 W/m^2 reach the ground. In the IR a backreflection from greenhouse gases delivers 340 W/m^2.

A nanogranular Pt/C material has a bandgap of 128 meV, which allows to absorb IR-Light. This radiation can be absorbed by a nanocrystalline Pt/C compound. Large absorber areas can be used. Silicon material absorbes only energies above 1.3 eV during daylight from the visible light. The green house gases, however, emit their radiation all day and night in the IR. The absorbed IR photons can be stored in the compound material as coherent Boson fields. A field gradient applied to such fields can move the Bosons and make them decay at the end of the field, and release electrons as a current. HaWilKo can produce a 1 cm^2 large sheet to demonstrate the energy harvesting in the IR.

DS 23.11 Wed 17:45 H 2032

Coordination compounds for focused electron beam induced deposition (FEBID) — •Iwona Szymańska. and Katarzyna Madajska — Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland

Focused electron beam induced deposition is a direct maskless nanolithography technique. The compounds applied as FEBID precursors should effectively generate volatile metal carriers, which are transported over a substrate. Next, they are irradiated by high-energy electrons and decompose forming nanomaterials [1]. Copper and silver exhibit high electrical and thermal conductivity and are extensively used in microelectronics.

Copper and silver carboxylate compounds were applied as CVD precursors [2,3]. Carboxylates are able to coordinate as monodentates, chelates, and bridges forming complexes of diverse nuclearity. Secondary ligands enable manipulating physicochemical parameters of precursors. Research was focused on the copper(II) and silver(I) carboxylate compounds, which seems to be promising for a FEBID process. The usefulness of a thermal analysis, EI MS spectrometry, and VT IR spectroscopy for the FEBID precursors selection was evaluated. The secondary ligand influence was studied basing on primary amines.

Acknowledgements: The authors wish to thank Nicolaus Copernicus University in Toruń (Statute Research no.103) for a financial support.

References: [1] I. Utke et al., Angewandte Chemie Int. Ed., 49 (2010) 9328; [2] A. Grodzicki et al., Coord. Chem. Rev., 249 (2005) 2232; [3] I.B. Szymańska,, Polyhedron, 65 (2013) 82.

DS 24: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials V (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Wednesday 15:00–17:45 Location: HL 001

Invited Talk DS 24.1 Wed 15:00 HL 001

Computational Approach to the Electronic Structure of Strongly Correlated Materials: Towards Theoretical Spectroscopy and Theory Assisted Material Design — •Gabriel Kotliar — Serin Physics Laboratory Rutgers University — Brookhaven National Laboratories

We will introduce a project, to build algorithms and a suite of open source codes, to compute the electronic structure of correlated materials. It involves different methods, to provide different compromises between speed and accuracy, and to treat different types of correlation (static and dynamic). The suite includes methods ranging from vertex corrected GW, rotationally invariant slave bosons and LDA+DMFT, and we will illustrate some of these methods (and their failures) in d and f electron systems.

DS 24.2 Wed 15:30 HL 001

Spectral properties of Sr2IrO4 from first principles — •Cyril Martins[1], Benjamin Lenz[2], and Silke Biermann[2,3] — [1]Laboratoire de Chimie et Physique Quantiques, UMR 5626, Université Paul Sabatier, 118 route de Narbonne, 31400 Toulouse, France — [2]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, Université Paris-Saclay, 91128 Palaiseau, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

The spin-orbit system Sr2IrO4 has raised tremendous interest recently, due to intriguing similarities to the high-Tc superconducting copper oxides.

We study the evolution of the electronic structure of Sr2IrO4 using a combination of ab-initio density functional theory and many-body techniques. The effects of spin-orbit coupling, distortions of the oxygen octahedra and Hubbard interactions are included on a first-principles level. We calculate the momentum-resolved spectral function and compare to recent photoemission data, finding good agreement with experiment.

DS 24.3 Wed 15:45 HL 001

Role of non-local correlations in doped Sr_2IrO_4 — •Benjamin Lenz[1], Cyril Martins[2], and Silke Biermann[1,3] — [1]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, Université Paris-Saclay, 91128 Palaiseau, France — [2]Laboratoire de Chimie et Physique Quantiques, UMR 5626, Université Paul Sabatier, 118 route de Narbonne, 31400 Toulouse, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

When doping the spin-orbit system Sr_2IrO_4 recent photoemission experiments found pseudogap behavior at low temperatures, which raises the question of its relation to the pseudogap found in high-Tc superconducting copper oxides.

Here, we study the evolution of the electronic structure of Sr_2IrO_4 upon electron- and hole-doping by combining ab-initio density functional theory and two quantum cluster techniques. Our treatment includes the effects of spin-orbit coupling, distortions of the oxygen octahedra and Hubbard interactions on a first-principles level. We show that short-range antiferromagnetic fluctuations are crucial to account for the electronic properties of the material even in the high-temperature paramagnetic phase. Furthermore, pseudogap features in the momentum-resolved spectral function of the emerging exotic metallic state are analyzed and found to be in good agreement with experiment.

DS 24.4 Wed 16:00 HL 001

Describing the coupled structural and metal-insulator transition in rare-earth nickelates with DFT+DMFT — •Alexander Hampel and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

Perovskite rare-earth nickelates, $R\mathrm{NiO}_3$, display a rich phase diagram, where all compounds with R from Pr to Lu undergo a metal-insulator transition (MIT) that is accompanied by a structural distortion. This distortion breaks the symmetry between formerly equivalent Ni sites and is related to a charge disproportionation driven by correlation effects, resulting in an insulating state. Here, we employ density functional theory together with dynamical mean field theory (DFT+DMFT) to explore the interplay between lattice distortions and electronic correlation effects in these compounds. By utilizing a symmetry-based distortion mode analysis, we are able to isolate the specific lattice distortion occurring at the phase transition. Calculating total energies within DFT+DMFT then allows us to relax the structures with respect to this distortion. We find, that the resulting distortion amplitudes and its variation across the series are in good agreement with experimental results. Our work highlights the capabilities of the DFT+DMFT method to describe complex materials with coupled electronic and structural degrees of freedom.

DS 24.5 Wed 16:15 HL 001

Magnetocrystalline anisotropy of FePt: LDA+DMFT study — •saleem Ayaz Khan[1], Junqing Xu[2], johan Schott[3], Ondřej Šipr[1], and Jan Minár[1] — [1]University of West Bohemia, Pilsen, Czech Republic — [2]LMU Munich, Germany — [3]Uppsala University, Sweden

In our recent work (Phys. Rev B, 94, 144436, 2016) we employed ab initio methods (FLAPW and KKR) to get a reliable value for the magnetocrystalline anisotropy (MCA) energy of FePt. The theoretical MCA energy of FePt (3.0 meV) is significantly larger than the experimental value (1.3 meV), implying that the LDA cannot properly describe the MCA of FePt. Considering that the MCA essentially arises from spin orbit coupling it appears that to obtain reasonable agreement with experiments, it is necessary to include orbital correlations. To account realistically for both the electronic and geometric structure of materials, we use a combined density functional and dynamical mean field theory, LDA+DMFT. Our computation is based on the fluctuation exchange approximation and an analytic continuation method for the self-energy. Our results show that dynamical correlation effects are important for a correct treatment of the 3d-5d hybridization in FePt, which in turn plays a significant role for the magnetocrystalline anisotropy

DS 24.6 Wed 16:30 HL 001

Diagnostics for plasmon satellites and Hubbard bands in transition metal oxides — •Steffen Backes[1], Hong Jiang[2], and Silke Biermann[1] — [1]Centre de Physique Théorique, École Polytechnique, 91128 Palaiseau, France — [2]College of Chemistry and Molecular Engineering, Peking University, China

The generally accepted picture of $SrVO_3$ is that of a correlated electron metal where a renormalized quasi-particle peak at the Fermi level coexists with upper and lower Hubbard bands, separated by Coulomb interaction U. Recently, this picture has become blurred with the rise in interest in additional plasmonic satellites. Distinguishing plasmonic features from Hubbard bands is a non-trivial question. In this talk we employ combined many-body perturbation theory and dynamical mean field theory ("GW+DMFT") to discuss the processes that give rise to these different satellites and show how to identify their origin in realistic materials. We present an application of this scheme to different transition metal oxides, which we find to exhibit both Hubbard and plasmonic satellites at similar energetic positions.

DS 24.7 Wed 16:45 HL 001

Phase transitions of the 2D Hubbard-Holstein model — •Teresa E. Reinhard[1], Uliana Mordovina[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

In the 2d Hubbard-Holstein model at zero temperature, a quantum phase transition between Mott and Peierls insulator can be observed. Whether a metallic phase emerges in between remains an open question [1,2]. As the emergence of the Mott phase is a many body effect, a description beyond the mean field level is crucial. At the same time, a method that can cope with two dimensions is needed.

To address this open question, we have extended Density Matrix Embedding Theory (DMET) from the purely electronic case [3,4] to coupled fermion-boson systems. DMET is an embedding theory which benefits from the exponentially decaying correlation in most quantum systems thus allowing a description beyond mean field at low cost.

We show the phase diagram of the 2d Hubbard-Holstein model at zero temperature obtained for different cluster sizes. [1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012) [2] S. Wouters, C. A. Jiménez-Hoyos, G. K.-L. Chan, arXiv:1605.05547 (2016) [3] R. T. Clay and R. P. Hardikar, Phys. Rev. Lett 95, 096401 (2005) [4] J. Bauer, EPL 90 27002 (2010)

DS 24.8 Wed 17:00 HL 001

A quantum embedding theory combining many-body perturbation theory with configuration interaction — •Marc Dvorak and Patrick Rinke — Department of Applied Physics, Aalto University School of Science, 00076-Aalto, Finland

We present a new quantum embedding theory called dynamical configuration interaction (DCI). It captures non-local and static correlation in an orbital active space with configuration interaction (CI) and high-energy, dynamic correlation in the complementary bath space with many-body perturbation theory (MBPT). The formulation is general, but we focus on molecular systems with an *ab-initio* Hamiltonian. The conceptual key to our approach is to replace the exact electronic Hamiltonian in the bath space with one of excitations defined over the correlated ground state. This transformation is naturally suited to the language and methodology of many-body Green's functions. Correlation in the bath is therefore described at the quasiparticle level with Green's functions instead of with the many-body wave function. Our approach avoids computational and conceptual difficulties associated with Green's function embedding and improves upon wave function methods by including dynamical correlation from the bath space. A major advantage to DCI is that it naturally treats ground and excited states on equal quantum mechanical levels. For ground state properties, we present dimer dissociation curves for H_2 and N_2 in excellent agreement with exact results. Excited states of N_2 give excellent agreement with experiment, and we demonstrate the scalability of our method by computing excited states of a free-base porphyrin molecule.

DS 24.9 Wed 17:15 HL 001

Real-Structure Effects and Correlation in Layered Sodium Cobaltates — Sophie Chauvin[1,2], Silke Biermann[1], Lucia Reining[2], and •Claudia Rödl[3] — [1]Centre de Physique Théorique, École polytechnique, CNRS, Université Paris-Saclay, 91128 Palaiseau, France — [2]Laboratoire des Solides Irradiés, École polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [3]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Na-doped layered cobaltates Na_xCoO_2 feature a rich phase diagram with a plethora of physical phenomena ranging from metal-insulator transitions over magnetism to charge ordering. These instabilities of the electronic structure are mostly attributed to correlation effects within the quasi-2D CoO_2 layers. Here, we focus on $Na_{2/3}CoO_2$, a doping for which the system is metallic and exhibits an experimentally established charge disproportionation on the Co atoms.

We study the electronic properties of the CoO_2 layers and investigate the impact of the intercalated Na atoms on the electronic structure in the ordered layered superstructure. The problem is tackled from an *ab-initio* point of view using density-functional theory (DFT) and many-body perturbation theory (MBPT). Moreover, we study the static charge-density response of the material to understand instabilities in the system. Our approach complements recent model calculations from extended dynamical mean-field theory (EDMFT). The calculated results are compared to experimental spectroscopic data.

DS 24.10 Wed 17:30 HL 001

Slave rotor approach to impurity models with correlated dp orbitals — •Jakob Steinbauer and Silke Biermann — École Polytechnique, Palaiseau, France

We propose a slave rotor method for the solution of many-orbital quantum impurity problems, which maps the original problem onto one with reduced degeneracy. This is particularly useful for the dynamical mean field theory treatment of transition metal oxides where the interactions between ligand states with d-electrons are all too often simply neglected. We derive a general formalism relying on an optimized effective model obtained from the variational principle of Feynman and Peierls and test the method in the atomic limit.

DS 25: Organic Thin Films, Organic-Inorganic Interfaces: Session I (joint session DS/CPP)

Time: Wednesday 16:00–18:15 Location: H 0111

Invited Talk DS 25.1 Wed 16:00 H 0111

Prospects of Engineering Chemistry and Electronic Character of Interfaces in Multifunctional (Bio)Organic-Inorganic Hybrids — •Maria Losurdo — Institute of Nanotechnology, CNR-NANOTEC, Bari, Italy

New opportunities for energy harvesting, plasmonics, active photonics, biomimetic catalysis, biosensing, immunosensing and cellular recognition are offered by novel hybrid heterojunctions combining, semiconductors, plasmonic metal nanostructures and (bio)-organic systems.

In order to design these (bio)-organic/inorganic platforms, the establishment of reliable and reproducible protocols for their functionalization is still needed, which require better understanding of the surface and interfacial electronic phenomena.

This contribution presents strategies for tailoring the chemistry and electronic character of interfaces in hybrids spanning from planar surfaces (semiconductors Si, III-Vs, TCOs, SiC) to nanosystems (plasmonic Au, Ga, Al) designed to enable applications in photovoltaics (hole transport organic layers and semiconducting new polymers), biomimetic catalysis (porphirins) and bio- immuno-sensing (proteins, DNA, cells).

The emphasis will be on functionalization methods, including plasma treatments of surfaces and interfaces, resulting assembly and nanostructures and how the interface chemistry determines the charge transfer enabling the specific functionality.

Future directions towards the rational design of those hybrids will be suggested.

15 min. break.

DS 25.2 Wed 16:45 H 0111

Synthesis and combined experimental and theoretical characterization of dihydro-tetraaza-acenes — •Bernd Kollmann[1], Zhongrui Chen[2], Daniel Lüftner[1], Olivier Siri[2], and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, NAWI-Graz, Universitätsplatz 5. 8010 Graz, Austria — [2]Aix Marseille Universite, CNRS, CINaM UMR 7325, 13288 Marseille, France

We present a combined experimental and theoretical study of electronic and optical properties of dihydro-tetraaza-acenes (DHTAn). Using a solvent-free condensation, we are able to synthesize DHTA5, DHTA6 and DHTA7 molecules. We investigate their gas-phase electronic structures of by means ab-initio density functional calculations employing an optimally-tuned range-separated hybrid functional. By comparing with the parent linear oligoacenes (nA) and based on computed ionization potentials and electron affinities, we predict DHTAn molecules to be more stable than acenes of the same length, where we expect DHTAn molecules to be persistent at least up to n = 7 rings. We further exploit the analogy with nA by analyzing the entire intramolecular π-band structure of the DHTAn molecules. This clearly reveals that the additional two electrons donated by the dihydropyrazine group are delocalized over the entire molecule and contribute to its π-electron system. As a consequence, the symmetry of the frontier orbitals of DHTAn differs from that of the parent nA molecule. This is also illustrated by the UV-vis absorption spectra which have been measured for DHTA5, 6 and 7 dissolved in dimethyl sulfoxide and analysed by means of excited state calculations with an time-dependent DFT framework.

DS 25.3 Wed 17:00 H 0111

photochromic phosphonic-acid diarylethene self-assembled monolayer switches on polar ZnO surfaces — •Qiankun Wang[1], Giovanni Ligorio[1], Valentin Diez-Cabanes[2], David Cornil[2], Björn Kobin[3], Stefan Hecht[3], Jérôme Conil[2], Emil J.W. List-Kratochvil[1], and Norbert Koch[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Laboratory for Chemistry of Novel Materials, University of Mons — [3]Department of Chemistry, Humboldt-Universität zu Berlin

Here, we investigate the interfacial chemical and switching 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 and density functional theory calculations. The observed work function increase is attributed to the introduction of a surface dipole; the binding modes of the phosphonic-acid linker were retrieved from the deconvolution of O 1s core level spectra, indicating the formation of mixed bidentate and tridentate binding. The quantification of core level spectra supports the picture of a densely packed SAM on both ZnO surfaces. Upon illumination with ultraviolet and visible light, respectively, we observe a 0.7 eV energy level shift at the onset of the highest occupied molecular orbital (HOMO) level of the PA-DAE molecules. This can further on be used to reversibly switch the energy level alignment at the ZnO/PA-DAE interface in device structures.

DS 25.4 Wed 17:15 H 0111

Investigation of sputter deposited nanostructured alloy films on polymer surfaces — Niko Carstens[1], Alexander Hinz[1], Oleksandr Polonskyi[1], •Thomas Strunskus[1], Matthias Schwartzkopf[2], Pallavi Pandit[2], Andre Rothkirch[2], Franziska Löhrer[3], Volker Körstgens[3], Simon Schaper[3], Peter Müller-Buschbaum[3], Stephan Roth[2], and Franz Faupel[1] — [1]Chair for Multicomponent Materials, CAU Kiel, 24143 Kiel — [2]DESY, 22607 Hamburg — [3]Physcis Department, TU Munich, 85748 Garching

The fabrication of functional materials with tailored plasmonic properties gained much interest in recent years. Vapor phase deposition techniques like sputtering are an attractive approach to produce self-assembled nanostructured films which exhibit plasmonic activity when the effective thickness is under the percolation threshold. As the local surface plasmon resonance can be tuned by the composition, alloy films are of special interest. In this study, the growth of miscible (AuAg) and immiscible (CuAg) systems on different polymer surfaces (PS and PMMA) by magnetron sputtering has been investigated. The correlation between optical properties and the stage of film growth was examined during deposition by means of in-situ reflection UV-Vis spectroscopy as well as time resolved GIWAXS and GISAXS investigations [1,2]. In addition, SEM investigations as well as ex-situ transmission UV-Vis spectroscopy were performed after film deposition.

[1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 9, 5629 (2017), [2] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015).

DS 25.5 Wed 17:30 H 0111

Anomalous Roughness Evolution of Organic Mixed Films — •Alexander Hinderhofer, Jan Hagenlocher, Martin Oettel, and Frank Schreiber — Institute of Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

The surface morphology and roughness of thin films and crystals depend on competing mechanisms, which either roughen or smooth the film surface during growth. Important roughening mechanisms, are kinetic roughening based on shot noise and roughening due to mound growth, which is facilitated by reduced interlayer transport, often associated with a step edge. While these issues have been well studied for growth of simple atomic species, comparatively little is known about organic systems. These are expected to exhibit a fundamentally different growth behavior, due to their different interactions (van-der-Waals) and thus different response to strain and due to their internal degrees of freedom.

We use in situ x-ray reflectivity and complementary atomic force microscopy to monitor crystallinity and roughness evolution during growth of organic binary mixtures of several compounds, i.e. pentacene (PEN), perfluoropentacene (PFP), diindenoperylene (DIP) fullerene (C60). A general trend of reduced roughness in the mixed films compared to the pure materials is observed. We will discuss this roughness evolution in relationship to the in-plane crystallinity of the thin films and will show that the growth behavior can be rationalized by a, compared to homoepitaxy, lowered step edge barrier for lower in-plane crystallinity.

DS 25.6 Wed 17:45 H 0111

Grain boundaries and charge carrier diffusion in large crystal MAPI thin films — •Richard Ciesielski[1], Frank Schäfer[1], Nicolai Hartmann[1], Nadja Giesbrecht[1], Thomas Bein[1], Pablo Docampo[2], and Achim Hartschuh[1] — [1]Department Chemie und Center for Nanoscience (CeNS), LMU München, Deutschland — [2]School of Electrical and Electronic Engineering, Newcastle University, United Kingdom

Micro- and nanocrystalline methyl-ammonium lead-iodide (MAPI)-based thin film solar cells today reach power conversion efficiencies of up to 20%. We investigate the impact of grain boundaries on charge carrier transport in large crystal MAPI thin films using time-resolved photoluminescence (PL) microscopy and numerical model calculations. While long-ranged diffusive charge carrier transport is observed within single crystals, no transport occurs across the grain boundaries. The observed PL transients are found to crucially depend on the microscopic geometry of the crystal and the point of observation. Our experimental results show no quenching or additional loss channels due to grain boundaries for the studied material, which thus do not negatively effect the performance of derived thin film devices.

DS 25.7 Wed 18:00 H 0111

Nanoporous thin films of organic semiconductors for gas sensing applications — •Jean-Nicolas Tisserant, Wolfgang Kowalsky, and Robert Lovrincic — TU Braunschweig, Institut für Hochfrequenztechnik c/o InnovationLab, Speyerer Str. 4 69115 Heidelberg

Organic semiconducting devices could find applications in high added-value products such as efficient sensors for the detection of toxic gases.(1) Nanoporous morphologies are particularly interesting in this scope because they offer enhanced interfacial areas compared to the corresponding planar materials. Processes such as the diffusion of an analyte molecule to the active area of a gas sensor (2) may thus be improved proportionally to the amount of interface added. We propose to use nanoporous thin films of semiconductors in an organic field-effect transistor (OFET) for sensing of an endocrine disruptor in air. In the strategy that we follow, organic semiconducting molecules were self-assembled into nanoporous 2D films following a recently developed method.(3,4) These films were biased in an OFET configuration to build an indirect sensor in which the non-covalent interaction between a sensing dielectric and the target molecule modifies the electrical characteristics of the transistor.

References: (1)Zhang, C., Chen, P. & Hu, W. Chem. Soc. Rev. 44, 2087-2107 (2015); (2)Zhang, F., Qu, G., Mohammadi, E., Mei, J. & Diao, Y. Adv. Funct. Mater. 27, 17-20 (2017); (3)Tisserant, J. N. et al. RSC Adv. 6, 23141-23147 (2016); (4)Tisserant, J.-N. et al. ACS Appl. Mater. Interfaces 9, 27166-27172 (2017)

DS 26: Annual General Meeting of the Thin Films division

Annual Report

Time: Wednesday 18:30–19:30 Location: H 0111

60 min. break

DS 27: New Twists for Nanoquakes on a Chip - Emerging Applications of Surface Acoustic Waves in Condensed Matter Physics (Focussed Session): Session I

Surface acoustic waves (SAWs) with gigahertz frequencies and micrometre size wavelength can be elegantly generated using piezoelectric transducers fabricated with standard integrated circuit technology. Their small propagation velocity, tight surface confinement, as well as low susceptibility to decoherence and dissipation have been exploited over the past decades in numerous devices, in particular for electronic and optical signal processing. Today, the interaction of SAWs with electrical, optical, magnetic, and mechanical excitations in condensed matter is a highly active field of research. It is driven by the vision to harness the power of this technique in a broad spectrum of emerging applications including advanced sensors, the control of magnetization and collective excitations, as well as the coherent interactions between charge and spin excitations, photons, and phonons down to the fundamental level of single quanta. We propose a symposium that brings together experts for emerging and future applications of surface acoustic waves. For the proposed symposium we have identified potential speakers covering the large palette of fields which this versatile technique is successfully applied or currently evolving towards. These encompass nanoscale acousto-optic integrated circuits and plasmonics, the control of single quantum systems and collective excitations in hybrid systems. Because the proposed symposium covers a wide range of frontier research in which SAWs are employed with greatest success, it will serve as an ideal platform for scientific exchange. Thus, it aims to foster new interactions between the different scientific communities. Its most important goal is to introduce this exciting field of research to the many young Masters and PhD students, and postdocs attending the joint DPG-EPS Spring meeting and gives them the opportunity to present contributed talks at the symposium or associated sessions.

Organized by

Hubert Krenner, Universität Augsburg, Germany, hubert.krenner@physik.uni-augsburg.de

Jorge Pedros, Universidad Politécnica de Madrid, Spain, j.pedros@upm.es

Chris Ford, University of Cambridge, UK, cjbf@cam.ac.uk

Time: Thursday 9:30–13:15 Location: H 2032

Invited Talk DS 27.1 Thu 9:30 H 2032

Coupling RF-driven acoustic wave devices with nanocavity optomechanics — •Kartik Srinivasan, Marcelo Wu, Marcelo Davanco, and Krishna Balram — National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

Nanocavity optomechanical systems are being developed for a variety of sensing and signal transduction applications. Optomechanical crystal cavities, which co-localize optical modes within a photonic bandgap and mechanical modes within a phononic bandgap, have been of particular interest due to the strong interactions they support. Here, I will describe our efforts in connecting such devices to radio frequency (RF) waves, through the development of a piezoelectric cavity optomechanics platform. Frequency and time-domain characterization of devices within this platform will be presented, as will efforts to improve the overall efficiency of microwave-to-optical transduction.

Invited Talk DS 27.2 Thu 10:00 H 2032

Quantum Spin-Mechanics with Color Centers in Diamond — •Hailin Wang — Department of Physics, University of Oregon, Eugene, OR 97403, USA

Quantum acoustics is an emerging field focusing on interactions between acoustic waves and artificial atoms that can be exploited in quantum science. Acoustic waves propagate at a speed that is five orders of magnitude slower than the speed of light and couple to artificial atoms through mechanical processes, enabling a new paradigm for on-chip quantum operation and communication.

Among the various artificial atoms or qubits that have been explored, nitrogen vacancy (NV) color centers in diamond are of special interest because of their robust spin coherence and the ease with which these qubits can be measured and controlled. In this talk, I will discuss our recent experimental advance in coupling NV centers to surface acoustic waves (SAWs). By exploiting strain coupling to orbital degrees of freedom, we are able to induce strong and coherent spin-mechanical interactions with SAW amplitudes at only a fraction of a picometer. This platform opens a new avenue for experimental exploration of spin-based quantum acoustics, including quantum control of both spin and mechanical degrees of freedom.

Invited Talk DS 27.3 Thu 10:30 H 2032

Acoustic Traps and Lattices for Electrons in Semiconductors — Martin Schuetz[1,2], •Johannes Knörzer[1], Géza Giedke[3,4], Lieven Vandersypen[5], Mikhail Lukin[2], and Ignacio Cirac[1] — [1]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany — [2]Physics Department, Harvard University, Cambridge, MA 02318, USA — [3]Donostia International Physics Center, Paseo Manuel de Lardizabal 4, E-20018 San Sebastián, Spain — [4]Ikerbasque Foundation for Science, Maria Diaz de Haro 3, E-48013 Bilbao, Spain — [5]Kavli Institute of NanoScience, TU Delft, P.O. Box 5046, 2600 GA Delft, The Netherlands

We propose and analyze a solid-state platform based on surface acoustic waves (SAWs) for trapping, cooling and controlling (charged) particles, as well as the simulation of quantum many-body systems. We develop a general theoretical framework demonstrating the emergence of effective time-independent acoustic trapping potentials for particles in two- or one-dimensional structures. As our main example we discuss in detail the generation and applications of a stationary, but movable acoustic pseudo-lattice (AL) with lattice parameters that are reconfigurable in situ. We identify the relevant figures of merit, discuss potential experimental platforms for a faithful implementation of such an acoustic lattice, and provide estimates for typical system parameters. With a projected lattice spacing on the scale of about 100nm, this approach allows for relatively large energy scales in the realization of fermionic Hubbard models, with the ultimate prospect of entering the low-temperature, strong-interaction regime.

Invited Talk DS 27.4 Thu 11:00 H 2032

Manipulating single electrons on the fly using a sound wave — •Christopher Bauerle — Institut Neel, CNRS Grenoble

Surface acoustic waves (SAW) provide a promising platform to realize quantum optics experiments with electrons at the single particle level. Earlier single-shot experiments have shown SAW-assisted electron transport between spatially separated quantum dots over a distance of 4 μm with an efficiency of about 92 % [1,2]. Here we go an important step further. We couple two quantum channels by a tunnel barrier along a region of 2 μm. At the ends of each channel respectively a quantum dot is placed serving as single electron source and detector. We demonstrate single electron transport over a distance of 22 μm with extremely high efficiency above 99 %. Changing the energy detuning in the coupling region we can partition the electron on-demand into two paths. By gradually changing the barrier height

we additionally observe tunnel oscillations of the probability that the electron ends up at the upper or the lower detector quantum dot. This finding demonstrates coherent manipulation of the electron quantum state on the fly. Our results pave the way for the implementation of a solid state flying qubit having high relevance in fundamental research and quantum information technology.

[1] Hermelin et al., Nature 477, 435-438 (2011) [2] McNeil et al., Nature 477, 439-442 (2011)

15 min. break.

DS 27.5 Thu 11:45 H 2032

Surface acoustic wave modulation of a coherently driven quantum dot in a pillar microcavity — •Bruno Villa[1,2], Anthony J. Bennett[1], David J. P. Ellis[1], James P. Lee[1,3], Joanna Skiba-Szymanska[1], Thomas A. Mitchell[2], Jonathan Griffiths[2], Ian Farrer[2], David A. Ritchie[1], Christopher J. B. Ford[2], and Andrew J. Shields[1] — [1]Toshiba Research Europe Limited, Cambridge Research Laboratory, 208 Cambridge Science Park, Milton Road, Cambridge CB4 0GZ, United Kingdom — [2]Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — [3]Engineering Department, University of Cambridge, 9 J. J. Thomson Avenue, Cambridge, CB3 0FA, United Kingdom

In this work we demonstrate the generation of a high-frequency pulsed single-photon stream. A quantum dot embedded in a pillar microcavity efficiently scatters photons when driven coherently with a narrow-band continuous wave laser. Simultaneously, the transition energy is periodically tuned by a surface acoustic wave (SAW) propagating along the substrate at 1 GHz. The combined action of the light and strain fields on the quantum dot yields a periodic signal displaying anti-bunching. In addition we are able to resolve multiple phonon sidebands in the emission spectrum.

DS 27.6 Thu 12:00 H 2032

Surface acoustic wave regulated single photon emission of a coupled quantum dot-nanocavity system — •Matthias Weiss[1], Stephan Kapfinger[1], Thorsten Reichert[2], Jonathan Finley[2], Achim Wixforth[1], Michael Kaniber[2], and Hubert Krenner[1] — [1]Lehrstuhl für Experimentalphysik 1, Universität Augsburg, 86159 Augsburg, Germany — [2]Walter Schottky Institut, TU München, 85748 Garching, Germany

Here we report on a coupled quantum dot-nanocavity system in the weak coupling regime, that is dynamically tuned by the coherent elastic field of a $f_{SAW} \cong 800\,\mathrm{MHz}$ surface acoustic wav (SAW).[1] The SAW induced strain fields lead to a dynamic modulation of the cavity resonance by a combination of mechanical deformation and photo-elastic coupling and of the QD by deformation potential coupling. These effects lead to a dynamical tuning of the energy splitting between the single QD and the cavity. By applying a phase locked stroboscopic laser excitation scheme and the use of time and spectral resolved detection the SAW induced modulation of the interaction can be observed. These measurements show clearly a spectral resonance between QD and cavity at a well defined time during the acoustic cycle and the resulting increase of the QD-cavity interaction by the Purcell effect. This leads to a precisely timed single photon emission as confirmed by a direct measurement of the second order photon correlation function, $g^{(2)}$, at the resonance.

[1] M. Weiß et al., Appl. Phys. Lett. 109, 033105 (2016)

DS 27.7 Thu 12:15 H 2032

Development of a SAW-driven source of single photons — •A. Rubino[1], T-K Hsiao[1], Y. Chung[1], S-K Son[1], H. Hou[1], A. Nasir[2], J Pedros[3], R. T. Phillips[1], G. Éthier-Majcher[1], M. Stanley[1], M. Atatüre[1], K. Niang[1], G. Rughoobur[1], A. Flewitt[1], T. Mitchell[1], J. P. Griffiths[1], I. Farrer[1], D. A. Ritchie[1], and C. J. B. Ford[1] — [1]U. of Cambridge — [2]The National Physical Laboratory (NPL) — [3]Universidad Politécnica de Madrid

We have developed devices in which both electrons and holes can be induced in an undoped GaAs/AlGaAs well by gates to form a lateral n-i-p junction. SAWs, generated by a transducer, collect electrons in the n-region and transport them into the p-region where they recombine with holes. If the stream is composed of single electrons, the recombination with holes should produce a stream of single photons We observe light emission in DC forward bias when the voltage applied is above the flat- band condition. Alternatively, we can bias the junction 100 mV below the flat-band condition, so that no current flows until a 1 or 3 GHz SAW drives a current and light emission, by pumping electrons over the hill in the intrinsic region. We have characterised this SAW-driven electroluminescence in the regime where less than one electron is transported per cycle on average. Time-resolved electroluminescence has been used to extract the electron recombination time and to quantify the contributions from electromagnetic crosstalk and the SAW. In a device without significant crosstalk, the degree of second-order coherence, g2(0), was measured using a Hanbury Brown and Twiss interferometer, and it shows the signature of antibunching.

DS 27.8 Thu 12:30 H 2032

SAW Transducers with Gouy Phase Adjustments for Minimal Beam Waist — •Madeleine Msall[1,2] and Paulo Santos[2] — [1]Bowdoin College, Brunswick, USA — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, DE

High frequency surface acoustic waves can effectively probe and control low-dimensional electron systems. SAW provide localized control of band structure through dynamic strain coupling that can be exploited for switching applications or to drive transport. Applications that rely upon SAW coupling to quasi 0-D systems (e.g., quantum dots) require highly tuned SAW cavities with near-field focusing transducers. IDTs are formed by electrode fingers placed on lines of equal phase, requiring pattern correction for both material anisotropy and the expected Guoy phase shift for a Gaussian beam. [1] Our models show that appropriate pattern adjustments can provide significant enhancement of local strain in sub-wavelength focal spots without frequency broadening. These model improvements inspire new strategies for creating high-Q cavities with optimized coupling between phonons and qubits.

[1] Holme, et al. 2003 DOI.org/10.1063/1.1590405

DS 27.9 Thu 12:45 H 2032

Multi-harmonic quantum dot optomechanics in fused $LiNbO_3$-(Al)GaAs hybrids — •Emeline Nysten[1,2], Yong Heng Huo[3,4], Hailong Yu[5], Guo Feng Song[5], Armando Rastelli[3], and Hubert J. Krenner[1,2] — [1]Lehrstuhl für Experimentalphysik 1, Universität Augsburg, Augsburg, Germany — [2]Nanosystems Initiative Munich (NIM), München, Germany — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler Universität Linz, Linz, Austria — [4]University of Science and Technology of China, Shanghai, China — [5]Chinese Academy of Sciences, Beijing, China

Surface acoustic waves (SAW) are used to control the emission of quantum dots (QDs) and, in particular, SAWs enable the injection of charge carriers into the dot or the modulation of their energy levels [1,2,3]. Here we explore the possiblility to enhance the interaction between the SAW and epitaxial GaAs QDs by tranferring them on a strong piezoelectric $LiNbO_3$ substrate by epitaxial lift-off [4]. By employing multi-harmonic transducers, we generated sound waves on $LiNbO_3$ over a wide range of radio frequencies. We monitored their coupling to and propagation across the semiconductor membrane, both in the electrical and optical domain. We demonstrate the enhanced optomechanical tuning of the embedded quantum dots with increasing frequencies. This effect was verified by finite element modelling of our device geometry and attributed to an increased localization of the acoustic field within the semiconductor membrane. References: [1]Appl.Phys.Lett. **93**, 081115 (2008), [2]Nano Lett. **10**, 3399-3407 (2010), [3]Phys.Rev.B **88**, 085307 (2013), [4]Appl.Phys.Lett. **106**, 013107 (2015)

DS 27.10 Thu 13:00 H 2032

Zero-group-velocity acoustic waveguides for high-frequency resonators — •Muhammad Hamidullah and Cinzia Caliendo — Institute of Photonics and Nanotechnologies, IFN-CNR, Via Cineto Romano 42, 00156 Rome, Italy

Zero group velocity (ZGV) Lamb-like modes resonator based on a silicon-on-insulator (SOI)/AlN suspended thin film was simulated to design high-frequency electroacoustic resonators that do not require metal strip gratings or suspended edges to confine the acoustic energy. The electroacoustic standing wave can be obtained with only one interdigital transducer (IDT) and no reflectors, thus reducing both the device size and the technological complexity. The ZGV resonant conditions in the SOI/AlN composite plate, i.e. the frequencies where the mode group velocity vanishes while the phase velocity remains finite, were investigated in the frequency range from few hundreds of MHz up to 1900 MHz with the wavelength range from 50 um to 22 um. Phase velocity at ZGV resonant condition (>15000m/s) is higher than bulk longitudinal phase velocity. By reducing the film thickness and the wavelength in sub-micrometer range, ultra-high frequency resonator

with a resonant frequency higher than 10 GHz can be achieved. Furthermore, as the energy is locally trapped in the source area, these modes are expected to be highly sensitive to the plate thickness and mechanical properties changes, therefore, can be exploited for sensing application.

Keyword: Lamb wave, thin film, zero group velocity, SOI, AlN

DS 28: 2D materials: Chalcogenides II (joint session HL/DS)

Time: Thursday 9:30–13:15 Location: A 151

DS 28.1 Thu 9:30 A 151

Excitation-induced transition from direct to indirect band gaps in monolayer TMDCs — •Daniel Erben[1], Alexander Steinhoff[1], Tim Wehling[1,2], Christopher Gies[1], and Frank Jahnke[1] — [1]Insitute for Theoretical Physics, University of Bremen, Germany — [2]Bremen Center for Computational Materials Science, University of Bremen, Germany

Monolayer transition metal dichalcogenides (TMDCs) are atomically thin semiconductors with a direct band gap, which allows their use as active material in optoelectronic devices. Often photoluminescence or photoemission spectroscopy experiments are employed for the characterization of TMDCs. Via laser pulse excitation these methods provide excited charge carriers that populate the valleys of the band structure. The Coulomb interaction of these excited carriers causes strong many-body renormalizations in the band structure, which consequently shift the valleys and the excitonic resonances by several hundred meV.
In this talk we give detailed insight into the many-body effects in monolayer MoS_2, $MoSe_2$, WS_2 and WSe_2 by evaluating the semiconductor Bloch equations including DFT-band structures and interaction-matrix elements. This provides a precise description for the interplay of the Coulomb interaction with the electron and hole populations. We describe the impact of these effects on the K- and Σ-valley in the band structure. Our calculations show a clear tendency to a direct-to-indirect band gap transition due to the renormalizations. Being reminiscent of the effect of strain on monolayers, this transition should also lead to a quenching of the photoluminescence.

DS 28.2 Thu 9:45 A 151

Microscopic description of localized quantum-dot-like states in MoS2 nanobubbles — •Christian Carmesin, Matthias Florian, Michael Lorke, Daniel Erben, and Frank Jahnke — Institute for Theoretical Physics, University of Bremen, Germany

Atomically thin layers of transition metal dichalcogenides (TMDCs) have emerged as a new class of optically active materials with recent applications reaching into the quantum-information technologies. The systematic engineering of local confinement potentials opens the possibility of the deterministic generation of single-photons. A possible platform are TMDC nanobubbles that develop if air is enclosed during the stacking of layers. We report on results of atomistic tight-binding calculations of different sizes and height-to-diamter ratios of these nanostructures and show that the formation of confined quantum-dot-like single-particle states is caused by an interplay of strain and dielectric screening.

DS 28.3 Thu 10:00 A 151

Optical properties of TMDC semiconductors in the 1,55μm telecom wavelength range — •Michael Lorke and Frank Jahnke — Institute für theoretische Physik, Universität Bremen

In the context of the current interest in atomically thin semiconductors, we study optical properties of highly excited and/or highly doped transition-metal dichalcogenides (TMDCs). We show that under such excitation conditions, transitions between the first and higher conduction bands are possible. These transitions are analogous to intersubband transitions in conventional quantum well devices. In this work we discuss the carrier density and temperature dependence of such transitions and show that they can be tuned into the technologically relevant 1,55μm telecom wavelength range. This opens the possibility to utilize TMDCs in novel devices ranging from quantum cascade lasers to novel infra-red photodetectors.

DS 28.4 Thu 10:15 A 151

Coupling of a monolayer of WSe2 to an InGaP bullseye cavity — •Oliver Iff[1], Vasilij Baumann[1], Monika Emmerling[1], Marcelo Davanco[2], Kartik Srinivasan[2], Sven Hoefling[1,3], and Christian Schneider[1] — [1]Technische Physik, Universitaet Wuerzburg, Am Hubland, Wuerzburg, Germany — [2]Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, Maryland, U.S.A. — [3]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, UK

Photonic cavities based on circular gratings can be used to enhance the emission of optically active materials. Here, we investigate the optical properties of such a cavity consisting of centric rings of InGaP which are completely surrounded by air, forming a floating membrane. The characterization was done via photoluminescence measurements using embedded quantum dots as light source and spatially mapping out the near field emission. Strikingly, the grating membrane can also be transferred via the dry-stamp method onto a given substrate without disturbing its optical modes and therefore opening up new ways of building coupled systems. Furthermore, the structures are optimized for wavelengths near 750nm, making it suitable for coupling to different kinds of 2D materials like WSe2 or MoSe2. A monolayer of WSe2 has been transferred onto the cavity showing improved photoluminescence of the charged exciton right at the centre position. This enables a new path to couple monolayer of 2D materials to photons in order to gain access to quantum electrodynamic effects including strong light-matter coupling.

DS 28.5 Thu 10:30 A 151

Exciton-phonon coupling in mono- and bilayer $MoTe_2$ — •Sophia Helmrich[1], Robert Schneider[2], Alexander W. Achtstein[1], Ashish Arora[2], Bastian Herzog[1], Steffen Michaelis de Vasconcellos[2], Mirco Kolarczik[1], Oliver Schöps[1], Rudolf Bratschitsch[2], Ulrike Woggon[1], and Nina Owschimikow[1] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany — [2]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany

We investigate excitonic transitions of mechanically exfoliated monolayer and bilayer molybdenum ditelluride ($MoTe_2$) by temperature-dependent photoluminescence spectroscopy. Based on identical scaling of the excitonic optical bandgap and the integrated area of the emission with temperature we conclude that ML and BL $MoTe_2$ have similar band alignment and excitonic behavior. Our experiments show that for identical excitation laser power the bilayer yields twice the intensity as the monolayer unlike for other transition metal dichalcogenides. From the emission lines we extract key parameters for exciton-phonon coupling processes demonstrating an unusually small coupling with acoustical phonons of $\gamma_{\mathrm{LA}} = (28 \pm 4)\,\mu\mathrm{eV\,K^{-1}}$ and $(14 \pm 4)\,\mu\mathrm{eV\,K^{-1}}$ for ML and BL $MoTe_2$, respectively, where the interactions with longitudinal optical phonons of $\Gamma_{LO} = (40.1 \pm 5.6)$ meV ((86.4 ± 12.6) meV) for ML (BL) $MoTe_2$ are comparable to values of other TMDs. These observations make $MoTe_2$ an attractive and robust material with a large luminescence yield for applications in the technically relevant near-infrared region.

DS 28.6 Thu 10:45 A 151

Giant Gap-Plasmon Tip-Enhanced Raman Scattering of MoS2 Monolayers on Au Nanocluster Arrays — •Mahfujur Rahaman[1], Alexander G. Milekhin[2,3], E. E. Rodyakina[2,3], A. V. Latyshev[2,3], Volodymyr M. Dzhagan[1,4], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107, Chemnitz, Germany — [2]Novosibirsk State University, Pirogov 2, 630090, Novosibirsk, Russia — [3]Rzhanov Institute of Semiconductor Physics RAS, Lavrentiev Ave. 13, 630090, Novosibirsk, Russia — [4]V. Lashkaryov Institute of Semiconductors Physics, Nat. Acad. of Sci. of Ukraine, 03028, Kyiv, Ukraine

We present the results on a gap-plasmon tip-enhanced Raman scattering study of MoS2 monolayers deposited on a periodic array of Au nanostructures on a silicon substrate forming a two dimensional (2D) crystal / plasmonic heterostructure. We observe a giant Raman enhancement of the phonon modes of the MoS2 monolayer located in a plasmonic gap between Au tip apex and Au nanoclusters. Tip-enhanced Raman (TER) mapping allowed us to determine the gap-

plasmon field distribution responsible for the formation of hot spots. These hot spots provided an unprecedented giant Raman enhancement of 5.6 * 108 and a spatial resolution as small as 2.3 nm at ambient conditions. Moreover, due to strong hot electron doping in the order of 1.8 * 1013 cm-2, we observed a structural change of MoS2 from 2H to 1T phase. Thanks to the very good spatial resolution, we were able to spatially resolve those doping sites. Our results open the perspectives of optical diagnostics in nanoscale for many other 2D materials.

DS 28.7 Thu 11:00 A 151

Doping dependent photoluminescence of ML WSe2 — Jhih-Sian Tu, •Sven Borghardt, Detlev Grützmacher, and Beata Kardynał — Peter Grünberg Institute 9 (PGI-9), Forschungszentrum Jülich, Germany

While free exciton states of monolayer transistion meatal dichalcogenides are well understood, photoluminescence spectra of WSe_2 contain number of low energy features that are not understood and collectively referred to as localized states. Such signal is not observed in spectra of materials with the lowest energy state being bright for example in the spectra of monolayer MoSe_2. In order to shed light on the origin of the sub-bandgap emission from WSe_2, we measured low temperature photoluminescence at a very wide range of both electron and hole doping levels. The spectra appear rich in structure which is very strongly doping dependent. The spectral, polarization and spatial correlations between the long wavelength emission features with the signal from the recombination of the bright exciton and trion states are consistent with the brightening of momentum-dark states either by phonon-mediated processes or by interactions of excitons with electrons or plasmons. Unexpectedly, while majority of the spectral features share polarization properties of excitons and trions, some show cross-polarization with the excitation laser.

15 min. break.

DS 28.8 Thu 11:30 A 151

Effective theory of monolayer TMDC double quantum dots — •Alessandro David, Andor Kormányos, and Guido Burkard — Department of Physics, University of Konstanz, D-78464, Germany

Monolayer Transition Metal Dichalcogenides (TMDCs) are promising candidates for the creation of quantum dots, because they are truly two-dimensional semiconductors with a direct band gap. One of their features is an intrinsic spin-orbit interaction that splits the spins in the conduction and valence band. In this work, we analyse theoretically the behaviour of a double quantum dot (DQD) system created in the conduction band of these materials, with two electrons in the regime of the (1,1) charge configuration. Motivated by recent experimental progress, we consider several scenarios, such as when the spin splitting is different in the two dots or when the the valley degeneracy in the TMDC is removed due to a ferromagnetic insulator substrate. Finally, we discuss in which cases it is possible to reduce the low energy subspace to the lowest Kramer's pairs, where novel interactions appear.

DS 28.9 Thu 11:45 A 151

transport properties of high-quality ultrathin two-dimensional superconducting Mo2C crystals and Heterostructures — •n. kang[1], l.b wang[1], c. xu[2], s. song[1], and w.c. ren[2] — [1]Peking University, Beijing, P. R. China. — [2]Institute of Metal Research, Shenyang, P. R. China.

There is particularly interesting in the studies on highly crystalline 2D superconductors. Recently, we have obtained high-quality ultrathin Mo2C crystals and graphene/Mo2C heterostructures by means of chemical vapor deposition method [1-3]. Here, we report on transport measurements on superconducting Mo2C crystals and heterostructures in the 2D limit. We observe magnetoresistance (MR) oscillations and negative MR at low magnetic fields for temperature far below superconducting transition temperature[2,3]. We discuss that these anomalous behaviors can be understood quantitatively by including the effects of inhomogeneous superconducting phase and quantum fluctuations. For graphene/ Mo2C heterostructures, we demonstrate the realization of highly transparent Josephson junction devices based on these strongly coupled heterostructures[3].

[1]. C. Xu, L. B. Wang, Z. B. Liu, L. Chen, J. K. Guo, N. Kang*, X, L. Ma, H. M. Cheng, and W. C. Ren*, Nature Mater, 14, 1135(2015).

[2] L. B. Wang, C. Xu, Z. B. Liu, L. Chen, X, L. Ma, H. M. Cheng, W. C. Ren*, and N. Kang*, ACS NANO, 10, 4504(2016).

[3] C. Xu, S. Song, Z. B. Liu, L. Chen, L. B. Wang, D. X. Fan, N. Kang*, X, L. Ma, H. M. Cheng, and W. C. Ren*, ACS NANO, 11, 5906 (2017).

DS 28.10 Thu 12:00 A 151

Nanoplatelets - a material system between strong confinement and weak confinement — •Marten Richter — Institut für Theoretische Physik, Technische Universität Berlin, Germany

Recently grown CdSe Nanoplatlets are often described to have a similar electronic structure as two-dimensional quantum wells and are promoted as colloidal quantum wells with monolayer precision width. Here we show, that nanoplatelets are not ideal quantum wells, but cover (depending on their size a strong confinement) an intermediate and a Coulomb interaction dominated regime [1]. For the analysis we show results from a solution of the full four dimensional exciton wave function and analyze different confinement regimes.

[1] Phys. Rev. Materials 1, 016001 (2016)

DS 28.11 Thu 12:15 A 151

Giant magnetic splitting inducing near-unity valley polarization in van der Waals heterostructures — •Philipp Nagler[1], Mariana V. Ballottin[2], Anatolie A. Mitioglu[2], Fabian Mooshammer[1], Johannes Holler[1], Jonas Zipfel[1], Michael Kempf[1], Nicola Paradiso[1], Christoph Strunk[1], Rupert Huber[1], Alexey Chernikov[1], Peter C. M. Christianen[2], Christian Schüller[1], and Tobias Korn[1] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]High Field Magnet Laboratory (HFML), Radboud University, The Netherlands

Atomically thin van der Waals heterostructures enable solid-state systems in the ultimate thickness limit. Type II band alignment of transition metal dichalcogenides (TMDCs) leads to the formation of interlayer excitons, which stem from spatially separated electron-hole pairs. These species are highly promising for future valleytronic devices since they combine ultra-long lifetimes with the peculiar spin-valley physics of the constitutent monolayers. Here, we demonstrate strong magnetic coupling of interlayer excitons in a $WSe_2/MoSe_2$ heterostructure to an external magnetic field up to 30 T. The observed g factor of -15 by far exceeds typical values of the g factor in TMDC monolayers and enables near-unity valley polarization of long-lived interlayer excitons at high fields. Our findings can be made plausible by taking into account the AB-stacking configuration of the heterostructure where K+ and K− valleys align in momentum space, leading to spin-allowed inter-valley optical transitions.

DS 28.12 Thu 12:30 A 151

Effective passivation of ultra-thin layers of InSe to enhance electrical properties — •Himani Arora[1,2], Younghun Jung[3], Sanghoon Chae[3], Daniel Rhodes[3], Ghidewon Arefe[3], Takashi Taniguchi[4], James Hone[3], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Department of Mechanical Engineering, Columbia University, New York, NY, 10027, USA — [4]Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

We report electrical properties of ultrathin layers of Indium Selenide (InSe), a member of the III-VI chalcogenides family, which has shown a mobility two orders of magnitude higher than MoS2, alongside better stability than black phosphorus.

InSe has light electron effective mass and high mobility enabling its usage for fast, high performance electronics. State-of-the-art InSe transistors reported so far, consist of 6 nm thick InSe flake contacted using graphene edge contacts and reaching a mobility of 1500 cm2V-1s-1 at RT in top-gate configuration. However, InSe being an air-sensitive material loses its conductance over time, resulting the transistor to become unfunctional.

In this study, we report an InSe-based transistor fully encapsulated in h-BN layers which enhanced its electrical properties compared to an un-encapsulated device. The transistor reached a high Hall mobility at RT, while retaining its performance for a long period of time.

DS 28.13 Thu 12:45 A 151

Impact of layer separation on the optoelectronic properties of van der Waals heterostructures — •Malte Hartmann[1], Matthias Florian[1], Alexander Steinhoff[1], Frank Jahnke[1], Julian Klein[2], Alexander Holleitner[2], Jonathan Finley[2],

Tim Wehling[1], Michael Kaniber[2], and Christopher Gies[1] — [1]Institut für theoretische Physik, Bremen, Deutschland — [2]Walter Schottky Institut, München, Deutschland

Dielectric screening plays an important role in the field of atomically thin transition-metal dichalcogenides (TMDs) and van der Waals heterostructures consisting of stacked 2D-materials. In each layer the field lines of the Coulomb interaction are screened by the adjacent material, which reduces the single-particle band gap as well as binding energies of exciton complexes and can be used to tailor the optoelectronic properties. By combining an electrostatic model for a dielectric hetero-multi-layered environment with semiconductor many-particle methods, we demonstrate that the electronic and optical properties are sensitive to the interlayer distances on the atomic scale. Spectroscopical measurements in combination with a direct solution of a three-particle Schrödinger equation reveal trion binding energies that correctly predict recently measured interlayer distances.

DS 28.14 Thu 13:00 A 151

Band Gaps and Carrier Relaxation in Thin Films of ZrS_3 — •Christopher Belke[1], Sonja Locmelis[2], Johannes C. Rode[1], Hennrik Schmidt[1], Bastian Hoppe[2], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

New varieties of two-dimensional crystals [1] are currently getting into focus of the material sciences. An example for such layered materials are Transition Metal Trichalcogenides. Here we study the compound ZrS_3: bulk crystals were synthesized by chemical gas transport; stoichiometry and structure were verified by powder X-ray diffractometry and energy-dispersive X-ray spectroscopy (EDX), and analyzed by absorption measurements. The latter indicate an indirect bandgap of about 1.8 eV and a direct bandgap of 2.3 eV, which differ slightly from literature values [2, 3]. Thin flakes are exfoliated and contacted. Conductivity measurements are investigated in response to illumination with LEDs of different wavelengths. We observe a pronounced rise in conductivity between 2.1 eV and 2.4 eV which is in good agreement with the direct bandgap found in the absorptions measurements. Measurements of charge carrier relaxation are described by a power-law dependence and reveal unexpectedly long relaxation times.

[1] A. K. Geim, I. V. Grigorieva, Nature 499, 419-425 (2013).
[2] M. Abdulsalam, D. Joubert, Eur. Phys. J. B. 88, 177 (2015).
[3] Y. Jin, X. Li, J. Yang, Phys. Chem. Chem. Phys. 17, 18665 (2015).

DS 29: Lithography III: Lithography and Structuring (joint session KFM/DS)

While high-resolution 2D lithography and structuring is relatively mature and also widely applied in industrial processes, work on its 3D variant is mostly focusing on fundamental aspects and process development. At the lower edge of possible 3D feature dimensions, certainly methods such as electron beam induced deposition, non-linear multi-photon-laser lithography and thermal scanning probe lithography techniques are required. This session discusses most of these dedicated 3D methods in detail. For the fabrication of complex 2D and 2.5D patterns, advanced electron beam and X-ray methods are continuously developed further. In addition, new methods such as high resolution Talbot lithography for relatively large areas are already entering industrial maturity. This session also discusses some of the latest developments in this field of binary lithography.

Organizer: Robert Kirchner - Technische Universität Dresden

Time: Thursday 9:30–12:50 Location: EMH 025

Invited Talk DS 29.1 Thu 9:30 EMH 025

3D Nanoprinting via Focused Electron Beams — •Harald Plank[1,2], Robert Winkler[1,2], Jason Fowlkes[3,4], and Philip Rack[3,4] — [1]Institute for Electron Microscopy and Nanoanalysis Graz University of Technology, 8010 Graz, Austria — [2]Graz Centre for Electron Microscopy, 8010 Graz, Austria — [3]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — [4]Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee 37996, USA

3D-printing of functional structures has emerged to an important technology in research and development. While being reliable on the micro and sub-micron scale, it becomes very challenging when aiming for nano-sized geometries. Among the very few direct-write techniques on that scale, Focused Electron Beam Induced Deposition is one of the promising candidates as this technology has recently done tremendous steps forward. In particular, this technology allows additive fabrication of complex, freestanding 3D nano-architectures on almost any material and surface morphology, which enables entirely new 3D nano-applications (e.g. plasmonics, artificial spin-ice or nano-probes). The contribution starts with an introduction of FEBID and sheds light on recent progress, which leverages this technology from a scientifically oriented fabrication tool into the status of a reliable and predictable 3D-nanoprinter. In the following, several applications are discussed to demonstrate the new possibilities of this generic fabrication technology. Finally, the talk gives an overview of ongoing activities together with future perspectives beyond current limitations.

DS 29.2 Thu 10:00 EMH 025

3D printing at the diffraction limit: sample injection for time-resolved serial crystallography — •Michael Heymann — MPI of Biochemistry, Am Klopferspitz 18, 82152 Martinsried

Continuous injection using the Gas Dynamic Virtual Nozzle (GDVN) is a proven sample delivery method for biological imaging using X-ray free-electron lasers. However, many important aspects of GDVN functionality have yet to be thoroughly understood and/or refined due to fabrication limitations. We report the application of 2-photon polymerization as a form of high-resolution 3D printing to fabricate GDVNs with submicron resolution. This allows rapid prototyping of a wide range of nozzle designs from standard CAD drawings to iteratively optimize crucial dimensions for optimal performance. To understand enzyme catalysis and protein conformational changes at the atomic scale, we pioneered mixing-injectors for time-resolved structural biology to record molecular movies of substrate turn-over. We experimentally validate 3D print accuracy, as well as fluid mixing dynamics using X-ray tomographic imaging. We developed mixing-injectors to mix nanocrystals with substrate and to subsequently deliver them into the X-ray interaction region just milliseconds after mixing. This method can determine the structures of transient states and thereby kinetic mechanisms. In a proof of principle experiment, we could follow the catalytic reaction of the M. tuberculosis β-lactamase with the 3rd generation antibiotic ceftriaxone by time-resolved serial crystallography with millisecond to second time resolution at 2Å spatial resolution.

DS 29.3 Thu 10:20 EMH 025

Fabrication of superior 2D and 3D nano-devices using NanoFrazor lithography — Colin Rawlings[1], Armin Knoll[2], Felix Holzner[1], and •Zhengming Wu[1] — [1]SwissLitho AG, Zurich, Switzerland — [2]IBM Zurich, Switherland

Thermal scanning probe lithography (t-SPL) has recently entered the lithography market as first true alternative or extension to electron beam lithography (EBL). The first dedicated t-SPL systems, called NanoFrazor, have been installed at research facilities in Europe, America, Asia and Australia by the company SwissLitho.

The application range for this new nanofabrication capability is broad and will be demonstrated with the discussion of a selection of examples. Applications that are enabled by the nm-precise 3D patterning include 3D phase plates and finely tuned coupled Gaussian optical microcavities. Furthermore, 3D shaped nanofluidic confinements

have been used to precisely control the movement of nanoparticles and nanowires. The high resolution 2D capability was applied e.g. to shape complex plasmonic structures. Furthermore, several superior nanoelectronic devices will be shown. Such devices are predominantly made from randomly dispersed nanowires or 2D materials. Therefore, they benefit strongly from the unique markerless overlay capability of the NanoFrazor lithography, but also from the fact that actually no charged particle beam is used during lithography, which can often damage sensitive materials. Finally, a few examples are shown, how the heated tips are also used for direct modification of surfaces by triggering of a local phase change or a chemical reaction.

DS 29.4 Thu 10:40 EMH 025

Innovations in photoresists and photopolymers for 2D / 3D micro and nano fabrication — •Anja Voigt, Christine Schuster, Jan Klein, Arne Schleunitz, and Gabi Grützner — micro resist technology GmbH, Koepenicker Str. 325, 12555 Berlin, Germany

Different methods for the manufacture of high resolution 2D and 3D features require a wide range of material solutions based on innovative photoresists and photopolymers. As a commercial resist supplier, micro resist technology aims at providing such solutions tailored for diverse lithography processes, comprising both materials and technology support. The following highlights will be presented:

E-beam lithography is a versatile patterning method for the generation of high resolution nano-patterns. Combining stepwise greyscale exposure and pattern reflow with a positive tone resist results in greyscale patterns of small dimensions.

Greyscale UV lithography of up to 100 micron thick resist films, either by direct laser writing or by conventional mask aligner exposure and a greyscale mask, can generate very deep greyscale micro-patterns. Both very thick films, and considerably smaller pattern features including sharp tips have been successfully fabricated using this technique.

Laser interference lithography is another method which allows the manufacture of nanoscale patterns * periodic patterns even on very large substrates. Whereas two photon absorption (2PA) allows the generation of real 3D patterns at micro and nanoscale.

The development of photoresist and photopolymer materials tailored to meet the requirements of the specific technologies will be presented.

20 min. break

Invited Talk DS 29.5 Thu 11:20 EMH 025

Diffractive X-ray Optics for Synchrotrons and Free Electron Lasers - a challenge from the lithographer's point of view — •Christian David — Paul Scherrer Institut, Villigen, Switzerland

X-rays are excellent probes for the investigation of matter using scattering, imaging and spectroscopic techniques, offering high penetration capability, spatial and temporal resolution, along with elemental and chemical sensitivity. Accelerator-based photon sources play a key role in these analytical techniques as they offer beams with unique brilliance.

This presentation will give an overview on developments of x-ray instrumentation and experimental techniques based on diffractive optics. These optical elements are designed for short wavelength radiation ranging from the vacuum ultraviolet to hard x-rays and play a key role in the shaping, direction, and detection for a variety of experiments. The key challenges lie in the fabrication of the diffractive structures by advanced nanolithography techniques, as they need to provide dimensions and placement accuracies down to the nanometer scale.

Many applications of these devices include x-ray imaging techniques. The x-ray optics developed at PSI provide spatial resolution down to the 10 nm range, and are designed exploit phase contrast mechanisms or spectroscopic information. Moreover, recent developments of optics for beam splitting and the manipulation of x-ray wave fronts open up new opportunities for time resolved measurements of ultra-fast processes at x-ray lasers.

DS 29.6 Thu 11:50 EMH 025

A high contrast multilayer process for electron beam lithography using different developers — •Philip Trempler[1], Frank Heyroth[2], Matthias Schirmer[3], Christian Kaiser[3], Tobias Mai[3], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther Universität Halle-Wittenberg 06099 Halle (Saale), Germany — [3]ALLRESIST GmbH, Am Biotop 14, 15344 Strausberg, Germany

We have developed a new multilayer resist system for the fabrication of three-dimensional nanostructures in a one-step electron beam exposure. The multilayer resist consists of three layers with different sensitivity and different process chemistry. The sensitivity of the three layers to different respective developers allows a very large controllable undercut in the middle layer. The low sensitivity bottom layer can be patterned in high detail almost independent from the pattern exposed in the two layers on top. At acceleration voltage of 30 kV the resist is ideally suited for the fabrication of for example T-gate structures by lift-off in a high reliability process with a very large process window.

DS 29.7 Thu 12:10 EMH 025

Fabrication of metal nanostructures with focused X-rays — •Andreas Späth, Florian Vollnhals, Fan Tu, Hubertus Marbach, and Rainer H. Fink — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen, Germany

Focused X-ray beam induced deposition (FXBID) is a novel technique for the fabrication of metallic nanostructures by illuminating gas phase precursors with focused soft X-rays in a zone plate based scanning transmission X-ray microscope (STXM). With this technique we have been able to produce localized Co and Mn nanostructures with growth rates and purity competitive with electron beam induced deposition (EBID) [1,2]. We demonstrate that our approach exhibits significant selectivity with respect to incident photon energy leading to enhanced deposition for resonant excitation of the precursor molecule. This finding opens a new field of photon energy selective deposition from precursor mixtures and deposition from various precursors within one production cycle. The impact of several deposition parameters on the growth rate, such as illumination time and precursor pressure are discussed with respect to a deeper understanding of deposition processes and optimization of the procedure. Furthermore, we discuss routes to the formation of magnetic deposits by in-situ cleaning techniques (e.g., co-dosing of reactive gases or annealing). The project is funded by the BMBF (05K16WED).

[1] A. Späth et al., RSC Advances, 2016, 6, 98344.
[2] F. Tu et al., J. Vac. Sci. Technol. B, 2017, 35(3), 031601.

DS 29.8 Thu 12:30 EMH 025

Printing Uniform Periodic Structures over Large Areas with Displacement Talbot Lithography — •Harun Solak — EULITHA AG, 5416 Kirchdorf, Switzerland

High-resolution periodic patterns such as linear gratings or two-dimensional arrays are required in many applications. This is especially true in photonics, where optimized interaction of light with periodic nanostructures enables creation of new or higher performance devices such as LEDs, lasers, photovoltaic cells, sensors and LCD screens. In such applications, patterns with periodicity approximately in the 0.1-1micrometer-range need to be printed on device surfaces. Current lithographic methods face significant challenges in terms of technical feasibility or cost in meeting the requirements. The recently introduced Displacement Talbot Lithography (DTL) method allows uniform printing of periodic patterns in a non-contact, proximity scheme [1]. The technique enables patterning on non-flat surfaces and in thick photoresist films up to the highest resolution possible at a given exposure wavelength. Photolithography systems specially designed to perform DTL exposures are now available and they find increasing use in various academic and industrial applications [2-3]. The capabilities of this new tool will be introduced with examples of applications. 1. H. Solak, C. Dais, F. Clube, Optics Express, Vol. 19, p. 10866 (2011). 2. H. Le-The, et al, Adv. Mater. Technol. 2017, 2, 1600238. 3. P. M. Coulon, et al Phys. Status Solidi B, 1700445.

DS 30: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VI (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Thursday 10:30–12:45 Location: HL 001

DS 30.1 Thu 10:30 HL 001

Core-level spectroscopy with the *GW* approximation — •Dorothea Golze and Patrick Rinke — Department of Applied Physics, Aalto University, Espoo, Finland

Inner-shell spectroscopy is an important tool to characterize molecules, liquids and adsorption processes at surfaces. We present a new, accurate method for computing X-ray photoelectron spectra based on the *GW* approximation that overcomes the limitations of density functional theory based approaches. Green's function theory in the *GW* approximation has become the method of choice for addition and removal energies of valence electrons in solids and is now increasingly being applied to molecules. However, *GW* core-level spectroscopy has thus far not received any attention. In most *GW* implementations, the self-energy is computed in the imaginary frequency domain followed by an analytic continuation to the real frequency axis. However, our calculations show that the analytic continuation becomes highly inaccurate for frequencies far away from the Fermi level and is not suitable for the computation of core excitations. Thus, we evaluate the self-energy on the real-frequency axis using the contour deformation (CD) technique. We implemented CD in combination with a resolution-of-the-identity approximation for the screened Coulomb interaction in the FHI-aims program package. Test calculations reveal that our implementation reproduces Turbomole reference calculations [1] perfectly. Furthermore, we present benchmark studies of small and medium-sized gas-phase molecules and discuss the potential of our method for more complex systems. [1] M. J. van Setten et al. JCTC, 2013, 232

DS 30.2 Thu 10:45 HL 001

***GW* and beyond from matrix resolvents** — •Jan Gesenhues[1], Dmitrii Nabok[2], Michael Rohlfing[1], and Claudia Draxl[2] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Theoretische Festkörperphysik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Typically GW calculations make use of either plasmon pole models or numerical integration in order to determine the screened Coulomb interaction W. We demonstrate how to obtain an analytical representation of W with the help of a matrix resolvent and present some standard GW results which have been obtained with the method. The analytical W is a useful starting point for subsequent calculations involving vertex corrections. On the other hand, the matrix resolvent technique itself can be applied upon a BSE-like equation of motion for the polarizability to include vertex corrections.

DS 30.3 Thu 11:00 HL 001

Electron-Magnon Scattering in Elementary Ferromagnets from First Principles: Lifetime Broadening and Kinks — Mathias C. T. D. Müller, •Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We study the electron-magnon scattering in bulk Fe, Co, and Ni within the framework of many-body perturbation theory implemented in the full-potential linearized augmented-plane-wave method. Starting from the *GW* approximation we obtain a Bethe-Salpeter equation for the two-particle (electron-hole) Green function, where single-particle Stoner excitations and collective spin-wave excitations (magnons) are treated on the same footing. We employ the solution of the Bethe-Salpeter equation to construct a self-energy that describes the scattering of electrons and magnons. The resulting renormalized electronic band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy, which are strongest in Fe. In the case of Co and Ni, the renormalization gives rise to kinks in the electronic band dispersion at low binding energies, which we attribute to electron scattering with spatially extended spin waves. Furthermore, we find a band anomaly at larger binding energies in iron, which results from a coupling of the quasihole with single-particle excitations that form a peak in the Stoner continuum. This band anomaly has, in fact, been observed in recent photoemission experiments at the same energy and momentum.

DS 30.4 Thu 11:15 HL 001

Effects of the Tamm-Dancoff approximation on the optical spectra of organic molecules — •Tobias Lettmann and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

When calculating excited state properties of electronic systems within the many-body perturbation theory (MBPT), the Bethe-Salpeter equation (BSE) needs to be solved. This is often done within the so called Tamm-Dancoff approximation (TDA), neglecting the coupling of resonant and anti-resonant excitations.

It is generally accepted that the TDA is justified for large, extended systems e.g. bulk crystals. However it has been shown that the TDA may no longer hold for some organic semiconductors[1]. In this talk we discuss the effects of the TDA on the resulting optical spectra of organic molecules of different sizes and investigate for which cases the TDA may still be justified.

[1] B. Baumeier et al: *J Chem. Theory Comput.*, 2012, **8**, 997

DS 30.5 Thu 11:30 HL 001

Ab-initio treatment of non-local electronic correlations with the dynamical vertex approximation — •Anna Galler[1], Patrik Thunström[2], Patrik Gunacker[3], Josef Kaufmann[3], Matthias Pickem[3], Jan M. Tomczak[3], and Karsten Held[3] — [1]Centre de Physique Theorique, Ecole Polytechnique, 91128 Palaiseau, France — [2]Department of Physics and Astronomy, Materials Theory, Uppsala University, 75120 Uppsala, Sweden — [3]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

Recently, approaches such as the dynamical vertex approximation (DΓA) or dual-fermion method have been developed. These diagrammatic approaches are going beyond dynamical mean-field theory (DMFT) by including non-local electronic correlations on all length scales as well as the local DMFT correlations. Here we present our efforts to extend the DΓA methodology to ab-initio materials calculations (AbinitioDΓA). Our approach is a unifying framework which includes both, GW and DMFT-type of diagrams, but also important non-local correlations beyond, e.g. non-local spin fluctuations. In our multi-band implementation we are using a worm sampling technique within continuous-time quantum Monte Carlo in the hybridization expansion to obtain the DMFT vertex, from which we construct the reducible vertex function in a ladder approximation. As a first application we show results for transition metal oxides. Support by the ERC project AbinitioDGA (306447) is acknowledged.

References: [1] A. Galler, P. Thunström, P. Gunacker, Jan M. Tomczak, and K. Held, Physical Review B 95, 115107 (2017)

DS 30.6 Thu 11:45 HL 001

Non-local correlations in effectively reduced spatial dimensions — •Jan M. Tomczak[1], Matthias Pickem[1], Benjamin Klebel[1], Anna Galler[2], Josef Kaufmann[1], Patrik Gunacker[1], Patrik Thunström[3], Thomas Schäfer[2], Alessandro Toschi[1], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, Austria — [2]Centre de Physique Théorique, Ecole Polytechnique, Palaiseau, France — [3]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Using the dynamical vertex approximation and its recent extension for electronic structure calculations, AbinitioDΓA[1], we explore the impact of spatial dimensions onto non-local correlations: (a) we compare magnitude and manifestations of non-local self-energies in ultra-thin films of transition-metal oxides to those in the bulk material. (b) we track the evolution of non-local correlations in the doped Hubbard model when continuously going from 3D to 2D. In particular we probe the limits of the "space-time separation" of electronic correlations evidenced in 3D[2]. Support by the ERC project AbinitioDGA (306447) and the Austrian Science Fund (FWF) projects I 2794-N35

and P 30213-N36 is acknowledged.

References: [1] A. Galler, P. Thunström, P. Gunacker, JMT, K. Held, PRB 95, 115107 (2017), [2] T. Schäfer, A. Toschi, JMT, PRB 91, 121107R (2015)

DS 30.7 Thu 12:00 HL 001

Does the optical signature of oxidized polyethylene stem from saturated or unsaturated carbonyl defects? — •Guido Roma[1], Fabien Bruneval[1], and Layla Martin-Samos[2] — [1]DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, F-91191 Gif sur Yvette, France — [2]CNR-Demokritos, Trieste, Italy

Polyethylene (PE), one of the simplest and most used aliphatic polymers, is generally provided with a number of additives, in particular antioxidants, because of its tendency to get oxidized. Carbonyl defects, a product of the oxidation of PE, are occurring in various forms, in particular saturated ones, known as ketones, where a C=O double bond substitutes a CH_2 group, and various unsaturated ones, i.e., with further missing hydrogens. Many experimental investigations of the optical properties in the visible/UV range mainly attribute the photoluminescence of PE to one specific kind of unsaturated carbonyls, following analogies to the emission spectra of similar small molecules. However, the reason why saturated carbonyls should not be optically detected is not clear. We investigated the optical properties of PE with and without carbonyl defects using perturbative GW and the Bethe-Salpeter equation in order to take into account excitonic effects. We discuss the calculated excitonic states in comparison with experimental absorption/emission energies and the stability of both saturated and unsaturated carbonyl defects. We conclude that the unsaturated defects are indeed the best candidate for the luminescence of oxidized PE, and the reason is mainly due to oscillator strengths.

DS 30.8 Thu 12:15 HL 001

Bethe-Salpeter equation beyond the Tamm-Dancoff approximation at finite momentum transfer: Absorption and loss spectra including excitonic effects — •Benjamin Aurich, Caterina Cocchi, and Claudia Draxl — Humboldt-University, Berlin, Germany

The state-of-the-art ab-initio method for computing optical properties of semiconductors is based on the Bethe-Salpeter equation (BSE) which describes the excitations of the system in terms of interacting electron-hole (e-h) pairs. For absorption spectra, typically no momentum transfer from light to the e-h pairs is considered, and the coupling between excitations and de-excitations of e-h pairs is usually neglected by using the Tamm-Dancoff approximation (TDA). This approach yields excellent agreement with experiment for many materials, but may break down for confined systems [1]. The TDA is also known to fail to describe the electron energy loss spectra for materials as simple as silicon [2]. We report on the extensions of the open-source code `exciting` [3] allowing for BSE calculations beyond the TDA and at finite momentum transfer using an exact diagonalization scheme [4]. We demonstrate the differences between TDA and non-TDA spectra at vanishing and finite momentum transfer for periodic molecular systems.

[1] M. Grüning et al., Nano Lett **9**, 2820 (2009)
[2] V. Olevano and L. Reining, Phys. Rev. Lett. **86**, 5962 (2001)
[3] A. Gulans et al., J. Phys. Condens. Matter **26**, 363202 (2014)
[4] T. Sander et al., Phys. Rev. B **92**, 045209 (2015)

DS 30.9 Thu 12:30 HL 001

Calculations of charge and spin susceptibilities and quasiparticle energy shifts within the CASTEP plane-wave DFT code — •Vincent Sacksteder[1], Evgeny Plekhanov[2], Phil Hasnip[3], Matt Probert[3], Stewart Clark[4], Keith Refson[1], and Cedric Weber[2] — [1]Royal Holloway University of London, UK — [2]Kings College London, UK — [3]University of York, UK — [4]University of Durham, UK

CASTEP is a pseudopotential based plane wave code which scales to the largest supercomputers and offers a wide feature set. Within CASTEP we have implemented calculation of the charge and spin susceptibility tensor, which describes the response to a perturbing charge or spin. We present corrections to the Kohn-Sham energies obtained by using the susceptibility tensor to screen Hartree-Fock exchange. In the static limit this is the SEX part of the COHSEX approximation, and if instead the dynamic susceptibility is used one obtains the GW approximation.

Our memory and CPU consumption scales linearly with the plane wave basis size, allowing thorough exploration of convergence with basis size, not only of the susceptibility itself, but of the SEX and GW quasiparticle shifts. We emphasize that our calculations are heavily parallelized, in exactly the same way as a standard DFT ground state calculation.

This work will allow first principles calculations of magnon spectra, exchange couplings, ionization potentials, and KKR and DMI coefficients.

DS 31: Poster Session II

Time: Thursday 11:15–13:15 Location: Poster F

DS 31.1 Thu 11:15 Poster F

Morphology and crystallinity of $Sr_xCo_yO_z$ films at different growth conditions and stoichiometry — •Patrick Schöffmann[1], Sabine Pütter[1], Jürgen Schubert[2], Willi Zander[2], Markus Waschk[3], Paul Zakalek[3], and Thomas Brückel[3] — [1]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Garching — [2]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich GmbH — [3]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. Because of the multivalent Co states and high oxygen mobility it is a promising material for energy and information applications. [1]

We aim at growing thin films of $SrCoO_{3-\delta}$ by molecular beam epitaxy and filling the oxygen vacancies by oxygen plasma assisted annealing. Achieving a 1:1 stoichiometry by co-evaporation of Sr and Co requires tuning of the individual growth rates, which is not straightforward as there are three constituents with different sticking coefficients.

We present the effect of the growth conditions on the stoichiometry, crystallinity and morphology of $Sr_xCo_yO_z$ films on STO and requirements for $Sr_1Co_1O_{2.5}$ films. First results of decreased oxygen vacancies by annealing in a low pressure oxygen atmosphere are discussed.

[1] H. Jeen et al., Nature Materials 12, 2013

DS 31.2 Thu 11:15 Poster F

Understanding and controlling the growth of carbon nanowalls — •Sebastian Tigges[1,2], André Giese[1], Axel Lorke[1,2], and Nicolas Wöhrl[1,2] — [1]Universität Duisburg-Essen, Faculty of Physics, 47057 Duisburg, Germany — [2]Center for Nanointegration Duisburg-Essen, 47057 Duisburg, Germany

Carbon nanowalls (CNWs) exhibit exceptional thermal as well as electrical conductivity. Their surface area may be controlled simply by adjusting process parameters. This makes them especially attractive for application in sensors and energy technology. Extensive research has been undertaken to understand the complex mechanisms contributing to the growth of CNWs. The most important challenge is proper understanding of growth mechanisms to directly control morphology/structure. Here, we investigate the different CNW structures that are obtained by tuning process parameters such as temperature, substrate bias, flow rate of precursor gas, and pressure in our inductively coupled plasma enhanced CVD system. CNW structures of varying height, inter-wall distance and morphology are obtained. They are characterized and distinguished via scanning electron microscopy and Raman spectroscopy. Plasma characterization is done by optical emission spectroscopy and quadrupole mass spectrometry. Particularly Raman spectroscopy shows important variation in both defect density and defect type. Furthermore formation of different CNW structures is observed, which changes with residual time of the complex precursor molecule used as carbon source. This way a simple growth model is derived.

DS 31.3 Thu 11:15 Poster F

Influence of O_2/N_2 Gas Compositions on PECVD de-

posited Silicon Oxide Films — •Philipp Moritz[1,2], Simon Homann[1,2], Lisa Wurlitzer[1,2], and Wolfgang Maus-Friedrichs[1,2] — [1]Institute of Energy Research and Physical Technologies, Clausthal University of Technology, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]Clausthal Centre of Material Technology, Clausthal University of Technology, Agricolastr. 2, 38678 Clausthal-Zellerfeld

Plasma enhanced chemical vapor deposition (PECVD) is an established process to deposit solid coatings. We used PECVD with a tetraethyl orthosilicate (TEOS) precursor to coat titanium substrates with silicon oxide. In order to this the substrate was exposed to TEOS with a carrier gas mixture of O_2 and N_2. For the experiments a dielectric barrier discharge plasma was used under atmospheric pressure. It causes a reaction of the TEOS to form a solid film of silicon oxide.

To optimize the stoichiometry and morphology of the deposited coating the gas composition of O_2 and N_2 is varied. The total gas flow is kept constant. Investigations with X-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) show significant differences in the stoichiometry and morphology of the coatings dependent on the gas composition.

DS 31.4 Thu 11:15 Poster F

Preparation and characterisation of carbon-free Cu(111) films on sapphire for graphene synthesis — •Jan Lehnert, Daniel Spemann, M.Hamza Hatahet, Michael Mensing, Christoph Gruner, Patrick With, Philipp Schumacher, Annemarie Finzel, Dietmar Hirsch, and Bernd Rauschenbach — Leibniz Institute of Surface Engineering (IOM), Leipzig, Germany

This work presents an investigation of unwanted carbon formed on polycrystalline Cu(111) thin films. The goal is to obtain carbon-free Cu films as a substrate for controlled graphene synthesis. Cu films were prepared by ion beam sputtering at room temperature on c-plane Al_2O_3. These films had been thermally treated in a temperature range between 300 and 1020 °C. The crystallinity of the Cu films was studied by XRD and RBS/channeling and the surface was characterised by Raman spectroscopy, XPS and AFM for each annealing temperature. RBS measurements revealed the diffusion of the Cu into the Al_2O_3 substrate at high temperatures of > 800 °C. Furthermore, a cleaning procedure using UV ozone treatment is presented to remove the carbon contamination from the surface which yields essentially carbon-free Cu films that open the possibility to synthesise graphene with controlled number of graphene layers. On these Cu substrates, graphene was synthesised by carbon ion implantation and subsequent annealing. These graphene layers were transferred to a SiO_2/Si waver using a standard wet-chemistry approach. Raman and AFM measurements were performed to investigate the quality of the transferred graphene layers.

DS 31.5 Thu 11:15 Poster F

Ge_2Fe thin films grown by solid-phase epitaxy — •Samuel Gaucher[1], Bernd Jenichen[1], Michael Hanke[1], Achim Trampert[1], Holm Kirmse[2], Steven C. Erwin[3], and Jens Herfort[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Humboldt-Universität zu Berlin, Berlin, Germany — [3]U. S. Naval Research Laboratory, Washington, D. C., USA

To grow an epitaxial semiconductor over a ferromagnetic metal, a solid-phase epitaxy (SPE) approach was recently developed, whereby amorphous Ge is crystallized slowly by annealing over Fe_3Si. It was realized that a sufficiently thin Ge layer would incorporate Fe and Si atoms to form an ordered superlattice, with 2D planes of Fe atoms interposed between tetragonal Ge formations. This crystal structure is understood as Ge_2Fe (with some Si on Ge sites), a compound that is not energetically stable as a bulk material. By growing Fe_3Si and Ge in the right proportions (1:3), it was possible to use SPE to achieve isolated single-crystalline Ge_2Fe films, directly on GaAs substrates, with thicknesses ranging from 8 to 20 nm. Ge_2Fe thin films are ferromagnetic at low temperature and show strong magnetocrystalline anisotropy, with thickness dependent coercivity on the order of 200 Oe along the easy magnetization axis. The material has a room temperature resistivity $\rho \sim 8 \times 10^{-6} \Omega$ m along the Fe basal planes, which decreases as a metal when temperature is lowered. Alike other thin Fe-Ge compounds, Ge_2Fe is a possible candidate to host topological magnetic skyrmions, among other interesting micromagnetic phenomena.

DS 31.6 Thu 11:15 Poster F

The impact of various substrate pretreatments on the growth of chalcogenide thin films — •Brigitte Baumkötter[1], Matthias M. Dück[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany — [2]JARA-FIT, RWTH Aachen University, Germany

Phase change materials (PCMs) are remarkable due to a unique combination of optical and electrical properties featuring a strong contrast between the crystalline and the amorphous phase. These characteristics have been used for optical data storages for a long time and are now about to revolutionize the field of electronic non-volatile memories.

The microstructure of a thin film may influence its properties, and is therefore an obstacle for measurements of reproducible material properties. However, utilizing thin films is mandatory due to the strong disorder dependence of many PCMs, which cannot be easily reproduced in a single crystal. Due to the anisotropic structure of materials from the pseudo-binary line GeTe-Sb_2Te_3 (GSTs) orientation dependent measurements are of special interest. Especially infrared spectroscopy enables new insights on the effect of disorder, which induces a metal to insulator transition in several PCMs of this class.

Besides texture, two major requirements for optical measurements are a thick film of around 500 nm and a low surface roughness. Therefore, an optimized thick film with a strong texture and a smooth surface is necessary. As the substrate and its surface has a crucial influence on the structure of grown films, this study focuses on the influence of different substrate pretreatments on the film quality.

DS 31.7 Thu 11:15 Poster F

Nanocrack networks: a systematic approach for surface tailoring of sputter deposited oxide thin films — •Alexander Vahl[1], Jan Dittmann[1], Bodo Henkel[1], Oral Cenk Aktas[1], Thomas Strunskus[1], Suman Kumar Sharma[2], and Franz Faupel[1] — [1]Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Multicomponent Materials, Kaiserstr. 2, 24143, Kiel, Germany — [2]Department of Physics, Malaviya National Institute of Technology, Jaipur 302017, India

Surface roughness is a critical parameter for various thin film applications, influencing properties like wetting and catalytic performance. Thermally induced nanocrack network formation is an efficient tool to modify the surface of thin films. We report on the fundamental process of nanocrack network formation, showcased at the example TiO2 and Al2O3 thin films deposited by pulsed reactive DC magnetron sputtering. In case of TiO2, the amount of oxygen during the deposition process was found to be crucial for the formation of crystalline anatase seeds in the as deposited thin film. In a post deposition heat treatment step, the preexisting structural features densified and gave rise to a connected network of nanoscopic cracks. In case of Al2O3, independent of the oxygen content the thin film showed high resiliency against crystallization and accordingly no connected nanocrack network was observed.

DS 31.8 Thu 11:15 Poster F

B-site Ordering in La2CoMnO6 Films: Influence of Lattice Strain — •Philipp Ksoll[1], Christoph Meyer[1], Sven Esser[2], Vladimir Roddatis[3], and Vasily Moshneaga[1] — [1]Erstes Physikalisches Institut, Georg-August-Universität Göttingen, Deutschland — [2]Lehrstuhl für Experimentalphysik VI, Institut für Physik, Universität Augsburg, Deutschland — [3]Institut für Materialphysik, Georg-August-Universität Göttingen, Deutschland

Physical properties of double perovsikte (DP) with general formula A2BB'O6 (A=rare earth or alkaline earth metals: B/B' = Co/Mn, Ni/Mn, Fe/Mo) depend strongly on the degree of B-site ordering. To optimize and control the structure, magnetism and electrical properties we further developed the metalorganic aerosol deposition (MAD) technique to grow DP films in a layer-by-layer (LL) mode under a precise control of oxygen atmosphere during deposition process. Epitaxial films of the prototype DP La2CoMnO6 have been LL-grown on (111)-oriented SrTiO3, LaAlO3 and Al2O3(0001) substrates and characterized by global (x-Ray, SQUID, Raman) and local (TEM) techniques. The role of substrate-induced epitaxial strain on the B-site ordering is discussed. Further on, a half-metallic ferromagnetic Sr2FeMoO6 films with transition temperatures well above room temperature, Tc˜450 K, will be obtained. Financial support by the DFG via projects Ro5387/3-1 and Mo2255/3-1 is acknowledged.

DS 31.9 Thu 11:15 Poster F

Well Ordered Iron Sulfide Layers on Au(111) — •Earl Davis, Giulia Berti, Helmut Kuhlenbeck, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft

The iron-sulfur world hypothesis of G. Wächtershäuser is an origin-

of-life theory which proposes that early life may have formed at the surface of sub-marine iron sulfide compounds. This involves the activation of carbon dioxide to form simple organic molecules. Theoretical and experimental studies have shown that the mineral greigite (Fe_3S_4) should be active for this.

With the goal of CO_2 activation, our aim was to prepare ordered iron sulfide layers. We found that such a layer can be prepared on Au(111) by deposition of iron in an atmosphere of S_2 molecules which are produced by an electrochemical sulfur source. According to XPS, the layer is sulfur terminated, and STM shows a homogeneous, well-ordered surface with a hexagonal symmetry. The same symmetry is found in LEED patterns and the hexagonal lattice parameter fits to what is expected for $Fe_3S_4(111)$. I/V LEED curves were measured in order to determine details of the structure. Additionally, initial reactivity experiments have shown that it is possible to hydrogenate the surface, which might offer routes to hydrogenation reactions.

DS 31.10 Thu 11:15 Poster F

Texture Optimization of Metastable $GeSb_2Te_4$ Thin Films — •Hannah Niehaus[1], Matthias M. Dück[1], Stefan Jakobs[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany — [2]2 JARA-FIT, RWTH Aachen University, Germany

Phase-change materials (PCM) are already established in optical data storage technologies. Currently these materials are also introduced into the market for electronic data storage, since they offer an attractive portfolio of properties. A prominent representative of PCMs is the material $GeSb_2Te_4$ (GST), whose electronic properties are governed by disorder-induced effects. GST exists in two different crystalline phases: a rocksalt-like metastable structure and a stable hexagonal one, which is obtained at higher annealing temperatures. Furthermore, this material undergoes a metal-to-insulator transition (MIT) independent of this structural transition. In this study we optimize the texture of GST thin films in the metastable phase in order to enable the investigation of the influence of atomic disorder on the electrical behavior. The material is deposited via sputter deposition on various substrates. In the optimization process parameters such as gas pressure, temperature and power are varied. The structure and quality of the thin films are characterized by x-ray reflectivity (XRR) and diffraction (XRD) as well as atomic force microscopy (AFM). The texture of GST thin films was optimized successfully which now allows systematic investigations of the influence of disorder on the MIT.

DS 31.11 Thu 11:15 Poster F

Characterization and optimization of rf sputtered $LiCoO_2$ thin films by post thermal annealing — •Marcel Couturier, Fabian Michel, Philipp Schurig, and Angelika Polity — Justus Liebig Universität, 35392 Gießen

$LiCoO_2$ thin films have been grown by rf-magnetron-sputter-deposition on platinum coated quartz substrates. The films were annealed at 700 °C for several hours in different atmospheres such as vacuum or under flux of oxygen to create phases which are favorable for battery applications. For structural characterization X-ray diffraction and Raman spectroscopy were used. HT-$LiCoO_2$-films with (003)-orientation after annealing under flowing oxygen and Co_3O_4-films with (311)-orientation after annealing in a vacuum could be observed. Furthermore, the stoichiometry could be determined using X-ray photoelectron spectroscopy, revealing a weak lithium deficiency in the grown films. Additional parasitic lithium phases near the surface of the films could be observed by analysis of the Li 1s photoelectron signal. Scanning electron microscopy images have shown changes in the surface morphologies of the films after undergoing the heat-treatment. Grains have slightly increased their volume. Moreover the shape changes after the annealing process in comparison to the untreated samples.

DS 31.12 Thu 11:15 Poster F

Deposition and optimization of a $LiCoO_2$ cathode layer for battery applications — •Sebastian Leonard Benz, Martin Becker, Christian Reindl, Angelika Polity, and Peter J. Klar — Justus Liebig Universität, 35392 Gießen

This work is about the deposition and characterization of Lithium Cobalt Oxide (LCO) thin films, deposited by rf magnetron sputtering. Different sputter process parameters such as gas flux, sputter power, deposition time and gas composition were considered. In addition, the influence of the used substrate was investigated. Different materials like glass, sapphire and metals were used as substrates. The main aim was to optimize the growth parameters for battery applications of LCO. Mostly X-ray-diffraction (XRD), as well in Bragg-Brentano as in four-circle geometry, was used to characterize the crystal structure and especially the out-of-plane orientation of the deposited thin films. By varying the parameters mentioned above, a (012) orientation has been achieved. Moreover, scanning electron microscopy (SEM) has been used to characterize the surface morphology. Furthermore, Raman spectroscopy gave insights into the crystal structure.

DS 31.13 Thu 11:15 Poster F

Electrically conductive long term stable ultrathin Gallium/Gallium(hydr)oxide layers — •Sebastian Runde[1], Heiko Ahrens[1], Frank Lawrenz[1], Amal Sebastian[1], Stephan Block[2], and Christiane A. Helm[1] — [1]Inst. f. Physics, Greifswald University, Germany — [2]Dept. for Biochemistry and Chemistry, Free University of Berlin, Germany

Single Gallium/Gallium(hydr)oxide Ga/GaOxHy layers were prepared by induced break-up after forced wetting. Multilayers were formed by repeating the deposition procedure. X-ray reflectivity shows a multilayer structure. The repeat unit consists of a Ga layer covered by a GaOxHy layer (thickness 2.9 nm). The multilayer thickness is proportional to the number of deposited layers. The multilayer-air roughness may be smaller than the substrate-multilayer roughness, which is attributed to the large surface tension of Gallium. The electric conductivity of a multilayer follows Ohm*s law. The sheet resistance decreases with the number of deposited layers. We suggest that induced break-up after forced wetting is an environmentally friendly way to produce large ultrathin conductive layers from fluid metals.

DS 31.14 Thu 11:15 Poster F

Interface tuning by metallic and insulting interlayers in manganite-titanite heterojunctions — •Stephan Melles, Birte Kressdorf, Joerg Hoffmann, Ulrich Ross, and Christian Jooss — University of Goettingen, Institute of Materials Physics, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany

New photovoltaic materials like complex oxides allow for fundamental studies of new conversion mechanisms which have the potential to overcome current efficiency limitations. Their interfaces play a crucial role in controlling charge transfer and charge separation, and determine the current-voltage ($I-V$) characteristics of such systems. Here, we present studies on interface design of manganite-titanite heterojunctions which are prepared by ion beam sputtering of thin films of hole doped $Pr_{0,66}Ca_{0,34}MnO_3$ (PCMO) on electron doped single crystalline $SrTi_{0.9975}Nb_{0.0025}O_3$ (STNO) substrates. The junction displays a rectifying $I-V$ characteristic and a pronounced photovoltaic effect, involving polaronic excitations [1]. Preliminary results show that the sputter deposition of Cr interlayers can either modify the junction to an ohmic contact or modify the rectifying characteristic and enhance the photovoltaic effect, depending on thickness and preparation conditions. Consequently, we started to prepare wedge-shaped Cr interlayers, allowing for a systematic thickness dependent analysis. The growth mode of Cr layers is investigated by SEM and AFM studies and the change of cross plane current voltage characteristics is studied. The interfaces are characterized by transmission electron microscopy. Reference: [1] B. Ifland et al., New J. Phys. 19 (2017) 063046

DS 31.15 Thu 11:15 Poster F

Synthesis and characterization of transition-metal germanides — •Yufang Xie[1,2], Ye Yuan[1,2], René Hübner[1], Jörg Grenzer[1], Mao Wang[1,2], Manfred Helm[1,2], Shengqiang Zhou[1], and Slawomir Prucnal[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany — [2]Technische Universität Dresden, D-01062 Dresden, Germany

Si was sufficient to fulfil the requirements of microelectronic industry for more than five decades. Further progress based on the miniaturisation of transistors is challenging. Therefore new materials and concepts are considered for the next generation of nanoelectronics. In this work, we present the formation of transition-metal germanides epitaxially grown on Ge wafer. Those materials have great promise for both the ohmic contacts to n-type Ge with extremely low specific contact resistivity and spintronics. The transition-metal germanides are synthesized by metal sputtering on Ge followed by millisecond range flash lamp annealing which is suitable for larger-area fabrication and compatible with CMOS technology. On one hand, orthorhombic NiGe whose contact resistivity is only around 1.2*10-6 Ω cm2, is beneficial for achieving high-performance Ge-based nano-electronic devices. On

the other hand, cubic FeGe with B20 phase is a Skyrmion-carrier material attractive for spintronics. In summary, the epitaxial transition-metal germanides materials can be obtained by a novel epitaxial approach which provides insight to their technological usage.

DS 31.16 Thu 11:15 Poster F

Surface plasmon resonance investigation of gold nanoparticle aggregation on self-assembled monolayers — •Navid Khangholi, Alfred Kick, Mathias Lakatos, and Michael Mertig — Technische Universität Dresden, Dresden, Germany

A new sensor principle based on Surface Plasmon Resonance is developed using AuNPs functionalised with carboxylic groups (AuNP-COOH) immobilised on self-assembled monolayers (SAM). The immobilisation of AuNP-COOHs occurs electrostatically between a positively charged SAM and negatively charged AuNP-COOHs. This SAM consists of a thiolated pH-sensitive polymer, poly (2-vinylpyridine) with a terminal thiol group (P2VP-SH), as a supporting layer on the gold surface of the SPR chip. This polymer responds to the pH changes, e.g. swelling and shrinking in acidic or basic environments, respectively. Swelling of P2VP with AuNP-COOHs occurs between pH 2.3 and 1.7. This induces an enhanced decrease of the SPR signal compared to the P2VP layers without AuNPs. This larger decrease of the SPR signal is due to the increase of the distance between the AuNPs and the gold substrate.

DS 31.17 Thu 11:15 Poster F

Perturbed angular correlation studies of H^2 plasma treated rutile — •Dmitry Zyabkin[1], Juliana Schell[2], Ulrich Vetter[1], Robinson Santos[3], and Peter Schaaf[1] — [1]Chair materials for Electronics, Institute of Materials Engineering and Institute of Micro- and Nanotechnologies MacroNano®, Gustav-Kirchhoff-Str. 5, 98693 Ilmenau, Germany — [2]European Organization for Nuclear Research (CERN), CH-1211 Geneva, Switzerland — [3]Instituto de Pesquisas Energéticas e Nucleares, IPEN, Saõ Paulo, Brazil

Hydrogenated titania has recently attracted enormous attention due to its compelling features and extended application [1]. Nonetheless, the origin of the improved features has stayed uncertain as well as H_2 stability under elevated temperatures. We report on recent perturbed $\gamma\gamma$-angular correlation (PAC) studies of TiO_2:H rutile thin films using the probe ^{111m}Cd, which was implanted at the online isotope separator ISOLDE at CERN. The films were synthesized by reactive magnetron sputtering and deposited on Si and quartz substrates, followed by an annealing step at 1173K for 5 hours. The subsequent H_2 plasma treatment was performed at various plasma temperatures up to 663K. After implantation with typically around 10^{12} probe atoms the samples were transported to the PAC setup and kept at 481K, 531K or 581K during the measurements in vacuum. Time-correlated R(t) spectra were fitted against electric quadrupole interaction parameter sets corresponding to fractions of probe atoms in specific local defect configurations.
[1] X.Chen *et al.* Chem. Soc. Rev., 2015,44, 1861-1885

DS 31.18 Thu 11:15 Poster F

Rf magnetron sputtering of solid electrolytes for battery applications — •Fabian Michel[1], Martin Becker[1], Jaroslava Obel[2], Martin Finsterbusch[3], Jürgen Janek[4], and Angelika Polity[1] — [1]Institute for Exp. Physics I and Center for Material Research (ZfM/LaMa), Justus-Liebig-Universität, 35392 Gießen — [2]Departement Chemie, Ludwig-Maximilian-Universität, 81377 München — [3]Forschungszentrum Jülich GmbH, 52428 Jülich — [4]Institute of Physical Chemistry and Center for Material Research (ZfM/LaMa), Justus-Liebig-Universität, 35392 Gießen

Lithium based solid electrolyte thin films were produced via rf magnetron sputtering. An optimization of the physical properties, which are important for battery applications, was done by varying the deposition parameters. Consequently compositions of the films were investigated using different techniques like X-ray photoelectron spectroscopy (XPS), inductively coupled plasma optical emission spectroscopy (ICP-OES) and Rutherford backscattering spectrometry (RBS). To evaluate the samples conductivity investigations were performed by electrochemical impedance spectroscopy (EIS). A maximum increase in ionic conductivity was sought after as was to gain knowledge about the influence of the different elements and sputtering parameters of the solid electrolyte with respect to the ionic conductivity. To monitor the improvements made, results were compared with earlier findings of investigations on solid electrolytes.

DS 31.19 Thu 11:15 Poster F

Chemical ordering in epitaxial (La,Sr)$CoO_{3-\delta}$ thin films prepared by RF magnetron sputtering — •Marcel Urban and Wolfgang Donner — TU Darmstadt, Materials Science, Structure Research, Darmstadt, Germany

The (La,Sr)CoO_3 based perovskites (LSCO) show promising properties regarding the application in solid oxide fuel cells and gas separation membranes, like the remarkable electronic and ionic conductivity at intermediate temperatures (below 800 K). These properties may be further improved by inducing cation and oxygen vacancy ordering, as observed in strained thin films [1].

Here we show recent results from epitaxially grown LSCO thin films. They were deposited on [001]-oriented $SrTiO_3$ single crystal substrates by means of radio frequency magnetron sputtering from a stochiometric $La_{0.5}Sr_{0.5}CoO_3$ target. The films were characterized *in situ* in terms of stoichiometry and surface structure by Auger electron spectroscopy and low-energy electron diffraction. Moreover, the crystal structure is examined by x-ray diffraction (XRD) using a four- circle single crystal diffractometer. Up to a thickness of about 50 unit cells the deposited films show a coherent, pseudomorphic growth whereas thicker films show an in-plane lattice relaxation. The coherent films exhibit Laue oscillations and a relatively small mosaicity. The deposition atmosphere can be used to tune the stoichiometry. In the next step, the induced ordering phase transition will be followed by in situ XRD during heat treatment of the films in different atmospheres.
[1] W. Donner et al., *Chemistry of Materials* 23.4 (2011): 984-988.

DS 31.20 Thu 11:15 Poster F

Melting and premelting behaviour of epitaxial thin films — •Constantin Wansorra and Wolfgang Donner — TU Darmstadt, Materials Science, Structure Research, Darmstadt, Germany

Despite the fact that melting of materials has been studied for more than a century [1], the melting behaviour of thin films is still topic of research [2]. Concerning bulk, it is now known that melting precursors [3] as the surface or grain boundaries are the reason for the absence of superheated solids. In thin films, the surface has a much higher impact on the properties of the material [4]. Therefore, research of their melting will produce a better understanding of high temperature stability and failure processes of the films.

We have prepared epitaxial films of low melting temperature metals on various substrates by Molecular Beam Epitaxy and studied structural changes near the melting temperature by reflection high-energy electron diffraction, scanning tunnelling microscopy and grazing incidence x-ray diffraction. We report on the changes in surface and interface roughness and the dewetting behaviour of the films. Furthermore, a technique of analysing the melting behaviour with x-ray diffraction is presented.
[1] Dash, *Reviews of Modern Physics* 71 (1999): 1737.
[2] Kahn, et al., *Springer Nature* 46 (2015): 3932.
[3] Rühm, et al., *Physical Review B* 68 (2003): 224110.
[4] Chen, et al., *Elsevier BV* 68 (2015): 97.

DS 31.21 Thu 11:15 Poster F

Direct observation of defect evolution in 2D single layer tungsten diselenide by low voltage high resolution transmission electron microscopy — •Robert Leiter, Yueliang Li, and Ute Kaiser — Electron Microscopy Group of Materials Science, University of Ulm, Albert- Einstein Allee 11, 89081 Ulm, Germany

Defects in two-dimensional transition metal dichalcogenides (TMDs) have received increasing attention in recent years due to their influence on their extraordinary mechanical, electrical, magnetic and optical properties. By controlled electron irradiation under the transmission electron microscope, such defects may tailor a material's unique properties. [1,2]

In this work, defect evolution in WSe_2 was observed in real time using our novel C_c- and C_s - corrected SALVE (Sub Ångström Low Voltage Electron microscopy) instrument [3] with atomic resolution. The combination of high time- and spatial resolution enabled the observation of many intermediate states, atom-by-atom and provides deeper understanding of its formation dynamics.
[1] Y.-C. Lin et al., Nat. Commun. 6, 6736 (2015)
[2] H.-P. Komsa and A. V. Krasheninnikov, Adv. Electron. Mater. 3, 1600468 (2017)
[3] M. Linck et al., Phys. Rev. Lett. 117, 076101 (2016)

DS 31.22 Thu 11:15 Poster F

Structural study of GaN nanostructures and thin films prepared by energy and mass selective ion-beam assisted MBE —

•Andriy Lotnyk, Sören Herath, Philipp Schumacher, Michael Mensing, Jürgen W. Gerlach, and Bernd Rauschenbach — Leibniz Institute of Surface Engineering (IOM), Permoserstr. 15, 04318 Leipzig, Germany

GaN is a widely used semiconductor material for optoelectronic applications. In this work, GaN nanostructures and thin films were produced on 6H-SiC(0001) and Al2O3(1-102) substrates by using a system for energy and mass selective ion-beam assisted molecular-beam epitaxy (IBA-MBE). The nanostructures were produced in two steps. In the first step of the deposition process, Ga-droplets were deposited on 6H-SiC at elevated temperatures. In the second step, a post-nitridation process of Ga droplets by either monoatomic or polyatomic, hyperthermal nitrogen ions was used for the synthesis of GaN nanostructures. The characterization of GaN nanostructures by aberration-corrected scanning transmission electron microscopy showed the formation of cubic GaN. The detailed structural investigation revealed different types of defects forming during the growth of nanostructures. The results on microstructure of GaN thin film will be also presented and the influence of ion energies on the real structure of GaN nanostructures and thin films will be discussed.

DS 31.23 Thu 11:15 Poster F

A route to epitaxial growth of periodic metal nanostructure arrays — •Denise Erb[1], Gerald Malsch[1,2], René Hübner[1], Kilian Lenz[1], Jürgen Lindner[1], Stefan Facsko[1], Manfred Helm[1,2], and Jürgen Fassbender[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden (Germany) — [2]Technical University Dresden, Institute of Solid State Physics, Dresden (Germany)

Epitaxial thin film growth on planar substrate surfaces is well-established for many materials. We show that it can also be feasible to grow nanostructures in an oriented manner on nanopatterned crystalline surfaces. Produced by a scalable procedure on large surface areas, such nanostructure arrays may find diverse applications in research and technology. On semiconductor substrates, nanoscale surface patterns with well-defined lateral periodicity form under low-energy ion irradiation via non-equilibrium self-assembly of vacancies and adatoms [1]. For appropriate process temperatures, the crystallinity of the substrate is retained during ion irradiation. When a material is then deposited onto the substrate by PVD under non-normal incidence, shadowing effects give rise to the formation of separated nanostructures [2], while a suitable lattice matching can induce epitaxial growth. In this contribution, we outline the patterning and growth procedure. As an example, we will present periodic Fe/Au nanostructure arrays and discuss their strongly anisotropic optical and magnetic properties. [1] X. Ou et al., Nanoscale 7, 18928 (2015) [2] Q. Jia, et al., Nano Research 15, 1 (2017)

DS 31.24 Thu 11:15 Poster F

Scanning Tunneling Microscopy and Spectroscopy of thin films of Strontium Ruthenates — •Marion A. van Midden, Tjaša Parkelj, Jernej Mravlje, Rok Žitko, Matjaž Spreitzer, and Erik Zupanič — Jožef Stefan Institute, Ljubljana, Slovenia

Because the energy scales of charge, spin, lattice, and orbital degrees of freedom of 4d- and 5d- transitional metal oxides are comparable, they exhibit a wide range of distinct electronic and magnetic properties. In the case of perovskite type transitional metal oxides these materials are also extremely sensitive to perturbations and can therefore be tuned via nonthermal parametrs such as doping, pressure, and magnetic fields. Growing thin films allows us to introduce strain via lattice mismatch with the substrate and thereby tune the properties of the film.

The films of $SrRuO_3$ were grown on $SrTiO_3$ using Pulsed Laser Deposition. The back-pressure in the system is below 10^{-9} mbar, which enables growth with a relatively small concentration of impurities. Growth was controlled *in-situ* using Reflected High-Energy Electron Diffraction. Using an ultra-high vacuum (UHV) suitcase the samples were transported to an UHV system equiped with Low-Energy Electron Diffraction and a Nanonis Joule-Thomspon Scanning Tunneling Microscope. Topography and spectroscopy measurements were done on clean surfaces and in the vicinity of defects.

DS 31.25 Thu 11:15 Poster F

Fe doping effect on the morphological, structural and photocatalytic properties of TiO2 thin layers — •fayçal bensouici[1], mustafa benyakhlef[1], mohamed bououdina[2], razika tala-ighil[1], mahdia toubane[1], and boudjemaa bouaouina[1] — [1]departement of physics,URMPE unite, UMBB university, 35000 boumerdes, algeria — [2]department of physics, college of science, university of bahrain, PO box 32038, kingdom of bahrain

Abstract: In this study, undoped and Fe3+ doped TiO2 thin films has been prepared via sol-gel method using the tetraethyl-orthotitanate as source of Ti and Fe(III) nitrate as source of Fe3+ doping. Scanning electron microscopy (SEM-EDX), X-ray diffraction (XRD), and UV*vis spectrum were employed to examine the effects of Fe element on morphology, structure, optical characteristics and photocatalytics behavior of TiO2 films. XRD patterns showed the presence of TiO2 anatase phases only, no other phase has been appeared. SEM image confirm the nanometric grain size of all samples and a low decrease in band gap were we increases the Fe doping percentage. It is also observed that no enhancement in photocatalytics activities of Fe doped TiO2 thin films.

DS 31.26 Thu 11:15 Poster F

Microstructure and mechanical properties of Mo2N/CrN multilayers deposited by DC magnetron sputtering — •boudjemaa bouaouina[1], cristophe tromas[2], dominique eyidi[2], céderic mastail[2], anny michel[2], sedik elhak abaidia[1], and grégory abadias[2] — [1]Département de physique, Unité de recherche URMPE, Université de Boumerdès 35000, Algerie — [2]Insitut Pprime, Department of Physics and Mechanics of Materials, Université de Poitiers-CNRS-ENSMA, 86962 Chasseneuil-Futuroscope, France

The multilayer films Mo2N/CrN were deposited by reactive magnetron sputtering at 600°C on Si substrates with different bi-layer periods λ ranging from 5 to 50 nm. The microstructure of the multilayer was investigated from X-ray diffraction and scanning electron microscopy (cross section images). Both films, Mo2N and CrN deposited at 600°C present a face centered cubic structure. As the bi-layer period was decreased, the grain size increases from 14 to 20 nm and are well crystallized with (200) preferred orientation. The nanohardness measurements show that the mechanical properties of Mo2N/CrN multilayers depend on the bi-layer period and the highest value of 29 GPa was obtained at the bilayer period of 10 nm.

DS 32: Invited Talk: Michael Heuken (joint session HL/DS)

Time: Thursday 12:30–13:00 Location: EW 201

Invited Talk DS 32.1 Thu 12:30 EW 201

Industrial Aspects of 2D Nanomaterials — •Michael Heuken[1,2], Annika Grundmann[1], Matthias Marx[1], Holger Kalisch[1], and Andrei Vescan[1] — [1]Compound Semiconductor Technology, RWTH Aachen University, Sommerfeldstr. 18, 52074 Aachen, Germany — [2]AIXTRON SE, Dornkaulstr. 2, 52134 Herzogenrath, Germany

2D nanomaterials such as graphene and layered transition metal dichalcogenides (MoS2) have attracted a lot of attention. They are very promising for future (opto)electronic devices. For TMDC, the realization of industrial fabrication is still a major challenge. To deposit large-area 2D films, high-productivity MOCVD systems are attractive allowing uniform growth on large substrates. Defined precursor fluxes and advanced temperature control enable homogeneous, precise and reproducible deposition processes. We report on the optimization of MoS2 growth on sapphire with respect to crystal quality, i. e. large crystals, and homogeneous substrate coverage, using an AIXTRON MOCVD reactor. Molybdenum hexacarbonyl and di-tert-butyl sulfide are used as metal-organic precursors, N2/H2 as carrier gases. Samples are characterized via atomic force microscopy, scanning electron microscopy, photoluminescence and Raman spectroscopy. For the deposition of graphene, an established CVD technology has been developed. Roll-to-roll-deposition equipment or technology for semiconductor grade layers on 300 mm wafers are available. Details of industrial requirements, state of the art and predicted market opportunities for 2D nanomaterials will be discussed.

DS 33: New Twists for Nanoquakes on a Chip - Emerging Applications of Surface Acoustic Waves in Condensed Matter Physics (Focussed Session): Session II

Surface acoustic waves (SAWs) with gigahertz frequencies and micrometre size wavelength can be elegantly generated using piezoelectric transducers fabricated with standard integrated circuit technology. Their small propagation velocity, tight surface confinement, as well as low susceptibility to decoherence and dissipation have been exploited over the past decades in numerous devices, in particular for electronic and optical signal processing. Today, the interaction of SAWs with electrical, optical, magnetic, and mechanical excitations in condensed matter is a highly active field of research. It is driven by the vision to harness the power of this technique in a broad spectrum of emerging applications including advanced sensors, the control of magnetization and collective excitations, as well as the coherent interactions between charge and spin excitations, photons, and phonons down to the fundamental level of single quanta. We propose a symposium that brings together experts for emerging and future applications of surface acoustic waves. For the proposed symposium we have identified potential speakers covering the large palette of fields which this versatile technique is successfully applied or currently evolving towards. These encompass nanoscale acousto-optic integrated circuits and plasmonics, the control of single quantum systems and collective excitations in hybrid systems. Because the proposed symposium covers a wide range of frontier research in which SAWs are employed with greatest success, it will serve as an ideal platform for scientific exchange. Thus, it aims to foster new interactions between the different scientific communities. Its most important goal is to introduce this exciting field of research to the many young Masters and PhD students, and postdocs attending the joint DPG-EPS Spring meeting and gives them the opportunity to present contributed talks at the symposium or associated sessions.

Organized by

Hubert Krenner, Universität Augsburg, Germany, hubert.krenner@physik.uni-augsburg.de

Jorge Pedros, Universidad Politécnica de Madrid, Spain, j.pedros@upm.es

Chris Ford, University of Cambridge, UK, cjbf@cam.ac.uk

Time: Thursday 15:00–15:45 Location: H 2032

DS 33.1 Thu 15:00 H 2032

Acousto-electric transport in epitaxial graphene coated by a ZnO piezoelectric film — •Yi-ting Liou, Alberto Hernández-mínguez, Jens Herfort, João marcelo Lopes, Abbes Tahraoui, and Paulo Santos — Paul-Drude-Institut, Berlin, Germany

We report on the transport of charge carriers in epitaxial graphene on SiC induced by surface acoustic waves (SAWs). SAWs are elastic vibrations propagating along a surface, which can be generated by applying a radio-frequency power to interdigital transducers (IDTs) deposited on piezoelectric materials. In this contribution, we report acousto-electric currents in epitaxial graphene covered by MgO and ZnO. The ZnO film provides a strong piezoelectric potential, which facilitates the acoustic transport in graphene using GHz SAWs. The 15-nm thick MgO layer is used as gate dielectric and also protects the graphene during the ZnO sputtering process. Raman spectra after the deposition of MgO and ZnO show no defect generated in graphene. In addition, the field-effect mobility at room temperature is about 2970 $cm^2\ V^{-1}\ s^{-1}$, which indicates that the electrical properties of graphene were preserved. The acousto-electric current was found to be of the order of 10 to 60 nA [1], which is up to 75 times larger than in a previous work using a 200 nm-thick SiO_2 layer instead of MgO [2]. Prospective work will include the investigation of acousto-electric transport while gate voltages are applied to further control the electrical properties of graphene.

[1] J. Phys. D: Appl. Phys. 50, 464008 (2017)
[2] Appl. Phys. Lett. 108, 193502 (2016)

DS 33.2 Thu 15:15 H 2032

Acoustically-driven surface phonon-plasmon polaritons in graphene/h-BN and graphene/h-BN/graphene heterostructures on piezoelectric substrates — •Rajveer Fandan[1], Jorge Pedrós[1], Jürgen Schiefele[2], Alberto Boscá[1], Javier Martínez[1], and Fernando Calle[1] — [1]Instituto de Sistemas Optoelectrónicos y Microtecnología, Universidad Politécnica de Madrid, Spain — [2]Instituto de Ciencia de Materiales de Madrid, CSIC, Spain

Surface plasmon polaritons (SPPs) in graphene couple strongly to surface optical (SO) phonons in the substrate leading to hybridized surface phonon-plasmon polaritons (SPPPs). Moreover, unlike conventional SPPs in metals, graphene SPPPs can be tuned in situ through the modulation of the carrier density by electrostatic gating, cover-

ing the mid-IR to THz range. Here we demonstrate that surface acoustic wave (SAW) can be used to generate propagating SPPPs in graphene/h-BN and graphene/h-BN/graphene heterostructures on AlN substrates over a broad energy range. h-BN between the graphene and the AlN substrate not only significantly changes the SPPP dispersion but also enhances the lifetime as compared to the previously studied graphene/AlN system[1]. The SPP dispersion of graphene splits into multiple branches due to the coupling with the SO phonons of both h-BN and AlN. In addition, hyperbolic phonon branches appear in the case of multilayer h-BN. Moreover, the addition of a second graphene layer is shown to further disperse and strengthen the SPPPs, providing greater robustness and tunability for future SAW-based plasmonic devices. [1] Schiefele et al., Phys. Rev. Lett. 111, 237405 (2013)

DS 33.3 Thu 15:30 H 2032

Sub-decay time control of the optical emission of lead halide perovskite nanowires at room temperature — •Lisa Janker[1], Lakshminarayana Polavarapu[2], Yu Tong[2], Alexander S. Urban[2], Jochen Feldmann[2], and Hubert J. Krenner[1] — [1]Experimentalphysik 1, Universität Augsburg — [2]Photonics and Optics Group, LMU München

The outstanding, composition-tunable optical properties of hybrid halide perovskites sparked extensive research effort worldwide leading to optoelectronic applications for photovoltaics, light emission and detectors. While most breakthrough studies focused on thin films, very recently, perovskite nanocrystals, platelets and nanowires (NWs) have been synthesized enabling size-tuning of the optical properties.

Here we report on the dynamic modulation of optical emission of $CsPbI_3$ NWs by a piezoelectric surface acoustic wave (SAW). SAWs have found various applications to probe and manipulate nanosystems at radio frequencies, e.g. to determine the mobilities in III-V semiconductor NWs.

We compare PL-transients recorded from a bundle of NWs without and with a SAW interacting with the NWs. Our experimental data clearly demonstrates that the PL-decay is periodically modulated in time by the SAW. Most strikingly, the period of this modulation is precisely $\frac{1}{2}$ T_{SAW}. The doubling of the modulation frequency points towards a field-induced displacement of the electron and hole forming an exciton. Such an electric field-driven nature of our approach promises deeper insight into excitonic properties of perovskite nanowires.

DS 34: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VII (joint session O/TT/MM/DS/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France Paul R. Kent, Oak Ridge National Laboratory, USA Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Thursday 15:00–17:45 Location: HL 001

Invited Talk DS 34.1 Thu 15:00 HL 001

Recent developments in FCIQMC: real-time propagation and improved convergence with walker number — •Ali Alavi — Max Planck Institute for Solid State Research, Stuttgart, Germany

The Full Configuration Interaction QMC method samples Slater determinants using an imaginary-time propagation of walkers, and can yield essentially exact ground- and excited states energies and wavefunctions for Fermionic systems. Recently we have extended this methodology to real-time propagation, enabling the calculation of spectral functions along the real-frequency axis. This method will be described in the talk, together with representative examples from molecular and lattice models. We will also describe a second development in the FCIQMC methodology which substantially improves the rate of convergence of the ground-state technique with respect to the number of walkers. With the new method, we can compute essentially the exact ground state energy of the benzene molecule, correlating 30 electrons (the entire valence) in the full set of 108 orbitals of a VDZ basis. Perspectives of the new methods will be discussed.

DS 34.2 Thu 15:30 HL 001

Quasi-Continuous LDA+DMFT calculations for SrVO3. — •Evan Sheridan, Christopher Rhodes, Evgeny Plekhanov, and Cedric Weber — King's College London, Theory and Simulation of Condensed Matter (TSCM), The Strand, London, United Kingdom.

The Dynamical Mean Field Theory (DMFT) is an extremely powerful tool in the treatment of strongly correlated electron systems and many DMFT calculations suffer from a computational bottleneck when it attempts to solve the Anderson Impurity Model (AIM).

Common among the early Anderson Impurity solvers was the Auxiliary Field Quantum Monte Carlo (AF-QMC) approach which relies on a discretisation of the imaginary time grid. AF-QMC solvers suffer from the notorious Suzuki-Trotter error,as a result of this , that has largely been ignored in recent years with the advent of Continuous Time-QMC (CT-QMC) solvers.

Here, we present a systematic study of how this issue can be overcome for realistic material properties using LDA+DMFT. We find that our quasi-continuous time method compares well to the state-of-the-art CT-QMC calculations for SrVO3, with the added advantage of linear scaling in temperature. The theoretical framework proposed is quite general and can be extended to cluster DMFT calculations.

DS 34.3 Thu 15:45 HL 001

High temperature superconducting oxychlorides: a light element model for cuprates — •Matteo d'Astuto[1,2], Blair Lebert[2,3], Ikuya Yamada[4], and Masaki Azuma[5] — [1]Institut NEEL CNRS/UGA UPR2940 25 rue des Martyrs BP 166 38042 Grenoble cedex 9 FRANCE — [2]IMPMC, UMR7590 UPMC-Sorbonne Universités - CNRS, Paris, France — [3]Synchrotron SOLEIL, Gif-sur-Yvette, France — [4]Nanoscience and Nanotechnology Research Center (N2RC), Osaka, Japan — [5]Materials and Structures Laboratory, TITech, Yokohama, Japan

The copper oxychloride cuprate $Ca_2CuO_2Cl_2$ (CCOC) system, with vacancy or Na doping on the Ca site, is unique among the high temperature superconducting cuprates (HTSCs) since it: lacks high Z atoms; has a simple I4/mmm 1-layer structure, typical of 214 (LSCO) cuprates, but which is stable at all doping and temperatures; and has a strong 2D character due to the replacement of apical oxygen with chlorine. It also shows a remarkable phase digram, with a superconducting T_C growing to the optimal doping without any minimum around 1/8 doping, despite the observation of charge modulations by near-field spectro-microscopy. Due to the reduced number of electrons, advanced calculations that incorporate correlation effects, such as quantum Monte Carlo are easier, but relatively little is known about CCOC (for a cuprate) from an experimental point of view. We are now filling this gap by a comprehensive experimental study covering the whole phase diagram, in particular of the (para)magnon and phonon dispersion..

DS 34.4 Thu 16:00 HL 001

Antiferromagnetic correlations in the metallic strongly correlated transition metal oxide $LaNiO_3$ — •Hanjie Guo[1], Zhiwei Li[1], Li Zhao[1], Zhiwei Hu[1], Chunfu Chang[1], Changyang Kuo[1], Wolfgang Schmidt[2], Andrea Piovano[2], Tunwen Pi[3], Oleg Sobolev[4], Daniel Khomskii[1], Liu Hao Tjeng[1], and Alexander Komarek[1] — [1]MPI CPfS, Dresden, Germany — [2]ILL, Grenoble, France — [3]NSRRC, Taiwan — [4]FRMII, Munich, Germany

The material class of rare earth nickelates with high Ni^{3+} oxidation state is generating continued interest due to the occurrence of a metal-insulator transition with charge order and the appearance of non-collinear magnetic phases within this insulating regime. The recent theoretical prediction for superconductivity in $LaNiO_3$ thin films has also triggered intensive research efforts. $LaNiO_3$ seems to be the only rare earth nickelate that stays metallic and paramagnetic down to lowest temperatures. So far, centimetre-sized impurity-free single crystal growth has not been reported for the rare earth nickelates material class since elevated oxygen pressures are required for their synthesis.

Here, we report on the successful growth of centimetre-sized $LaNiO_3$ single crystals by the floating zone technique at oxygen pressures of up to 150 bar. Our crystals are essentially free from Ni^{2+} impurities and exhibit metallic properties together with an unexpected but clear antiferromagnetic transition.

DS 34.5 Thu 16:15 HL 001

First-principles quantum Monte Carlo study of correlated materials — •Huihuo Zheng — Argonne Leadership Computing Facility, Argonne National Laboratory, Lemont, USA

Strongly correlated electronic systems have become an important subject of condensed matter physics, because of many fascinating phenomena arising in these systems such as metal-insulator transition, high temperature superconductivity, etc. Accurate characterization of the electron-electron correlations in these systems from first principles is essential for us to understand how these phenomena emerge from microscopic interactions. I will present our efforts in modeling correlated materials using the first-principles quantum Monte Carlo (QMC) method by showing two representative *ab intio* studies (vanadium dioxide and graphene) and a density-matrix downfolding theory for constructing low energy effective models from *ab initio* simulations. Using QMC, we correctly characterized the electronic structure of vanadium dioxide and unveiled the electronic origin of the metal-insulator transition which has been a mystery for decades. For graphene, we computed the electron screening from σ bonding electrons and illustrated how the emergent physics from underlying Coulomb interactions results in the observed weakly correlated semimetal. On the other hand, the downfolding approach we developed provides a way to quantitatively identify important microscopic interactions relevant to the macroscopic physics.

DS 34.6 Thu 16:30 HL 001

Reduced Density Matrix Theory for Coupled Fermion-Boson Systems — •Florian Buchholz[1], Iris Theophilou[1], Michael Ruggenthaler[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]MPSD, Hamburg, Germany — [2]CCQ, The Flatiron Institute, New York, United Sates — [3]Nano-bio Spectroscopy Group, San Sebastián, Spain

Reduced density matrix (RDM) theory proved to be successful in describing a wide range of many-body problems that are not easily accessible by the more common many-body perturbation theories or density functional theory. Especially as RDM theories are non-perturbative, they are advantageous in strong coupling scenarios.

However, RDM theory was to our knowledge never applied to systems with more than one active particle type. The focus of this talk is to analyze the possibilities and problems of an extension to coupled fermion-boson theories. Comparing a typical bilinear interaction term of the form $c_i^+ c_j (a_k^+ + a_k)$, where c^+/c and a^+/a indicate fermion and boson creation/annihilation operators, respectively and the fermionic 2-body interaction term $c_i^+ c_j^+ c_k c_l$, the former should have a considerably reduced definition space, which we hope to be exploitable. On the other hand, the bilinear interaction has a very different structure than the 2-body interaction and it is not clear at all, how to define a RDM that carries all information to compute experimental observables of a coupled fermion-boson system.

Specifically, I will illustrate some of the peculiarities of the fermion-boson interaction for simple model systems and present some ideas to deal with those.

DS 34.7 Thu 16:45 HL 001

Critical temperatures as function of magnetic anisotropy in two-dimensional systems from first-principles calculations — •Daniele Torelli — Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

Recent observation of ferromagnetic out-of-plane order in monolayer CrI_3 highlights the importance of a microscopic understanding of anisotropy in ground state magnetic systems. Single-ion anisotropy accounts mainly for spin-orbit coupling interaction and, in particular for two-dimensional (2D) materials, it's crucial to escape the Mermin-Wagner theorem. Here we investigate the variation of critical temperatures as functions of anisotropy in Heisenberg model systems using Metropolis Monte Carlo simulations. Results for square, hexagonal and honeycomb lattices are compared with equivalent simulations in the Ising model, which is confirmed to represent the limit with infinite anisotropy. Based on a new developed computational 2D materials database, we predict a vast number of 2D structures with high critical temperatures. As testing system, relevant Heisenberg exchange couplings and magnetic anisotropy energy in CrI_3 monolayer are extracted from first principle calculations and energy mapping analysis, yielding to an estimation of Curie temperature in good agreement with experimental results.

DS 34.8 Thu 17:00 HL 001

Oxygen vacancy-induced absorption of visible light in SrNbO3 — •Marcello Turtulici, Steffen Backes, and Silke Biermann — Centre de Physique Théorique, Ecole Polytechnique, 91128 Palaiseau, France

SrNbO3 has recently attracted attention as a bright red photocatalyst. Several, mutually contradicting, models have been proposed in the literature in order to explain the strong absorption in the visible spectrum, and no consensus even on the basic nature of the mechanism has been reached. In this work we investigate the optical properties of this material by means of state-of-the-art Density Functional Theory and many-body perturbation theory techniques. We evidence a high sensitivity of the optical properties on deviations from the ideal crystal structure. In particular, the optical properties should strongly depend on the presence of oxygen vacancies, which give rise to additional absorption channels in the visible frequency range. Most notably, the experimentally observed red color is likely due to transitions between orbitals of dominant Nb-eg character, which are enhanced by the strong hybridization of the quite extended 4d-states of Nb with oxygen p-states.

DS 34.9 Thu 17:15 HL 001

Transient charge and energy flow in the wide-band limit — Fabio Covito, •Florian Eich, Riku Tuovinen, Michael Sentef, and Angel Rubio — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Thanks to recent advances in ultra-fast pump-probe spectroscopies and nano-thermometry it is possible to study charge and energy flow at atomic time and length scales. In order to analyze the transient dynamics of nanoscale devices theoretically, the wide-band limit is a commonly used approximation. Here we investigate the applicability of the wide-band limit to the study of charge and heat transport through nanojunctions exposed to voltage biases and temperature gradients. We find that while this approximation faithfully describes the long-time steady-state charge and heat transport, it fails to characterize the short-time transient behavior of the junction. In particular, we find that the charge current flowing through the device shows a discontinuity when a temperature gradient is applied, while the energy flow is discontinuous when a voltage bias drives the dynamics and even diverges when the junction is exposed to both a temperature gradient and a voltage bias. We discuss this pathological behavior and propose two possible solutions.

DS 34.10 Thu 17:30 HL 001

From DFT to Coupled Cluster Theory - Understanding Oxygen Activation on Coin Metal Nanoparticles — •Wilke Dononelli and Thorsten Klüner — Institut für Chemie, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

In this study we focus on one of the most fundamental catalytic model reactions, the oxidation of CO on a metal catalyst. We studied the activation of molecular oxygen via dissociation or direct reaction of CO and O_2 within density functional theory (DFT) and high level CCSD(T) calculations. Therefore we use Au_{13} and Au_{55} nanoparticles (NPs) and a periodic Au(321) surface as model systems and compare the catalytic activity of the gold substrates to Ag and Cu based, as well as bimetallic NP catalysts. Part of the DFT calculations were performed, using the well-established PBE functional as implemented in the Vienna ab initio simulation package (VASP). Hybrid and double hybrid DFT calculations on the NPs were performed in Gaussian09. CCSD(T) calculation were performed in Gaussian09 using conventional CCSD(T) for the M_{13} (M=Au,Ag,Cu) NPs and CCSD(T)/PBE in a QM/QM embedding scheme using the ONIOM approach for M_{55} NPs. For systems of 55 metal atoms PBE gives the same results as double hybrids or even CCSD(T). For smaller M_{13} NPs interaction energies differ between PBE and higher levels of theory, which might be explained by the molecule like character of these NPs.

DS 35: Lithography IV: Lithography and Structuring (joint session KFM/DS)

This second lithography session focuses mainly on the application of advanced methods for quantum applications and the fabrication of lower dimensional systems. With the mass production of transistors devices at the 10 nm level with transmissive optical masks and with extreme UV reflective masks being at the horizon for mass fabrication, the industrial photomask fabrication is currently facing a significant technology transition and new technology requirements needed to keep pace with. The session also looks into those industrial challenges. Finally, the session focuses on important characterization methods required for the above mentioned state-of-the art lithography methods and their characterization.

Organizer: Robert Kirchner - Technische Universität Dresden

Time: Thursday 15:00–18:10 Location: EMH 025

Invited Talk DS 35.1 Thu 15:00 EMH 025

Electron Beam Lithography and Ion Beam Patterning for Applications in Quantum Technology — •Jörg Stodolka, Michael Kahl, Axel Rudzinski, and Sven Bauerdick — Raith GmbH, Dortmund, Germany

Electron Beam Lithography and Ion Beam Patterning allow to fabricate structures with nm resolution and accuracy, which is required for many devices based on quantum technology. After a general overview we present two specific applications.

First, we show an approach for a deterministic realization of photonic devices with very high process yield utilizing cathodoluminescence spectroscopy (CL) in combination with electron beam lithography: An electron beam is used to write nanopatterns in resist at positions that are preselected by local generation of light detected by CL.

Second, we present a method for scalable and maskless fabrication of silicon vacancy (VSi) defect arrays in silicon carbide using focused ion beam. The photoluminescence spectrum and optically detected magnetic resonance of the generated defect spin ensemble are used to analyze the synthesized centers and their desired defect state. The reliable production of VSi defects with a dedicated focused ion beam system allowing single ion implantation could pave the way for applications in quantum photonics and quantum information processing.

DS 35.2 Thu 15:30 EMH 025

Technology for fabrication of suspended sub-5 nm silicon nanowires and applications thereafter — Nikolay Petkov[1] and •Yordan M. Georgiev[2] — [1]Tyndall National Institute, University College Cork, Lee Maltings, Dyke Parade, Cork, T12R5CP, Ireland — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Bautzner Landstrasse 400, 01328 Dresden, Germany

Si nanowires (Si NWs) are very promising as channels for field effect transistors (FETs) and also as sensing devices. When the NW diameter is in the sub-10 nm range, quantum confinement of carriers is observed at room temperature, which is very appealing from scientific and application point of view.

This paper will present a technology for fabrication of sub-5 nm suspended Si NWs on silicon-on-insulator wafers. News of 20 nm width are first defined in the top Si layer by electron beam lithography and reactive ion etching. Then the NWs are subjected to three consecutive cycles of rapid thermal oxidation in oxygen atmosphere and wet etching in hydrofluoric acid. The resulting suspended Si NWs have high-quality crystalline structure and sub-5 nm size.

The possible applications of such NWs will be discussed, including FET-based Si NW chemo-/biosensors as well as gate all around (GAA) FETs. Additionally, the development of self-aligned nickel silicide NW contacts will be presented. The formation mechanism was examined by in-situ electron microscopy as a function of NW diameter and surface oxide.

DS 35.3 Thu 15:50 EMH 025

Photomask Manufacturing Technology - An Overview — •Christian Buergel, Torben Heins, and Martin Sczyrba — AMTC Dresden, Raehnitzer Allee, 0199 Dresden, Germany

Semiconductor devices are designed as vertical stacks of electrical components (e.g. transistors, capacities, wiring and connections), which are manufactured layer by layer during wafer processing.

Pattern formation on the wafer is done by using projection lithography and photomasks are key elements for the lithography. At least one photomask is required for each layer, where the mask contains the design information and is used as master for the desired geometries. The design, as represented on the photomasks, is replicated as a 4x demagnified image onto the wafer in the desired amount, hence enabling rapid and cost effective semiconductor production.

This presentation will give a broad overview of the manufacturing chain of a photomask. It will introduce into required processes like data preparation and manipulation for mask writing, resist and absorber material processing, metrology and inspection as well as mask repair and its qualification.

DS 35.4 Thu 16:10 EMH 025

Simulation of Ion Beam induced Surface Dynamics — •Alrik Stegmaier and Hans Hofsäss — 2. Physikalisches Institut, Georg-August Universität Goettingen

Structuring of surfaces through ion beam irradiation can be used to create self organizing dune-like waves, dimples, flat surfaces or chaotic patterns. The final structures are a result of the interplay of sputtering, redeposition, projectile implantation, transport and viscous flow, void/bubble formation and the initial surface conditions.

Accurate simulations of structuring are possible through molecular dynamics simulations, but these simulations are computationally too expensive to allow for a prediction of up to micrometer scale structure. A much faster approach is available through the use of continuum models. For this the net effect of the irradiation is expressed as the local change in surface height as a function of and up to forth order spacial derivatives of the local surface height. Typically the resulting equations of motion are taylor-expanded up to second order. Such an approach can be accurate when the surface is relatively flat and shadowing is not important, but the parameters often need to be empirically readjusted for experiments at different impact angles, ion energies or materials.

Here we present a new software package that allows for the rapid simulation of surface dynamics for arbitrary, nonlinear equations of motion that can also include nonlocal effects. With this software we explore nonlinear expansions to some of the common models, the effects of shadowing at flat impact angles and parameter determination through binary collision approximation simulation.

20 min. break

DS 35.5 Thu 16:50 EMH 025

NFFA-Europe: enhancing European competitiveness in nanoscience research and innovation — •Dimitrios Kazazis — Paul Scherrer Institut, 5232 Villigen, Switzerland

NFFA-Europe is a European open-access resource for experimental and theoretical nanoscience. It brings together advanced infrastructures throughout Europe, specialized on growth, nanolithography, nanocharacterization, theory, simulation and fine-analysis with Synchrotron, FEL and Neutron radiation sources to create a multi-site research platform that enables European and international researchers to carry out advanced project proposals impacting science and innovation. NFFA-Europe coordinates access to infrastructures on different aspects of nanoscience research that are not currently available at single specialized sites. Technique and tool selection, proposal construction and submission are all done through a single and intuitive web portal. The access to the combined infrastructures through NFFA-Europe is centrally coordinated and free of charge for all technologically feasible and internationally peer-reviewed and approved user projects. Not only do the approved projects have access to the combined infrastructures, but they also benefit from the competences and the technical support of the NFFA sites as well as a contribution towards travel and subsistence costs. NFFA-Europe's internal joint research activities address

key bottlenecks of nanoscience and nanotechnology i.e. nonostracture traceability, protocol reproducibility, in-operando nanomanipulation and analysis, open data etc. (www.nffa.edu)

DS 35.6 Thu 17:10 EMH 025

Fresnel-Mirror-Setup for Interference Lithography — •Arrigo Facchini[1], Bodo Fuhrmann[2], Hartmut S. Leipner[2], Georg Schmidt[1,2], and Roland Scheer[1] — [1]Martin Luther University Halle-Wittenberg Institute of Physics, D-06099 Halle (Saale), Germany — [2]Martin Luther University Halle-Wittenberg Interdisciplinary Center of Materials Sciences, D-06099 Halle (Saale), Germany

Interference lithography is one of many alternative lithography techniques for the fast fabrication of large area regular nano- and microscale patterns. A variety of more or less complex setups using Lloyd*s interferometers or beam splitters are described in literature.

In particular, rigid Lloyd*s interferometer setups allow the fast change of the periodicity by simply changing the angle of incidence. They have, however, the drawback that for smaller angles of incidence (larger periodicity) the illuminated area decreases and as a consequence also the possible sample size.

Here a robust Fresnel mirror setup is presented, which overcomes this problem and allows the fast fabrication of regular patterns in the *m-range with freely selectable periodicity. The maximum sample size is only determined by the setup chosen.

DS 35.7 Thu 17:30 EMH 025

Analysis of rough nanostructured surfaces by EUV-scatterometry — •Analía Fernández Herrero, Frank Scholze, and Victor Soltwisch — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany

Lamellar-gratings are commonly-used as diffractive optical elements or in state-of-the-art integrated electronic circuits. For the control of the lithographic manufacturing process in semiconductor manufacturing a rapid in-line characterization of the nanostructures is indispensable. With shrinking structure sizes, roughness gains influence on the device performance. Therefore the analysis of nanostructured surfaces demands the development of new metrology tools capable of destruction-free measurements, which, at the same time, deliver statistical information, relevant for the study of the imperfections. Small angle X-ray scattering under grazing incidence has already been investigated for the determination of the geometry parameters of such structures. Several reports stress the importance of the identification of the roughness contributions. Using EUV or soft X-ray radiation, with longer wavelengths, larger incidence angles can be used reducing the beam footprint on the samples without compromising the surface sensitivity. We present a new experimental tool to be developed at the PTB soft X-ray beamline at the electron storage ring BESSY II for the measurement of small structures and roughness contributions based on soft X-ray and EUV scatterometry.

DS 35.8 Thu 17:50 EMH 025

GISAXS reconstruction of profiles of gratings produced by quadruple patterning — •Mika Pflüger[1], Victor Soltwisch[1], R. Joseph Kline[2], Frank Scholze[1], and Michael Krumrey[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany — [2]National Institute of Standards and Technology (NIST), Gaithersburg, United States

New approaches are needed for the fast, non-destructive dimensional measurement of complex nanostructures produced in the semiconductor industry. One technique being considered is Small-Angle X-ray Scattering (SAXS), which has already been used to reconstruct the line profile of gratings with low uncertainties. Grazing-Incidence SAXS (GISAXS) additionally provides surface sensitivity, but the interpretation of the scattering is complicated by multiple scattering effects.

To produce structures beyond the diffraction limit of a single lithographic exposure, self-aligned double patterning (SADP) can be used. In SADP, sidewalls are deposited on the original line and the original line is removed, such that the sidewalls form lines with a doubled structure density. If the sidewall width and the original linewidth do not match, an alternating pitch error is introduced, impacting the performance of the resulting structures.

We present GISAXS measurements of a sample series produced by self-aligned quadruple patterning with varying pitch errors. From the intensities of the grating diffraction orders, we quantify the pitch errors and compare our results to previous SAXS measurements of the same samples.

DS 36: Organic Thin Films, Organic-Inorganic Interfaces: Session II (joint session DS/CPP)

Time: Friday 9:30–11:00 Location: H 0111

DS 36.1 Fri 9:30 H 0111

Infrared studies of device relevant organic/inorganic interfaces: energetic and morphological insights — •Sabina Hillebrandt[1,2], Sebastian Beck[1,2], and Annemarie Pucci[1,2] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — [2]InnovationLab, Heidelberg, Germany

Organic electronic devices consist of stacked layers as well as inorganic materials. The device performance is mainly influenced by the interfaces of these 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 self-assembled monolayers (SAM) in this context to engineer the surface of certain electrode materials, e.g. indium tin oxide (ITO) and metal surfaces, in order to improve charge injection at the organic/inorganic interface. With their inherent dipole SAMs are ought to improve the energetic alignment at the interface as well as to change the surface energy and thus the contact angle. Infrared (IR) spectroscopic studies supported by density functional theory (DFT) calculations reveal in addition to the molecular orientation of such SAMs the influence on that orientation on the subsequent organic semiconductor material. Furthermore, energy transfer between the electrode material and its modification and the organic semiconductor can be investigated, giving a deep insight into the energetic and morphological interplay at the interface.

DS 36.2 Fri 9:45 H 0111

Probing the orientation of phosphorescent Iridium complexes by impedance spectroscopy — •Markus Schmid, Thomas Lampe, Alexander Hofmann, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Impedance spectroscopy (IS) is a powerful, non-destructive method to analyze organic semiconductors and their interfaces. In organic bilayer devices, that contain one polar material, IS can be used to measure the interfacial charge density between the two semiconductors. This polarization results from partially aligned permanent dipole moments. If the permanent molecular dipole moment is known, conclusions about the molecular orientation are possible [1].

In this study we present results from IS for different polar Iridium complexes that are commonly used as emitters in organic light emitting diodes. By calculating their permanent dipole moment and their transition dipole moment via density functional theory we relate the average orientation of both vectors in the film. Additionally, the measured alignment of the molecules is compared to molecular dynamic simulations. We find good agreement between both, the often studied orientation of the transition dipole moment and the simulations.

[1] Jäger, Lars, *et. al.* AIP Advances **6**, 095220 (2016)

DS 36.3 Fri 10:00 H 0111

Comparative in-situ studies of Au sputter growth on homo and di-block co-polymer — •Pallavi Pandit[1], Matthias Schwartzkopf[1], Andre Rothkirch[1], Bjoern Fricke[1], Marc Gensch[1], Alexander Hinz[2], Oleksandr Polonskyi[2], Thomas Strunskus[2], Simon Schaper[3], Franziska C. Löhrer[3], Volker Körstgens[3], Franz Faupel[2], Peter Müller-Buschbaum[3], and Stephan V. Roth[1,4] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]CAU zu Kiel, LS Materialverbunde, 24143 Kiel — [3]Physik-Department, LS Funktionelle Materialien, 85748 Garching — [4]KTH, Teknikringen 56-58, SE-100 44 Stockholm

Nanostructured gold (Au) attracts great technological interest and it is a promising candidate for functional, optical and electronic applications. A tailored metal nanoparticle-polymer interface improves the functionality of the system; attributed to the polymer-metal interac-

tions, which are dominated by their interfacial interactions. Sputter deposition technique has been used for depositing metallic layer of few nanometer thicknesses in a controlled fashion on polymer surfaces [1]. To this end, we have investigated the morphological changes occurring at the metal-polymer interface during deposition using GISAXS and GIWAXS [2]. Optical properties of the system have also been studied in-situ and are correlated with the morphological properties of the gold nanocluster on polystyrene, polymethelmethacrlate and the corresponding di-block co-polymer. [1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 9, 5629 (2017). [2] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015).

DS 36.4 Fri 10:15 H 0111

Graphene based biosensing surfaces studied by IR-nanopolarimetry — •Karsten Hinrichs[1], Timur Shaykhutdinov[1], Christoph Kratz[1], Felix Rösicke[2], Cristoph Arenz[3], Norbert H. Nickel[2], and Jörg Rappich[2] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Schwarzschildstr 8, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekuléstr. 5, 12489, Berlin, Germany — [3]Institut für Chemie der Humboldt-Universität zu Berlin. Brook-Taylor-Str. 2, 12489 Berlin, Germany

AFM-IR based nanopolarimetry [1] for analysis of large area graphene pre-functionalized by diazonium compounds [2] and recognition of cysteine-modified peptide nucleic acid (PNA) [3] is presented. Homogeneity of the biosensing surfaces and the secondary structure of the PNA was studied by AFM-IR measurements. AFM-IR in a sensitive modus with synchronization between the pulse rate of the quantum cascade laser used as IR light source and the resonance of the cantilever can provide IR spectra in several seconds only. This facilitates direct insight into chemical composition, intermolecular interactions, and molecular orientation in nanoscale sub-ensembles.

[1] T. Shaykhutdinovet al, Supramolecular Orientation in Anisotropic Assemblies by IR Nanopolarimetry. ACS Macro Letters 2017, 598-602. [2] F. Rösicke et al, Chem. Commun. 53 (2017) 9308-9311. [3] K. Hinrichs et al, Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry 2018.

DS 36.5 Fri 10:30 H 0111

Study of reactive ion beam planarization process of a negative tone resist for smoothing aluminium mirrors — •Melanie Ulitschka, Jens Bauer, Frank Frost, and Thomas Arnold — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, 04318 Leipzig

Mirror optics are a key component for a wide range of optical systems in lithography, imaging, as well as aerospace industry. For such a specific field of applications lightweight, good machinable aluminum alloys are suitable since the reflection coefficient ranges from the UV to the IR spectral region with values well above 90%. The surface error topography after commonly manufacturing by single-point diamond turning meets the requirements for applications in the infrared spectral range. To use the aluminum mirrors in the shortwave visible and UV-spectral range one technological solution is the coating of the Al optics with a nickel-phosphorous layer and a metallization layer on top to realize ultra-smooth highly reflective surfaces. Further reduction of the surface roughness of aluminum optics and a simplification of this process chain is preferable.Ion beam planarization processes are a promising technology to transfer the ultra-smooth surface of a planarization layer into the underlying aluminum substrate. An equal etch rate for planarization layer and aluminum is the prerequisite for the transfer process. The contribution comprises investigations on the influence of different ion beam parameters on the chemical modification of the layer during the etch process, the effect of thermal pre-treatment of the planarization layer and the etch rate selectivity of layer and substrate.

DS 36.6 Fri 10:45 H 0111

Structure-Dependent Emission of 1-(Pyridin-2-yl)-3-(quinolin-2-yl)imidazo[1,5-a]quinoline — •Georg Albrecht[1,3], Jasmin Martha Herr[2,3], Hisao Yanagi[3], Richard Göttlich[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, JLU Giessen, Germany — [2]Institute of Organic Chemistry, JLU Giessen, Germany — [3]Nara Institute of Science and Technology, Japan

1,3-disubstituted imidazo[1,5-a]pyridines are receiving increased interest for applications in material science, mainly regarding organic light emitting diodes (OLED). In this work we studied the related 1-(pyridin-2-yl)-3-(quinolin-2-yl)imidazo[1,5-a]quinoline (PCIC) as a new and oxidation-stable blue emitter. Thin films were prepared by physical vapor deposition onto quartz glass, single crystals were grown from solutions or by entrainer sublimation. Thin films and crystals were characterized by AFM, XRD, optical absorbance and mainly by steady-state and time-resolved emission and compared to results obtained in solution. Storage of the originally amorphous thin film samples revealed an interesting crystallization behaviour, which could be resolved by fluorescence microscopy and comparison to the results obtained at single-crystals. A clear trend of red-shifted emission was observed for different crystalline phases relative to amorphous samples, corresponding to the change in molecular arrangement.

DS 37: 2D Materials: Session III (joint session DS/CPP/HL)

Time: Friday 9:30–12:30 Location: H 2032

Invited Talk DS 37.1 Fri 9:30 H 2032

Tunable Electronic Structures, Magnetism, and Axis-Dependent Conduction Polarity in Ge and Sn-based 2D Materials — •Joshua Goldberger — The Ohio State University, Columbus, OH USA

Here, we will discuss recent developments in the synthesis, properties, and applications of two classes of Ge- and Sn-based 2D materials; the ligand-functionalized Ge/Sn graphane analogues, and the exfoliatable van der Waals Zintl phases. First, the Ge/Sn graphane analogues have generated much excitement as their electronic structures are predicted to range from trivial insulators, to semiconductors with tunable gaps, to semimetallic, to topological insulators, depending on the substrate, chemical functionalization and strain. Through the synthesis and characterization of a large family of ligand-functionalized germananes, we will show how the electronic structure can be manipulated via surface chemistry. Second, we will highlight a new family of chemically and thermally robust exfoliatable 2D materials having a stoichiometry of ASn2Pn2, where A is a cation, and Pn is a pnictogen. This class of materials can be designed to exhibit a broad range of phenomena including the topological insulating compound, SrSn2As2, as well as the magnetic compound, EuSn2As2. Also, we will show that NaSn2As2 simultaneously exhibits opposite sign conduction polarities along its in-plane and cross-plane axes. Using a variety of advanced transport measurements we establish the band structure origins of this behavior. Together, these materials show how the inherent anisotropy in 2D materials can be rationally tailored to give rise to new phenomena.

DS 37.2 Fri 10:00 H 2032

Chemical and optical properties of transition metal dichalcogenide monolayers at the nanometer and subnanometer scale — •Luiz Tizei[1], Alberto Zobelli[1], Ching-Hwa Ho[2], Kazu Suenaga[3], Alexandre Gloter[1], Mathieu Kociak[1], and Odile Stéphan[1] — [1]Laboratoire de Physique des Solides, University of Paris-Sud, CNRS, Orsay, France — [2]National Taiwan University of Science and Technology, Taipei, Taiwan — [3]AIST, Tsukuba, Ibaraki, Japan

Defects and interface play an important role in material properties. Therefore, their characterization at the nanometer scale is crucial. Here, core-loss EELS and high angle annular dark field imaging have been used to identify single Cr atoms in WSe_2 monolayers. These atoms are always located at the metal site (W) with a 3+ formal valence, as deduced from EELS fine structure comparison with known references and X-ray photoelectron spectroscopy (XPS). Furthermore, Cr atoms are observed systematically close to single our double Se vacancies, indicating a possible electron doping of the system. Moreover, semiconducting 2H phase TMD monolayers present spin-split valence and conduction bands due to spin-orbit coupling. These two near band edge states are separated by from a few tens to a few hundred meV and can be measured by EELS with high spatial resolution. As an example, we will show measurements of the near band edge losses as a function of position across an interface between two TMDs. Results will be compared to calculated loss functions, tacking into account the materials' dielectric function.

DS 37.3 Fri 10:15 H 2032

Excitonic Phonon Sidebands in Monolayer Transition Metal Dichalcogenides — •Dominik Christiansen[1], Malte Selig[1], Gunnar Berghäuser[2], Robert Schmidt[3], Iris Niehues[3], Robert Schneider[3], Ashish Arora[3], Steffen Michaelis de Vasconcellos[3], Rudolf Bratschitsch[3], Ermin Malic[2], and Andreas Knorr[1] — [1]Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, Gothenburg, Sweden — [3]Physikalisches Institut und Zentrum für Nanotechnologie, Universität Münster, 48149 Münster, Germany

Monolayers of transition metal dichalcogenides (TMDs) show an extraordinarily strong Coulomb interaction, leading to the formation of tightly bound excitons. Because of a complex quasi-particle band structure, TMDs possess a variety of bright sates (addressable by light) and dark states (addressable by phonons). Here, we present a joint experiment-theory study on the influence of exciton-radiative and exciton-phonon interaction on the absorption line shape of different monolayer TMD materials. Solving the TMD Bloch equations in the quantum kinetic limit, we predict the appearance of spectrally asymmetric phonon-induced sidebands that are accompanied by a pronounced polaron-red shift. We analyze the influence of the interplay of phonon emission/absorption processes and dark intra- and intervalley excitonic states on the asymmetry of the absorption line shape.

D. Christiansen, et. al, Phys. Rev. Lett. 119, 187402 (2017)

DS 37.4 Fri 10:30 H 2032

Lifetime of Valley Excitons in Monolayer Transition Metal Dichalcogenides — •Malte Selig[1], Samuel Brem[2], Florian Katsch[1], Gunnar Berghäuser[2], Ermin Malic[2], and Andreas Knorr[1] — [1]Nichtlineare Optik und Quantenelektronik von Halbleitern, Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, Gothenburg, Sweden

In monolayers of transition metal dichalcogenides, weak screening leads to the formation tightly bound excitons which dominate the optical properties of these ultrathin materials. A pronounced circular dichroism leads to a spin and valley selective excitation of excitons at the corners of the hexagonal Brillouin zone. A microscopic understanding of the lifetime of such optically injected spins is of crucial interest for future technological applications. Here, based on a Heisenberg of motion formalism for excitons, we perform microscopic momentum and spin resolved computations to investigate the impact of exciton phonon coupling and intervalley exchange coupling on the valley lifetime of excitons. In our analysis, we also include recently discussed indirect dark excitons [1,2]. In the absence of low lying dark states we find valley lifetimes below 1 ps, which increases by orders of magnitude if the material is indirect.

[1] M. Selig et al., Nat. Commun. 7, 13279 (2016)
[2] M. Selig et al., arXiv:1703.03317 (2017)

DS 37.5 Fri 10:45 H 2032

Interface sensitive structure determination of silicon nanoribbons on Gold surfaces — •Peter Roese[1,2], Philipp Espeter[1,2], Karim Shamout[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1, Technische Universität Dortmund, Germany — [2]DELTA, Technische Universität Dortmund, Germany

In the last years there has been much progress in the growth and analysis of 2D-materials beyond graphene on metallic surfaces. Especially, silicon based two-dimensional silicene and one-dimensional silicon nano-ribbons came into scientific focus due to their promising electronic properties. Beside the exact knowledge of the fascinating electronic and chemical properties of such systems, the structural information is of great interest for precise DFT calculations. In this context the interaction between the silicon nano-ribbons and the substrate plays an important role. Techniques like STM or LEED provide information about the electronic structure of such systems but neither chemical information about the atomic bonds nor information about the interface. Photoelectron spectroscopy and diffraction easily provide information about atomic bonds and the interface between silicon nano-ribbons and the substrate, recently shown by Espeter et al [8]. The structure of silicon nano-ribbons on Ag(110) has recently been resolved whereas their exact structure on Au(110) and the effect of the interface needs to be analyzed in detail. Based on previous works, we present first photoelectron diffraction results of silicon nano-ribbons on Au(110).

15 min. break.

DS 37.6 Fri 11:15 H 2032

Disclosing the nature of excitons in van der Waals materials: The role of layer stacking in hexagonal boron nitride — •Wahib Aggoune[1,2], Caterina Cocchi[2,3], Dmitrii Nabok[2,3], Karim Rezouali[1], Mohamed Akli Belkhir[1], and Claudia Draxl[2,3] — [1]Laboratoire de Physique Théorique, Faculté des Sciences Exactes, Université de Bejaia, 06000 Bejaia, Algeria — [2]Institut fur Physik and IRIS Adlershof, Humboldt-Universitat zu Berlin, Berlin, Germany — [3]European Theoretical Spectroscopic Facility (ETSF)

With the example of bulk hexagonal boron-nitride, a prototypical van der Waals (vdW) crystal, we demonstrate that the electronic and optical properties of these materials can be tuned by layer patterning. By modifying the stacking, energy, intensity, and character of the electron-hole (e-h) pairs can be selectively modulated. Depending on the specific layer arrangement, lowest-energy excitons are localized within a single layer or delocalized in the three-dimensional space. Only in specific stackings charge-transfer e-h pairs appear above the absorption onset, triggered by the spatial distribution of the electronic states involved. Our results, obtained within a first-principles many-body framework, provide all the ingredients to identify, predict, and tailor the character of the e-h pairs in vdW materials.

DS 37.7 Fri 11:30 H 2032

Evidence for low-dimensional charge transport in carbon nitride polymers — •Christoph Merschjann — Helmholtz-Zentrum-Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

Carbon nitride (CN) polymers have gained much interest in recent years due to their potential application as both dark- and photocatalysts for various renewable-energy tasks, including water-splitting and CO_2 reduction, and others. Given their layered, van-der-Waals bound structure, these materials resemble graphite, and are hence often called "graphitic carbon nitrides" (g-C_3N_4). The main technical advantage of CNs is the abundance of their constituents (C, N, and H) and the absence of precious metals. However, compared to metal-based catalysts, the activity of CN materials is still rather low, a fact that has been largely attributed to their low conductivity. Recently, we found evidence that this low conductivity is due to polaronic hopping motions of photoexcited electrons and holes, which predominantly move vertical to the graphitic planes of the material. Backed-up by very recent transient-spectroscopy studies, we will discuss the validity of such a low-dimensional transport scenario, and its consequences for applications in catalysis as well as in organic electronics in general.

DS 37.8 Fri 11:45 H 2032

Deterministic Positioning of Single-Photon Emitters in Monolayer WSe_2 on the Nanoscale — •Johannes Kern[1], Iris Niehues[1], Philipp Tonndorf[1], Robert Schmidt[1], Daniel Wigger[2], Robert Schneider[1], Torsten Stiehm[1], Steffen Michaelis de Vasconcellos[1], Doris E. Reiter[2], Tilman Kuhn[2], and Rudolf Bratschitsch[1] — [1]Institute of Physics and Center for Nanotechnology, University of Münster, Germany — [2]Institute of Solid State Theory, University of Münster, Germany

Single-photon emitters are an important building block for photonic quantum technology. Here, we deterministically position single-photon emitters in monolayer WSe_2 on the nanoscale [1]. The atomically thin semiconductor is placed on top of a gapped single-crystalline gold rod which results in a folding of the monolayer around the metal nanostructure. At the gap position, local strain is induced in the atomically thin semiconductor. Excitons localize there and radiatively decay via single-photon emission.

[1] J. Kern et al., "Nanoscale positioning of single-photon emitters in atomically thin WSe2", Adv. Mater. 28, 7101-7105, (2016).

DS 37.9 Fri 12:00 H 2032

Pulsed Laser Deposition of Monolayer WSe_2 — •Avaise Mohammed[1], Hiroyuki Nakamura[1], Peter Wochner[1], Shyjumon Ibrahimkutty[1], Armin Schulz[1], Kathrin Müller[1], Krystian Nowakowski[2], Keita Matsuda[3], Johannes Geurs[1], Yijin Zhang[1], Mona Stadler[4], Kenji Watanabe[5], Takashi

Taniguchi[5], Benjamin Stuhlhofer[1], Georg Cristiani[1], Gennady Logvenov[1], Michael Jetter[4], Peter Michler[4], Jurgen Smet[1], Ulrich Starke[1], and Hidenori Takagi[1,6] — [1]MPI-FKF — [2]University of Twente — [3]Nagoya University — [4]IHFG, University of Stuttgart — [5]NIMS — [6]IFMQ, University of Stuttgart

Ultrathin WSe_2 films were deposited using a custom built hybrid-Pulsed Laser Deposition (PLD) system on different substrates. Raman spectroscopy and atomic force microscopy were used to identify the monolayer (ML) WSe_2. Synchrotron based grazing incidence X-ray diffraction revealed WSe_2 films to have a compressive strain on Al_2O_3 r-cut substrates. Angle resolved photoelectron spectroscopy confirmed the valance band structure of ML WSe_2 on epitaxial graphene with a clear spin splitting of 480 meV. Photoluminescence signal was identified from ML WSe_2 deposited on hexagonal BN. The results give evidence for PLD to be an excellent approach for the growth of monolayer transition metal chalcogenides.

DS 37.10 Fri 12:15 H 2032

Gate-dependent spin dynamics of dark trion states in monolayer WSe_2 — •Manfred Ersfeld, Frank Volmer, Maximilian Heithoff, Christopher Franzen, Christoph Stampfer, and Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

We explore the spin dynamics in WSe_2 monolayers by time-resolved Kerr rotation measurements. The longest spin lifetimes of up to 150 ns are observed at 5 K when resonantly pumping into charged exciton states (trions). We explain these long spin lifetimes by the formation of dark trion states which exhibit equal recombination lifetimes independently measured by time-resolved reflectivity [1]. We show that the spin lifetimes of the dark trion states strongly depend on the chemical potential which we tune by applying a gate voltage to the WSe_2 flake through a SiO_2/Si^{++} substrate. The formation of the dark trion states require intervalley scattering driven by short range scattering centres. Additional photoluminescence measurements indicate that this short range scattering is caused by localized states and gets strongly diminished with increasing temperature which may also be relevant for the overall strong decrease of both the spin amplitude and the spin lifetime of the dark trion states with increasing temperature.

[1] F. Volmer et al., Phys. Rev. B 95, 235408 (2017)

DS 38: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VIII (joint session O/TT/MM/DS/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Friday 10:30–12:45 Location: HL 001

DS 38.1 Fri 10:30 HL 001

Ab initio photoluminescence in 2D materials — •Pedro Melo[1,4], Andrea Marini[2,4], Matthieu Verstraete[1,4], and Zeila Zanolli[3,4] — [1]NanoMat / CESAM, ULiege Belgium — [2]ISM CNR, Italy — [3]RWTH Aachen Germany — [4]ETSF

The theoretical study of photoluminescence (PL) has been hindered in the past due to lack of predictive ab initio numerical techniques [1,2,4]. We present a complete theoretical framework for the computation of PL where electrons, nuclei, and photons are quantised. The intrinsic non-equilibrium nature of the process is fully taken into account [3]. Starting from the Keldysh contour, we arrive at a set of equations for the Green's functions of electrons, phonons, and photons where the different kinds of interactions are treated on the same footing. These equations are then simplified by using the generalised Baym-Kadanoff ansatz and the completed collision approximation [3]. This reduces the problem to a set of decoupled equations for the density matrix that describe all kinds of static and dynamical correlations. We show how the micro-macro connection relates the observable spectrum with the time-dependent microscopic dynamics, via the Bethe-Salpeter equation. Finally, we present the results of our numerical studies on 2D materials, such as WS2, where we relate the evolution of the carrier populations in the Brillouin zone with the changes in the PL spectrum of the material, for a range of experimental setups. [1] M. F. Pereira and K. Henneberger, PRB 58, 2064 (1998). [2] K. Hannewald, et al, PRB 67, 233202 (2003). [3] P. M. M. C. de Melo and A. Marini, PRB 93, 155102 (2016). [4] S. W. Koch, et al, Nat Mat 5, 523 (2006).

DS 38.2 Fri 10:45 HL 001

Strain on molybdenum disulfide sheets with defects from first principles — •Mohammad Bahmani[1], Mahdi Faghihnasiri[2], and Thomas Frauenheim[1] — [1]BCCMS, Physics Department, Bremen University, Bremen, Germany — [2]Physics Department, Shahrood University of Technology, Shahrood, Iran

Single layer of transition metal dichalcogenides(TMDCs) are under intense investigations since the discovery of unique characteristics of 2D and Vann der Waals layered materials. They are predicted to be the most promising structure for various future nanoscale devices. They have also novel applications in spintronic and optoelectronic. As a result of thermal equilibrium and the kinetics of processing, all real materials contain structural defects which show significant effects on their electrical, optical, vibrational, magnetic, and chemical properties. Besides, mechanical strain has very much influence on the electronic properties of 2D materials, particularly TMDCs. For example, 0.5% biaxial strain force direct band gap in molybdenum disulfide(MoS2) to become indirect since it breaks the crystalline symmetry. Therefore, I study different types of point defects such as single and double sulfur(S), single molybdenum(Mo) vacancies, and removing a Mo with its three upper S neighbors. I also substitute a Mo vacancy with one and two S atoms. Furthermore, as the second aim of this study, I showed the modification of defect states under uniaxial and biaxial compression and tensile strain. For the case of one S vacancy, this moves shallow states into the valance band and importantly breaks the degeneracy of degenerate states.

DS 38.3 Fri 11:00 HL 001

Competion of magnetic interactions and in-field behavior of cycloidal Uranium compound UPtGe. — •Leonid Sandratskii — Max Planck Institute of Microstructure Physics, Halle, Germany

Stimulated by recent high-field experiment [1] performed on unique actinide system with cycloidal magnetic structure, UPtGe, I performed a series of calculations aiming to understand the nature of the sequence of magnetic phase transitions caused by the applied magnetic field. The physics of the system is determined by the fine balance of the exchange interaction, magnetic anisotropy, and Dzyaloshinskii-Moriya interaction. This balance of interactions governs, in particular, the in-field behavior of the system. The physical consequences of the variation of the localization of the U 5f electrons is investigated.

[1] A. Miyake, A. Nakamura, Y. Shimura, Y. Honma, D. Li, F. Honda, M. Tokunaga, D. Aoki, doi.org/10.11316/jpsgaiyo.71.1.0_2062.

DS 38.4 Fri 11:15 HL 001

Electron correlation effects in the electronic structure of 4f-atoms adsorbed on metal and Graphene substrates — •Alexander B. Shick[1], Dmitry S. Shapiro[2], and Alexander I. Lichtenstein[3] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]nstitute of Radio Engineering and Electronics, Russian Academy of Sciences, Moscow — [3]Institute of Theoretical Physics, University of Hamburg, Germany

Surface supported single magnetic atoms, the so-called "single-atom magnets", open new opportunities in a quest for the ultimate size limit of magnetic information storage. Initially, the research mainly focused on 3d-atoms on surfaces. Recently, the attention was turned to the 4f-atoms, culminating in the experimental discovery of magnetically stable Ho atom on MgO(001) substrate [1], and Dy atom on graphene/Ir(111)[2]. We address the electronic and magnetic character of 4f-atoms on metal and Graphene substrate making use of a combi-

nation of the DFT with the exact diagonalization of Anderson impurity model (DFT+ED) [3]. The spin and orbital magnetic moments of Dy@Ir(111) and Dy/Graphene/Ir(111) are evaluated and compared with experimental XMCD data. The magnetic anisotropy energy is estimated, and the magnetic stability is discussed. The role of 5d-4f interorbital exchange polarization in modification of the 4f-shell energy spectrum is emphasized. [1] F. Donati et al., Science 352, 318 (2016). [2] R. Baltic et al., Nano Lett. 16, 7610 (2016). [3] A. B. Shick, D. S. Shapiro, J. Kolorenc, A. I. Lichtenstein, Sci. Rep. 7, 2751 (2017).

DS 38.5 Fri 11:30 HL 001

Interlayer trions in the MoS_2/WS_2 van der Waals heterostructure — •Thorsten Deilmann and Kristian Sommer Thygesen — CAMD, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Electronic excitations in van der Waals heterostructures can have interlayer or intralayer character depending on the spatial localisation of the involved charges (electrons and holes). In the case of neutral electron-hole pairs (excitons), both types of excitations have been explored theoretically and experimentally. In contrast, studies of charged trions have so far been limited to the intralayer type.

Here we investigate the complete set of interlayer excitations in a MoS_2/WS_2 heterostructure using a novel ab-initio method, which allows for a consistent treatment of both excitons and trions at the same theoretical footing. Our calculations predict the existence of bound interlayer trions below the neutral interlayer excitons. We obtain binding energies of 18/28 meV for the positive/negative interlayer trions with both electrons/holes located on the same layer. In contrast, a negligible binding energy is found for trions which have the two equally charged particles on different layers.

DS 38.6 Fri 11:45 HL 001

The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining — •Miguel Marques[1] and Antonio Sanna[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck Institut für Microstrukture Physics, Weinberg 2, 06120 Halle, Germany

Starting from the experimental data contained in the inorganic crystal structure database, we use a statistical analysis to determine the likelihood that a chemical element A can be replaced by another B in a given structure. This information can be used to construct a matrix where each entry (A,B) is a measure of this likelihood. By ordering the rows and columns of this matrix in order to reduce its bandwidth, we construct a one-dimension ordering of the chemical elements, analogous to the famous Pettifor scale. The new scale shows large similarities with the one of Pettifor, but also striking differences, especially in what comes to the ordering of the non-metals.

DS 38.7 Fri 12:00 HL 001

Novel two-dimensional topological insulators from first principles materials screening — •Thomas Olsen and Kristian Thygesen — Technical University of Denmark

We have applied first principles calculations to find new stable two-dimensional materials with non-trivial band topology. The novel materials include more than 10 quantum spin Hall insulators, quantum anomalous Hall insulators and topological crystalline insulators protected by mirror symmetry. We also discuss the dual topological nature of the band structure in the presence of both time-reversal and mirror symmetry and show that odd mirror Chern numbers always imply a quantum spin Hall effect.

DS 38.8 Fri 12:15 HL 001

Nanoparticles Classification with Self-Organisation Map (SOM) on 3D Electrostatic Potential Surface (EPS) — •Baichuan Sun and Amanda Barnard — Molecular & Materials Modelling, Data61 CSIRO, Door 34 Goods Shed, Village St, Docklands, VIC 3008, Australia

State-of-the-art deep learning (DL) algorithms are having tremendous impact across all scientific fields, and Material Science (MS) is no exception. A combination of computational chemistry simulations and DL techniques requires a hybrid computation/data research workflow, which represents a revolutionary approach to MS studies. There is a gap between the ab initio characterisation of nanomaterials with electronic structure simulations and its analytics with DL frameworks which stems from difficulties in representing quantum mechanical properties in such a way that is suitable for artificial neural networks. To overcome this issue we are evaluating the efficiency of visualising the 3-D Electrostatic Potential Surface (EPS) with Self-organising Maps (SOM), and integrating them directly into reliable DL frameworks. A Self-organisation Map classifies high-dimensional data into low-dimensional (normally 2D) space without supervision, while retaining the intrinsic topological relationship of the data set. As we will show, it is possible to represent a 3D molecular EPS with a single 2D snapshot, or "fingerprint" of the particle, provided they are orientationally invariant. In this study we demonstrate how Ag nanoparticles 3-D EPS self-organising texture maps can be used to classify nanoparticles based on the energy of the Fermi level.

DS 38.9 Fri 12:30 HL 001

Regulation of structure and high thermoelectric performance of 1D SnTe via encapsulation within single-walled carbon nanotube — Andrij Vasylenko[1], •Jamie Wynn[2], Sam Marks[1], Paulo V. C. Medeiros[3], Quentin M. Ramasse[4], Andrew J. Morris[4], Jeremy Sloan[1], and David Quigley[1] — [1]University of Warwick, Coventry, UK — [2]University of Cambridge, Cambridge, UK — [3]Daresbury Campus, Darsbury, UK — [4]University of Birmingham, Birmingham, UK

We present the extreme case of nanostructuring, exploiting capillarity of single-walled carbon nanotubes (SWCNTs) for synthesis of the smallest possible thermoelectric SnTe nanowires with cross sections as small as a single atom. By adapting high-throughput ab initio random structure searching, we discover several structures of SnTe that can be formed within SWCNT and compare results with experimentally obtained encapsulated SnTe nanowires. From first principles, we demonstrate that by choosing the appropriate diameter of a template SWCNT, we can manipulate the structure of 1D SnTe and its thermoelectric performance. The demonstrated technique opens a practical route towards nanostructural manipulation of electrical and thermoelectric properties of the 1D materials. The best candidate 1D SnTe structures demonstrate strongly enhanced ZT over a unprecedentedly broad temperature range with a maximum value of 3.25.