Thin Films Division
Fachverband Dünne Schichten (DS)

Patrick Vogt
Technische Universität Chemnitz
Institut für Physik / Halbleiterphysik
Reichenhainer Str. 70
09126 Chemnitz
patrick.vogt@physik.tu-chemnitz.de

Overview of Invited Talks and Sessions

(Lecture halls CHE 89 and CHE 91; Poster P1A)

Invited Talks

DS 2.1	Mon	9:30–10:00	CHE 89	**In situ fabrication of (Bi,Sb)-based topological insulator - superconductor hybrid devices** — •Peter Schüffelgen
DS 2.2	Mon	10:00–10:30	CHE 89	**Atomic monolayers as two-dimensional topological insulators** — •Ralph Claessen
DS 2.3	Mon	10:30–11:00	CHE 89	**Exceptional Topology of Non-Hermitian Systems** — •Jan Carl Budich
DS 7.1	Mon	11:15–11:45	CHE 89	**Atom-by-atom engineering of topological states of matter** — •Cristiane Morais Smith
DS 7.2	Mon	11:45–12:15	CHE 89	**Topological Insulator Lasers** — •Mordechai Moti Segev
DS 20.1	Wed	9:30–10:00	CHE 89	**Progress and challenges of organic and hybrid based thermoelectrics** — •Mariano Campoy-Quiles
DS 20.3	Wed	10:15–10:45	CHE 89	**Thermoelectric microdevices - challenges and perspectives** — •Gabi Schierning
DS 25.1	Wed	11:15–11:45	CHE 89	**Organic thermoelectrics: fundamentals, challenges and recent results** — •Martijn Kemerink
DS 25.3	Wed	12:00–12:30	CHE 89	**Tuning the Thermoelectric Performance of Hybrid Polymer/Nanoparticle Composites via Stoichiometric Control** — •Katherine A. Mazzio, Danny Kojda, Britta Ryll, Jens Niederhausen, Rodrigo Rubio-Govea, Klaus Habicht, Simone Raoux

Invited talks of the joint symposium SYNC

See SYNC for the full program of the symposium.

SYNC 1.1	Mon	9:30–10:00	HSZ 01	**Photonic Reservoir Computing and its Application to Optical Communication** — •Ingo Fischer, Apostolos Argyris
SYNC 1.2	Mon	10:00–10:30	HSZ 01	**Metal-oxide resistance switching memory devices as artificial synapses for brain-inspired computing** — •Sabina Spiga
SYNC 1.3	Mon	10:30–11:00	HSZ 01	**Towards brain-inspired photonic computing** — •Wolfram Pernice
SYNC 1.4	Mon	11:15–11:45	HSZ 01	**Photonic Recurrent Ising Sampler** — •Charles Roques-Carmes, Yichen Shen, Cristian Zanoci, Mihika Prabhu, Fadi Atieh, Li Jing, Tena Dubček, Chenkai Mao, Miles Johnson, Vladimir Čeperić, John Joannopoulos, Dirk Englund, Marin Soljačić
SYNC 1.5	Mon	11:45–12:15	HSZ 01	**Beyond von Neumann systems: Computational memory for efficient AI** — •Irem Boybat

Invited talks of the joint symposium SYSD

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:55	HSZ 02	**Disentangling transport in topological insulator thin films down to the nanoscale** — •Felix Lüpke

SYSD 1.2	Mon	9:55–10:20	HSZ 02	**Spintronics with Terahertz Radiation: Probing and driving spins at highest frequencies** — •Tom Sebastian Seifert, Tobias Kampfrath
SYSD 1.3	Mon	10:20–10:45	HSZ 02	**Non-radiative voltage losses in organic solar cells** — •Johannes Benduhn
SYSD 1.4	Mon	10:45–11:10	HSZ 02	**Multivalent ions for tuning the phase behaviour of protein solutions** — •Olga Matsarskaia
SYSD 1.5	Mon	11:10–11:35	HSZ 02	**Network Dynamics under Constraints** — •Malte Schröder
SYSD 1.6	Mon	11:35–12:00	HSZ 02	**Exciton spectroscopy of van der Waals heterostructures** — •Philipp Nagler

Invited talks of the joint symposium SYAS

See SYAS for the full program of the symposium.

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

Invited talks of the joint symposium SYWH

See SYWH for the full program of the symposium.

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

Invited talks of the joint symposium SYED

See SYED for the full program of the symposium.

SYED 1.1	Thu	9:30–10:00	HSZ 01	**Ultrafast electron dynamics at laser-irradiated surfaces** — •Baerbel Rethfeld
SYED 1.2	Thu	10:00–10:30	HSZ 01	**Unraveling Momentum-Dependent Electron-Phonon Coupling and its Role in the Origin of Charge Density Wave Phases** — •Bradley Siwick, Martin Otto, Jan-Hendrik Pohls, Laurent Rene de Cotret, Mark Sutton
SYED 1.3	Thu	10:30–11:00	HSZ 01	**Light MATTERs!!!** — •Hrvoje Petek, Andi Li, Zehua Wang, Marcel Reutzel
SYED 1.4	Thu	11:15–11:45	HSZ 01	**Quantum localization and delocalization of charge carriers in molecular organic crystals** — •Jochen Blumberger
SYED 1.5	Thu	11:45–12:15	HSZ 01	**Single-Atom Catalysis (SAC): How Structure Influences Reactivity** — •Gareth Parkinson

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Thu	9:30–10:00	HSZ 02	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

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

Invited talks of the joint symposium SYCL

See SYCL for the full program of the symposium.

SYCL 1.1	Fri	9:30–10:00	HSZ 02	**Topology and transport in nanostructures with curved geometries** — •Carmine Ortix
SYCL 1.2	Fri	10:00–10:30	HSZ 02	**Properties of domain walls and skyrmions in curved ferromagnets.** — •Volodymyr Kravchuk
SYCL 1.3	Fri	10:30–11:00	HSZ 02	**3D Mesoscopic Magnetic Architectures: Fabrication, Actuation & Imaging** — •Laura Heyderman
SYCL 1.4	Fri	11:15–11:45	HSZ 02	**3D nanostructures for superconductivity and magnetism** — •Oleksandr Dobrovolskiy
SYCL 1.5	Fri	11:45–12:15	HSZ 02	**Effect of Curvature on Topological Defects in Chiral Condensed and Soft Matter** — •Avadh Saxena

Sessions

DS 1.1–1.4	Mon	9:30–11:40	HSZ 105	**Focus: Diamond Technology and Electronics (joint session KFM/DS/HL)**
DS 2.1–2.3	Mon	9:30–11:00	CHE 89	**Focus Session: Topological Phenomena in Synthetic Matter I (joint session DS/O)**
DS 3.1–3.4	Mon	9:30–10:30	CHE 91	**Thin Film Applications I**
DS 4.1–4.12	Mon	9:30–13:00	POT 81	**2D semiconductors and van der Waals heterostructures I (joint session HL/DS/O)**
DS 5.1–5.8	Mon	10:30–12:45	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions I (joint session O/HL/CPP/DS)**
DS 6.1–6.5	Mon	10:45–12:00	CHE 91	**Thin Film Applications II**
DS 7.1–7.2	Mon	11:15–12:15	CHE 89	**Focus Session: Topological Phenomena in Synthetic Matter II (joint session DS/O)**
DS 8.1–8.6	Mon	15:00–16:30	CHE 89	**Layer Deposition I: Inorganic Thin Films**
DS 9.1–9.5	Mon	15:00–16:15	CHE 91	**Optical Analysis of Thin Films**
DS 10.1–10.10	Mon	15:00–17:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions II (joint session O/HL/CPP/DS)**
DS 11.1–11.11	Mon	15:00–18:30	POT 81	**2D semiconductors and van der Waals heterostructures II (joint session HL/DS)**
DS 12.1–12.5	Mon	16:30–17:45	CHE 91	**Thermoelectric and Phase Change Materials**
DS 13.1–13.5	Mon	16:45–18:00	CHE 89	**Layer Deposition II: Deposition Methods**
DS 14.1–14.8	Tue	9:30–11:30	CHE 89	**2D Materials and their Heterostructures I (joint session DS/O/HL)**
DS 15.1–15.6	Tue	9:30–11:00	CHE 91	**Organic Thin Films, Organic-Inorganic Interfaces I (joint session DS/CPP)**

DS 16.1–16.11	Tue	9:30–13:00	POT 81	**2D semiconductors and van der Waals heterostructures III (joint session HL/DS)**
DS 17.1–17.6	Tue	11:15–12:45	CHE 91	**Organic Thin Films, Organic-Inorganic Interfaces II (joint session DS/CPP)**
DS 18.1–18.5	Tue	11:45–13:00	CHE 89	**Transport Properties**
DS 19.1–19.8	Tue	14:00–16:00	POT 81	**2D semiconductors and van der Waals heterostructures IV (joint session HL/DS/O)**
DS 20.1–20.4	Wed	9:30–11:00	CHE 89	**Focus Session: Organic-based Hybrid Thermoelectrics I**
DS 21.1–21.5	Wed	9:30–10:45	CHE 91	**Layer Properties I: Electronic Properties**
DS 22.1–22.12	Wed	9:30–13:00	POT 81	**2D semiconductors and van der Waals heterostructures V (joint session HL/DS/O)**
DS 23.1–23.11	Wed	10:30–13:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions III (joint session O/HL/CPP/DS)**
DS 24.1–24.5	Wed	11:00–12:15	CHE 91	**Layer Properties II: Optical Properties**
DS 25.1–25.4	Wed	11:15–12:45	CHE 89	**Focus Session: Organic-based Hybrid Thermoelectrics II**
DS 26.1–26.9	Wed	15:00–17:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions IV (joint session O/CPP/DS/HL)**
DS 27.1–27.8	Wed	15:00–18:15	POT 81	**Focus Session: Functional Metal Oxides for Novel Applications and Devices I (joint session HL/DS)**
DS 28.1–28.18	Wed	15:00–18:00	P1A	**Poster: Thin Film Properties: Structure, Morphology and Composition**
DS 29.1–29.10	Wed	15:00–18:00	P1A	**Poster: 2D Materials and their Heterostructures**
DS 30.1–30.14	Wed	15:00–18:00	P1A	**Poster: Organic Thin Films and Thin Oxides**
DS 31.1–31.9	Wed	15:00–18:00	P1A	**Poster: Layer Deposition and Layer Properties**
DS 32.1–32.9	Wed	15:00–18:00	P1A	**Poster: Optical Analysis of Thin Films**
DS 33.1–33.8	Wed	15:00–18:00	P1A	**Poster: Thin Films: Applications, Transport and Phase Change Materials**
DS 34	Wed	18:15–19:15	CHE 91	**Annual General Meeting of the Thin Films Division**
DS 35.1–35.5	Thu	9:30–10:45	CHE 89	**2D Materials and their Heterostructures II (joint session DS/O/HL)**
DS 36.1–36.5	Thu	9:30–10:45	CHE 91	**Thin Oxides and Oxide Layers I (joint session DS/HL/O)**
DS 37.1–37.10	Thu	9:30–13:00	POT 81	**Focus Session: Functional Metal Oxides for Novel Applications and Devices II (joint session HL/DS)**
DS 38.1–38.6	Thu	11:00–12:30	CHE 89	**2D Materials and their Heterostructures III (joint session DS/HL)**
DS 39.1–39.5	Thu	11:00–12:15	CHE 91	**Thin Oxides and Oxide Layers II (joint session DS/HL)**
DS 40.1–40.6	Thu	15:00–16:30	CHE 89	**Thin Film Properties: Structure, Morphology and Composition I**
DS 41.1–41.9	Thu	15:00–17:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions V (joint session O/HL/DS/CPP)**
DS 42.1–42.6	Thu	15:00–16:30	POT 81	**Focus Session: Functional Metal Oxides for Novel Applications and Devices III (joint session HL/DS)**
DS 43.1–43.6	Thu	16:45–18:15	CHE 89	**Thin Film Properties: Structure, Morphology and Composition II**
DS 44.1–44.13	Fri	9:30–13:00	HSZ 04	**Magnetic Coupling and Anisotropy in Thin Films (joint session MA/DS)**
DS 45.1–45.6	Fri	9:30–11:00	CHE 89	**Thin Film Properties: Structure, Morphology and Composition III**
DS 46.1–46.6	Fri	11:15–12:45	CHE 89	**Thin Film Properties: Structure, Morphology and Composition IV**
DS 47.1–47.1	Fri	14:00–14:45	HSZ 02	**Overview Talk: Wiesendanger (joint session O/CPP/DS)**

Annual General Meeting of the Thin Films Division

Wednesday 18:15–19:15 CHE 91

DS 1: Focus: Diamond Technology and Electronics (joint session KFM/DS/HL)

Time: Monday 9:30–11:40 Location: HSZ 105

Invited Talk DS 1.1 Mon 9:30 HSZ 105
Doped CVD diamond layers for electronic device applications: Experimental and theoretical study — •Ken Haenen — Institute for Materials Research (IMO), Hasselt University, Diepenbeek, Belgium — IMOMEC, IMEC vzw, Diepenbeek, Belgium

While diamond is considered to be the ultimate wide band gap semiconductor due to its combination of superlative properties, the full understanding of the connection between growth conditions and subsequent layer properties is still lacking. In this presentation, focus is first devoted to the deposition of heavily and lightly B-doped CVD diamond films. Employing microwave plasma enhanced CVD in combination with Ib (100)-oriented high pressure high temperature (HPHT) substrates, the influence of the [C]/[H] ratio on key material properties is presented. This includes the surface morphology, crystal quality, and electrical transport properties by employing a wide range of characterization techniques, i.e.. Hall effect in a wide temperature range, FTIR spectroscopy, Raman spectroscopy, X-ray absorption spectroscopy, XPS, AFM, optical microscopy, and transmission electron microscopy. First principles density functional calculations (DFT) were performed to model the interaction of B with the H-terminated diamond surface, corroborating the observed increase of B-doping incorporation with used methane concentration. The insight offered by the combination of experiment and theory clearly provides a pathway to more efficient doping and enhanced crystal quality. Finally, the use of said layers in Schottky barrier diodes is presented.

Invited Talk DS 1.2 Mon 10:00 HSZ 105
Research and development for fabrication of diamond wafers for industrial use — •Hideaki Yamada — AIST, Osaka, Japan

Figure of merits of diamond as a candidate material in power electronics are superior to those of other materials, such as Si, SiC, and GaN. Especially, recent increase of the power density in power devices for high-frequency use require extremely high thermal conductivity of diamond. On the other hand, because of its stable quantum state under the standard condition, variety of sensors with wide dynamic-range and quantum computing have been studied. Therefore, in addition to its mechanical and optical applications, use of diamond in spintronics as well as electronics have been attracted researchers for variety of future applications in industry. One of the bottle necks for realization of them is in technique to fabricate diamond wafers with large area and sufficient quality under acceptable cost. We have developed techniques to enlarge seed substrates, and process them to wafers. To understand mechanism of the crystal growth, we simulated the growth environment numerically and compared them with experimental results. Our recent trials, achievement and future prospective to solve above issues aiming at realization of the industrial use of diamond will be presented with the related current state-of-the-art.

20 min. break

Invited Talk DS 1.3 Mon 10:50 HSZ 105
Diamond: Material of the future for high power, high frequency devices and quantum applications — •Shannon Nicley — Department of Materials, University of Oxford, Oxford, UK

Diamond is an exceptional material in many ways, not only for its well known hardness and highest room temperature conductivity, but also electronic properties like high electron and hole mobilities and a high electronic breakdown field strength. These properties predict that diamond electronic devices should have superior high power and high frequency performance over other semiconductor materials. Diamond is also a promising solid-state host for atomic scale defects for quantum applications. The realisation of diamond electronic devices and the full implementation of diamond quantum applications have both been limited in part by our ability to reliably grow high quality single crystal diamond. Control over the incorporation of dopant atoms such as boron and phosphorus is key for high power applications, and the ability to grow high purity, low-strain diamond as well as precisely place quantum defects remain areas of active investigation. I will give an overview of the growth of synthetic diamond and review recent progress in the control of boron and phosphorus doping. I will also present a very recently developed method for the deterministic and accurate placement of optically coherent NV centres using a laser writing technique. I will discuss the challenges in this field and give an outlook for both extreme electronic device and quantum applications.

DS 1.4 Mon 11:20 HSZ 105
Preliminary study of diamond based Kinetic Inductance Detectors — •Francesco Mazzocchi, Dirk Strauss, and Theo Andreas Scherer — Karlsruhe Institute of Technology (IAM-AWP), Hermann Von Helmholtz Platz 1, 76344 Eggenstein-Leopoldshafen

Kinetic Inductance Detectors (KIDs) have proven themselves as a very versatile cryogenic detector technology capable of applications in various fields due to their flexibility of design, sensibility and ease of production. We have recently proposed a polarization sensitive Lumped Elements KID as sensor for an innovative polarimetric diagnostics based on quantum cascade lasers (QCL) for application in the nuclear fusion. Each detector unit is composed by 4 pixels arranged at the vertices of a square, each pixels being sensible to only one polarization direction. The current system is based on niobium nitride (NbN) superconductor over High Resistivity Silicon (HRSi) substrate. Such material delivers good performances but its relatively high dielectric constant and loss tangent lead to increased substrate losses. Using a transparent substrate may improve this aspect and also the radiation resistance of such devices. Diamond is the substrate of choice, being a material already widely studied and used in the fusion environment as high power microwave window, due its outstanding optical and mechanical performances. In this work we present the preliminary design study and simulations for a diamond based Kinetic Inductance Detector with both single and poly-crystalline diamond (SCD/PCD) substrates taken into account.

DS 2: Focus Session: Topological Phenomena in Synthetic Matter I (joint session DS/O)

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

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

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

Invited Talk DS 2.1 Mon 9:30 CHE 89

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

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

Invited Talk DS 2.2 Mon 10:00 CHE 89

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

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

Invited Talk DS 2.3 Mon 10:30 CHE 89

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

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

DS 3: Thin Film Applications I

Time: Monday 9:30–10:30 Location: CHE 91

DS 3.1 Mon 9:30 CHE 91

Intrinsic oxygen vacancy driven universal 1/f noise behaviour of yttrium oxide-based Resistive Random Access Memory devices — •Eszter Piros[1], Martin Lonsky[2], Stefan Petzold[1], Jens Müller[2], and Lambert Alff[1] — [1]Institute of Materials Science, ATFT, Technische Universität Darmstadt, Darmstadt, Germany — [2]Institute of Physics, Goethe- University Frankfurt, Frankfurt am Main, Germany

Resistive Random Access Memory (RRAM) is an outstanding next-generation memory candidate due to its excellent performance and scaling potential. However, further improvement of device reliability and variability is required. In this respect, the choice of materials can play a key role. Y_2O_3 is a very interesting material for resistive switching as 25% of the anion sublattice is unoccupied. Yttria-based devices show gradual switching under DC and nanosecond-regime voltage pulse operation [1], and thus can be utilized in multi-bit and neuromorphic applications. To assess device reliability and to gain insight into the charge transport characteristics, low-frequency noise measurements were performed on Y_2O_3-based RRAM devices at several intermediate resistance states and as a function of DC switching cycles. A universal noise behaviour was observed with a frequency exponent of $\alpha \approx 1.2$ that is independent of the device resistance and the number of DC switching cycles. The noise magnitude is found to systematically decrease with DC cycling and to increase with the maximum applied voltage in the reset process.

[1] S. Petzold et al., Semicond. Sci. Technol. 34, 075008 (2019)

DS 3.2 Mon 9:45 CHE 91

Heavy ion irradiation effects on emerging memories: OxRAM, FeRAM and PCM — •Tobias Vogel[1], Nico Kaiser[1], Eszter Piros[1], Maximilian Lederer[2], Ricardo Olivo[2], Tarek Ali[2], Anna Lisa Serra[3], Thomas Kämpfe[2], Stefan Petzold[1], Gabriele Navarro[3], Christelle Charpin-Nicolle[3], Christina Trautmann[1,4], and Lambert Alff[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Fraunhofer IPMS, Dresden, Germany — [3]CEA LETI, Grenoble, France — [4]GSI Helmholtzzentrum, Darmstadt, Germany

Emerging memory classes such as oxide based resistive random-access memory (OxRAM), ferroelectric random-access memory (FeRAM) or phase-change memory (PCM) are discussed as the successor of flash technology for highly-scaled device technology. Thereby, radiation hardness is of particular interest, enabling applications e.g. in space conditions. Here, Resistive Random-Access Memory (RRAM) devices are promising for applications in harsh radiation environments due to their superior data retention upon ionizing radiation, especially compared to flash technology. [1] In this study, we compare the effect of heavy ion irradiation, the most hazardous kind of ionizing irradiation, on the structural and electrical properties of different emerging memory classes: Phase Change Memory (PCM) based on GST, Ferroelectic Random Access Memory (FeRAM) and OxRAM based on HfO_x. [1] S. Petzold et al., Heavy Ion Radiation Effects on Hafnium Oxide-Based Resistive Random Access Memory, IEEE Trans. Nucl. Sci. 66, 1715 (2019).

DS 3.3 Mon 10:00 CHE 91

Simulation of resistive switching in HfOx based RRAM and the role of low temperature tetragonal and hexagonal hafnia phases in conductive switching — •Nico Kaiser[1], Stefan Petzold[1], Enrique Miranda[2], Alexander Zintler[1], Leopoldo Molina-Luna[1], and Lambert Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, Germany — [2]Departament d Enginyeria Electrònica, Universitat Autònoma de Barcelona, Spain

HfOx is a promising candidate for the functional layer in Resistive Random Access Memory (RRAM) with the potential to replace conventional FLASH memory and being implemented in emerging technologies such as neuromorphics or in-memory computing. Although resistive switching was intensively investigated in recent years, the exact mechanism and the role of oxygen vacancies is not completely understood and highly debated. In this study, we developed an electrical conduction model utilizing two antiserially connected memdiodes (diodes with memory). In this way, all switching modes observed in stoichiometric monoclinic (m-HfO2) and oxygen-vacancy-stabilized low-temperature tetragonal (LTP t-HfOx) phase can be simulated. The separation of conduction characteristics via memdiodes allows to evaluate the role of both electrode-oxide interfaces separately. Through experimental thin film characterization methods such as XRD, XPS and electrical measurements, we investigate the physical properties of HfOx phases. Using TEM, we identify HfOx structures and their fingerprints in EELS which can be used to identify the role of LTP t-HfOx and hcp-HfOx in the switching process.

DS 3.4 Mon 10:15 CHE 91

Towards a large-scale quantum simulator at room temperature — •Philipp J. Vetter[1], Thomas Unden[1], Nikolas Tomek[1], Tamara Sumarac[2], Elana K. Urbach[2], Timo Weggler[1], Maximilian G. Hirsch[1], Hideyuki Watanabe[3], Kohei M. Itoh[4], Boris Naydenov[5], Mikhail D. Lukin[2], Martin B. Plenio[6], and Fedor Jelezko[1] — [1]Institute for Quantum Optics and Center for Integrated Quantum Science and Technology, Universität Ulm — [2]Department of Physics, Harvard University — [3]Correlated Electronics Group, Electronics and Photonics Research Institute, National Institute of Advanced Industrial Science and Technology, Tsukuba — [4]Department of Applied Physics and Physico-Informatics, Faculty of Science and Technology, Keio University — [5]Helmholtz-Zentrum Berlin für Materialien und Energie — [6]Institute for Theoretical Physics and Center for Integrated Quantum Science and Technology, Universität Ulm

Quantum simulators enable the study of strongly-correlated many-body systems that may exhibit exotic phases, such as spin liquids and supersolids. We present our progress of creating a large-scale quantum simulator at room-temperature, which is based on the nitrogen vacancy center in diamond, coupled to surrounding nuclear spins. We demonstrate the fabrication of a 1 nm thin 13C layer in diamond which is polarized and coherently controlled by the NV center. Furthermore, 2D-Materials which offer a clearly identifiable symmetry and thickness are transferred onto the diamond surface. The nuclear spins within the transferred flake are sensed via the NV center aiming for full polarization by tailored pulse schemes.

DS 4: 2D semiconductors and van der Waals heterostructures I (joint session HL/DS/O)

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

DS 4.1 Mon 9:30 POT 81

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

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

DS 4.2 Mon 9:45 POT 81

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

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

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

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

[1] B. Buades *et al.*, Optica **5**, 000502 (2018)

[2] D. Christiansen *et al.*, Phys. Rev. B **100**, 205401 (2019)

[3] M. Selig *et al.*, 2D Mater. **5**, 035017 (2018)

DS 4.3 Mon 10:00 POT 81

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

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

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

DS 4.4 Mon 10:15 POT 81

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

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

DS 4.5 Mon 10:30 POT 81

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

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

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

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

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

DS 4.6 Mon 10:45 POT 81

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

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

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

30 min. break

DS 4.7 Mon 11:30 POT 81

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

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

DS 4.8 Mon 11:45 POT 81

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

We study the influence of the $(GaSe)_n/(MoS_2)_m$ heterostack composition on the band alignment and the interlayer exciton energy using *ab initio* calculations.

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

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

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

DS 4.9 Mon 12:00 POT 81

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

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

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

DS 4.10 Mon 12:15 POT 81

In-plane anisotropy of the photon-helicity induced linear Hall effect in few-layer WTe_2 — •Simon Steinhauser[1,2], Paul Seifert[1,2], Florian Sigger[1,2], Jonas Kiemle[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], Christoph Kastl[1,2,4], Ursula Wurstbauer[1,2,5], and Alexander Holleitner[1,2] — [1]Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, D-85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstrasse 4, D-80799 München, Germany — [3]Advanced Materials Laboratory, Tsukuba, Ibaraki 305-0044, Japan — [4]Molecular Foundry, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley, California 94720, USA — [5]Institute of Physics, University of Münster, Wilhelm-Klemm-Strasse 10, D-48149 Münster, Germany

Using Hall photovoltage measurements, we demonstrate that a linear transverse Hall voltage can be induced in few-layer WTe_2 under circularly polarized illumination. We find that the photon-helicity induced Hall effect is strongly anisotropic with respect to the crystal axis. Our results are consistent with the Berry curvature and its dipolar distribution due to the breaking of inversion symmetry. We also studied how the Hall voltage changes with varying layer numbers. Time resolved optoelectronic autocorrelation spectroscopy shows the comparatively long spin lifetime of carriers caused by the momentum-indirect electron and hole pockets in WTe_2.

DS 4.11 Mon 12:30 POT 81

Characterization of interlayer excitons in $MoSe_2$-WSe_2 heterostructures in high magnetic fields — •Johannes Holler[1], Michael Kempf[3], Jonas Zipfel[1], Mariana Ballottin[2], Anatolie Mitioglu[2], Philipp Nagler[1], Michael Högen[1], Alexey Chernikov[1], Peter Christianen[2], Christian Schüller[1], and Tobias Korn[3] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]High Field Magnet Laboratory (HFML EMFL), Radboud University Nijmegen, Netherlands — [3]Institut für Physik, Universität Rostock, Germany

In the recent years, the research on transition-metal dichalchogenides

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

Here, we study these IEXs in $MoSe_2$-WSe_2 heterostructures. In low-temperature PL measurements in magnetic fields of up to 30T, we observe a giant valley-selective splitting and a resulting near-unity valley polarization. In time-resolved measurements, we track the buildup of IEX valley polarization in the magnetic field. We also find a clear dependence of the magnetic-field behavior of the IEX on the stacking angles.

DS 4.12 Mon 12:45 POT 81

Defect-related photoluminescence of WS_2 monolayers — •Marcel Ney, Aswin Asaithambi, Lukas Madauss, Marika Schleberger, Axel Lorke, and Günther Prinz — Faculty of Physics and CENIDE, University Duisburg-Essen, Germany

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

We will present low-temperature photoluminescence-spectroscopy (PL) measurements, which show the influence of laser-irradiation with different excitation powers on WS_2 monolayers grown on a standard Si/SiO_2 substrate via a chemical vapor deposition (CVD) process.

In the PL investigations, we observed a defect-related emission D_1, which can be assigned to adsorbate-decorated defect complexes [1]. The nature of this defect-related state investigated by laser-power-dependent measurements, will be presented in this contribution. During a laser excitation cycle, a laser-activated emission with a higher energy than the defect-related emission D_1, occurs. Furthermore, another defect-related emission D_2 was observed. Due to the annealing properties after laser-irradiation we identify this emission as a monosulfur vacancy decorated with physisorbed adsorbates [2].

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

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

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

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

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

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

Invited Talk DS 5.1 Mon 10:30 GER 38

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

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

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

DS 5.2 Mon 11:00 GER 38

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

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

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

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

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

DS 5.3 Mon 11:15 GER 38

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

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

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

DS 5.4 Mon 11:30 GER 38

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

We report an efficient implementation of renormalized second-order single-particle energies for periodic systems in an all-electron numeric atomic orbital framework. Starting from second-order perturbation theory, which is single-electron self-interaction free as a virtue of the first-order and second-order exchange diagrams, we use the Dyson equation to sum up infinite number of diagrams [1,2]. In our implementation we use Ewald summation for the long-range part of the Coulomb interaction. This results in an integrable singularity in k-space, which has to be carefully evaluated in order to ensure proper convergence with k-point mesh density. For this purpose we develop an approach based on a generalization of the Gygi-Baldereschi method. The dependence on the starting point of the perturbation theory is examined. The new approach shows a competitive or even superior performance for the description of band-energies compared to the current state-of-the-art methods such as hybrid functionals and G^0W^0 approximation. Thus, with a good starting point this method becomes a powerful tool for the prediction of band energies for a variety of materials.
[1] J. Sun and R. J. Bartlett, J. Chem. Phys. 104, 8553 (1996).
[2] A. Grüneis *et al.*, J. Chem. Phys. 133, 074107 (2010).

DS 5.5 Mon 11:45 GER 38

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

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

DS 5.6 Mon 12:00 GER 38

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

Strong many-body effects in solid state materials are the reason for features such as satellites in electronic excitation spectra. Many-body perturbation theory approaches based on the Green's function formalism are the state-of-the-art in their understanding, commonly applied in terms of the GW approximation to the self-energy, which neglects the so-called vertex correction in Hedin's equations. Although successful for some observables such as band gaps, this approximation cannot sufficiently well describe satellite peaks observed in experiment. Vertex corrections beyond GW can be taken into account thanks to time-dependent density-functional theory[1]. However, only adiabatic approximations have been considered so far. Here we make use of a non-adiabatic approximation[2] to investigate dynamical vertex corrections within a model self-energy. We compare our results to calculations where a static vertex is included and report first successes in terms of a correction to the satellites in the spectral function of sodium.
[1] R. Del Sole et al. *Phys. Rev. B*, 49, 8024 (1994)
[2] M. Panholzer et al. *Phys. Rev. Lett.*, 120, 166402 (2018)

DS 5.7 Mon 12:15 GER 38

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

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

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

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

DS 5.8 Mon 12:30 GER 38

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

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

DS 6: Thin Film Applications II

Time: Monday 10:45–12:00 Location: CHE 91

DS 6.1 Mon 10:45 CHE 91

Konforme Einbettung hocheffizienter Spektrometergitter mittels Atomlagenabscheidung — •Kristin Pfeiffer[1], Vivek Beladiya[1,2], Torsten Harzendorf[1], Thomas Flügel-Paul[1], Dirk Michaelis[1] und Adriana Szeghalmi[1,2] — [1]Fraunhofer-Institut für Angewandte Optik und Feinmechanik, Albert-Einstein-Str. 7, 07745 Jena — [2]Friedrich-Schiller-Universität Jena, Institut für Angewandte Physik, Albert-Einstein-Str. 15, 07745 Jena

Hocheffiziente Beugungsgitter, welche als dispersive Kernkomponenten in Spektrometern zum Einsatz kommen, stellen höchste Anforderungen an die Empfindlichkeit und Auflösung der optischen Gitter. Im vorliegenden Fall wird ein Spektrometergitter für das SWIR2-Band untersucht. Die wesentliche Herausforderung liegt hierbei in einer nahezu polarisationsunabhängigen Beugungseffizienz von mehr als 80 %.

Das betrachtete optische Design kombiniert ein Grundgitter aus Kieselglas (SiO2) mit einer hochbrechenden Einbettung aus TiO2. Das TiO2-Material wird hierzu konform mittels plasmagestützter Atomlagenabscheidung (PEALD) aufgebracht. Der PEALD-Prozess ist ein zentraler Aspekt in der Realisierung des Spektrometergitters, da sowohl die optische Qualität als auch die Konformität des eingebetteten Materials einen wesentlichen Einfluss auf die optische Effizienz des Gitters haben. Im Tagungsbeitrag wird im Speziellen der Einfluss der PEALD-Prozessparameter auf die Einbettung des Gitters und dessen Transmissionseffizienz für TM- bzw. TE-polarisiertes Licht betrachtet.

DS 6.2 Mon 11:00 CHE 91

Large area plasmonic sensor for refractive index based on partial-circular pair arrays — •Fanzhou Lv, Jiaxu Chen, Yudie Huang, Shiyao Jia, Zhihang Wang, Yi Wang, and Wenxin Wang — Harbin Engineering University, No. 145 Nantong Str, Nangang District, Harbin, China

Plasmonics is a rapidly developing branch in nanophotonics that embodies the feature of generating exceptional optical field enhancements in nanometer volumes. As a result of that, a considerable amount of high sensitivity sensors are attempting to construct based on localized surface plasmon resonance (LSPR). Here, a large area nanoarrays consist of partial-circular pairs is proposed as an example for refractive index sensing. First, the large area sample is fabricated by utilizing artificial alumina membranes with tetragonal lattice in physical vapor deposition (PVD) process and easy to implement to application. In addition, angle-resolved photonic spectroscopy is used to characterize the optical property variation of partial-circular pair (PCP) arrays as function of incident angle in the range of visible light. On one hand, for the symmetry-split nanoarray, a low-quality dipolar resonance is witnessed at normal incidence. On the other hand, after breaking the symmetry of unit in nanoarray, a strong Fano-like resonance is generated with high-quality factor. Besides, a pronounce coupling- induced reflection peak is observed within a broad spectral range, which is beneficial for improving the sensitivity of the refractive index sensor. In short, the optical phenomenon from symmetry breaking inspired us to optimize the designed PCP array as a refractive-index sensor.

DS 6.3 Mon 11:15 CHE 91

Novel Ion Detector with High Sensitivity for Multi-Ion Sensing — •Kun-Lin Liou, Ying-Chun Shen, Chien-Ping Wang, Yu-Lun Chueh, Chrong Jung Lin, and Ya-Chin King — National Tsing-Hua University 101, Sec. 2, Kuang-Fu Road, Hsinchu 30013, Taiwan, R. O. C

Nowadays, the ion sensor plays an important role in our daily lives. From pH level, heavy metal monitoring and evaluating bio-medical ion balance, these applications become more accessible as sensing technologies matures. The ion sensitive FET has compact size, cost-effective and fast response time; however, it is limited by the Nernst limit. The proposal ion detector with coupling structure not only can achieve high sensitivity, its sensing range can also be dynamically adjusted by setting suitable biasing conditions to alleviate such a challenge. Here, we especially focused on comparing the effect of various kinds of sensing film, their corresponding thickness and sensing region size on the sensing characteristics of the new detector. This new detector can deliver an output responsivity as high as 150 mV/pH. Moreover, the preliminary measurement results on sodium ion sensing obtained by calix[4]arene film are demonstrated. With a sensing gate isolated from the transistor channel, the proposal sensor has fully sensing capability to other kinds of ion such as heavy metal ion and so on. It also suggests that the proposed device can be integrated into sensors array for the detection of multiple ions simultaneously. Further optimization of coating material in the sensing membrane is expected to enhanced the performance of this new ion detector.

DS 6.4 Mon 11:30 CHE 91

Synthesis of Rutile-TiO_2 Nanorod Arrays for Efficient Solar Water Splitting via Microwave-Assisted Hydrothermal method — •Amin Qasim — University of Zakho,Duhok,KRG-Iraq

Using a microwave-assisted hydro thermal method (MWAHM) a single crystalline of vertically aligned TiO_2 nanorod (NR) arrays has been demonstrated via the novel ultra-rapid synthetic method for the production. High-quality NR arrays with controlled film thickness were achieved with fine control of the growth conditions as well. The effect of the different reaction conditions of MWAHM such as reaction time and growth temperature on the morphology, crystal orientation, and photo catalytic activity have been systematically investigated. In a typical condition of the MWAHM using 0.4 cm3 of titanium(IV) n-butoxide (TBO) at 180°C for 40 minutes, a small diameter and short length 124 nm and 2.93 m of TiO_2 nanorods respectively, are grown on fluorine-doped tin oxide (FTO) substrate. However, the photo current density produced TiO_2 NRs of 2.90 mA cm-2 with a maximum photo conversion efficiency of about 2.7 % which confers excellent photo-electrochemical performance. In comparison with the typical hydro thermal method (HM) synthesized NRs, the ultra-fast MWAHM synthesized NRs offers five times more efficiency photoelectrochemical (PEC) water splitting than the hydro thermal method (HM). The results suggest that these dense and aligned one-dimensional TiO_2 nanorods are promising for hydrogen generation from water splitting based on PEC cells.

DS 6.5 Mon 11:45 CHE 91

Sputter deposition of tungsten oxide and study of its electrochromic behavior for various electrolytes — •Mario Gies, Martin Becker, Fabian Michel, and Angelika Polity — Institute of Exp. Physics I and Center for Materials Research (LaMa), Justus Liebig University Giessen, Germany.

In this work, tungsten oxide films were prepared by means of various types of the sputter deposition, i.e. ion-beam and radio-frequency (rf)-sputter deposition. The focus was on optimizing the layers especially for use as a component in an electrochromic device. Layers were deposited from a metallic tungsten target under various gas mixtures of argon, oxygen and additional hydrogen. The choice of different gas mixtures allows to tune the optical characteristics of the synthesized films. Glass coated with fluorine-doped tin oxide (FTO) was used as substrate in order to establish an electrical contact for electrochemical measurements. The as-grown rf-sputtered layers were found to be amorphous. Ion-beam sputtered films were deposited under ambient as well as elevated growth temperatures. As a consequence, in addition to amorphous samples, crystalline films were grown. The different layers were investigated on the basis of their structural and compositional characteristics. Finally, the electrochromic properties of selected samples were examined in electrochemical measurements using different electrolytes.

DS 7: Focus Session: Topological Phenomena in Synthetic Matter II (joint session DS/O)

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

Invited Talk DS 7.1 Mon 11:15 CHE 89

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

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

Invited Talk DS 7.2 Mon 11:45 CHE 89

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

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

DS 8: Layer Deposition I: Inorganic Thin Films

Time: Monday 15:00–16:30 Location: CHE 89

DS 8.1 Mon 15:00 CHE 89

High quality vanadium dioxide thin films grown by a simple and low cost spray pyrolysis technique — •Oisín Murtagh[1], David Caffrey[1], Karsten Fleischer[2], Daragh Mullarkey[1], and Igor Shvets[1] — [1]School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College, University of Dublin, Dublin 2, Ireland — [2]School of Physical Sciences, Dublin City University, Dublin 9, Ireland

Vanadium dioxide is a well-known electronic phase change material due to strong electron correlation. In this presentation the details of VO2 thin film growth on Al2O3(0001) substrates using a low temperature solution based method (spray pyrolysis) and a subsequent annealing step in an inert atmosphere are described. The dependence of the growth on solvent, precursor, growth temperature and annealing conditions are examined. The resulting films show high crystallinity, homogeneity and a metal-insulator transition (MIT) at 70°C accompanied by a resistivity change of over 4 orders of magnitude. Structural, morphological, chemical and electronic properties are characterised using XRD, XPS, profilometry, AFM and 4 point probe electrical measurements. Triggering of the MIT through the application of an electric-field is also shown using microlithographic channels. The simplicity, scalability and cost of this growth method make it a promising candidate for large scale implementation of VO2 in modern applications, with an emphasis on non-conventional computing electronics.

DS 8.2 Mon 15:15 CHE 89

Optical temperature management for high-quality ZnO molecular beam epitaxy — •Maximilian Albert[1], Christian Golla[1], Christian Kaspari[2], Thomas Zettler[2], and Cedrik Meier[1] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]LayTec AG, Seesener Str. 10-13, 10709 Berlin, Germany

Zinc oxide is a wide gap semiconductor with a high exciton binding energy and significant nonlinear susceptibility. ZnO grown by molecular beam epitaxy (MBE) has already been used in various photonic or plasmonic structures taking advantage of those properties. For these structures the crystal quality is of great importance, which crucially depends on growth parameters, such as growth rate and substrate temperature. Both parameters are challenging to manage and analyze in-situ due to the non-opaque substrates and films. Therefore, novel techniques have to be researched and investigated. In our case we investigate a combined optical approach, promising insights into both growth temperature and growth rate of ZnO. We find that emissivity-corrected pyrometry together with band gap thermometry and reflectometry can address all needs and substantially improves quality control and monitoring of the growth process.

DS 8.3 Mon 15:30 CHE 89

Tailoring material properties of SiOx thin films by applying an electric field during plasma enhanced atomic layer deposition — •Vivek Beladiya[1,2], Martin Becker[3], Marek Sierka[3], and Adriana Szeghalmi[1,2] — [1]Institute of Applied Physics, Friedrich Schiller University, Jena, Germany. — [2]Fraunhofer Institute for Applied Optics and Precision Engineering IOF, Jena, Germany. — [3]Otto Schott Institute of Materials Research, Friedrich Schiller University, Jena, Germany.

SiO2 is a widely used metal oxide in microelectronics, optics, barrier coatings, and solar cells. Excellent optical, mechanical, chemical and structural properties are required for the optimum performance of these devices. These properties can be tailored by controlling ion energies by varying average bias voltage at the substrate stage during oxygen plasma in PEALD process.

In this work, the effect of applied average-bias voltage on SiO2 thin films properties, deposited in two different deposition tools were investigated. The average bias voltage up to -300 V was applied during the oxygen plasma exposure. A very low average-bias voltage (< -10 V) was sufficient to alter material properties indicating an influence on the surface chemical reactions. The stoichiometric and dense SiO2 thin films with low OH content were deposited by applying substrate biasing. The observed experimental trends were supported by atomistic simulations. It is shown that relevant surface reaction can be influenced by applying electric field during plasma step.

DS 8.4 Mon 15:45 CHE 89

Synthesis of Porous Silicon, Nickel and Carbon Thin Films by Vapor Phase Dealloying — •Stefan Saager, Bert Scheffel, Olaf Zywitzki, and Thomas Modes — Fraunhofer-Institut für Organische Elektronik, Elektronenstrahl- und Plasmatechnik FEP

Porous thin films have various application fields, e.g., for energy conversion in fuel cells, energy storage in lithium ion batteries or supercapacitors as well for catalysis, filtration and sensing. We synthesized porous thin films by co-evaporating a low-vapor-pressure material (e.g., Si, Ni or C) together with zinc and depositing a compact layer of resulting composite. High-rate deposition process up to 100 nm/s was realized by electron beam evaporation of the materials from two graphite crucibles with a fast deflected electron beam in high vacuum. Immediately after deposition, the coated stainless steel substrates were heated up in vacuum to a temperature above 500 °C and thereby zinc is removed selectively. Due to it's higher vapor pressure against that of remaining component, zinc is expelled from the layer and vacancies are generated by so called vapor phase dealloying. We investigated the feasibility of vapor phase dealloying process for the elements silicon, nickel and carbon. The elemental composition and the morphology of the layers prior and after thermal annealing were analyzed by scanning electron microscopy, by energy-dispersive X-ray spectrometry and by X-ray diffraction.

DS 8.5 Mon 16:00 CHE 89

Growth of epitaxial (110) oriented Mn2Au thin films via Molecular Beam Epitaxy — •Daniel Casey, Daragh Mullarkey, and Igor V. Shvets — School of Physics, Trinity College Dublin, The University of Dublin, Dublin 2, Ireland

Here we explore the crystallographic nature and growth of antiferromagnetic Mn2Au (110) oriented thin films deposited by molecular beam epitaxy.

By co-evaporating Mn and Au from separate Knudsen cells, (110) oriented films were obtained when deposited on a Pt (111) seed layer on Al2O3 (0001) substrates. A combination of high-resolution X-ray diffraction, low and high energy electron diffractions are used to elucidate the epitaxial relation of these films. The influence of substrate temperature during growth on the quality of the Mn2Au thin films is also explored.

DS 8.6 Mon 16:15 CHE 89

Superconducting titanium nitride thin films deposited by plasma enhanced atomic layer deposition — •Luisa Ehmcke[1], Stefanie Haugg[1], Kaline Furlan[2], Gerold Schneider[2], Robert Blick[1], and Robert Zierold[1] — [1]Center for Hybrid Nanostructures (CHyN), University of Hamburg, 22761 Hamburg, Germany — [2]Institute of Advanced Ceramics, Hamburg University of Technology, 21073 Hamburg, Germany

Titanium nitride is a widely used material in microelectronics due to its low resistivity and high thermal stability. Moreover, titanium nitride is a type 1 superconductor with a critical bulk temperature of 5.6 K.

Herein, we report about thin film titanium nitride, which was grown by plasma enhanced atomic layer deposition (PE-ALD) by utilizing tetrakis(dimethylamino)titanium (TDMAT) and a nitrogen/hydrogen mixture as precursor. By investigating the sheet resistance, the critical temperature, and the critical field the deposition process was optimized with respect to plasma power, plasma time, gas composition, and process temperature. We observed (i) a transition to an effective 2D electronic system and (ii) weak antilocalization in our films in low temperature magnetotransport studies [1,2]. These observations in combination with structural and compositional analysis prove the low impurity content of our thin film samples.

[1] Postolova et al., Sci. Rep., (2017) DOI: 10.1038/s41598-017-01753-w [2] Gupta et al., J. Magn. Magn. Mater., (2019) DOI: /10.1016/j.jmmm.2019.166094

DS 9: Optical Analysis of Thin Films

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

DS 9.1 Mon 15:00 CHE 91

Optical constants of nickel and gold from 0.06 to 6.0 eV at 300 K — •Stefan Zollner and Farzin Abadizaman — New Mexico State University, Las Cruces, NM, USA

Using spectroscopic ellipsometry, we performed high-precision measurements of the optical constants of gold and nickel thin films at room temperature from the mid-infrared to the near-ultraviolet spectral region. Gold shows typical Drude behavior in the infrared with a single species of charge carriers and several optical interband transitions with an onset of 2.54 eV. However, deviations from a simple Drude model are noticed at the longest wavelengths, possibly due to diffraction or the anomalous skin effect. For nickel, measurements were performed in UHV after preparing a clean surface by annealing in vacuum. The optical constants of Ni require a description with two species of Drude charge carriers with vastly different damping constants, and several interband transitions. The energies of the interband transitions can be determined by subtracting the Drude response from the optical constants. Several different representations of the optical constants of Ni and Au will be discussed, including a frequency dependent scattering rate and a renormalized effective mass. Tabulated optical constants as well as model line shapes fitted to the data will be presented.

DS 9.2 Mon 15:15 CHE 91

Validation of Optical Constants in the EUV Spectral Range — •Qais Saadeh[1], Victor Soltwisch[1], Frank Scholtze[1], and Philipp Naujok[2] — [1]Physikalisch-Technische Bundesanstalt (PTB), Abbestraße 2-12, 10587 Berlin, Germany — [2]OptiX fab GmbH, Hans-Knöll-Str. 6, 07745 Jena, Germany

After the introduction to high volume manufacturing, continuous development of EUVL systems and components will require the use of advanced materials, for example as absorber layers on next generation photomasks. In the EUV or soft X-ray spectral range the optical parameters of many materials are often not well known or based on theoretical calculations and interpolations. Thus, highly accurate measurements of the optical constants of thin layers obtained from different material compositions are necessary for the realistic modelling of new photomasks designs. Reflectometry is a widely used method for the determination of film thickness, especially in the X-ray spectral range. The same approach can also be used in EUV with a different focus. The aim is then to reconstruct the optical material parameters, the real and imaginary part of the refractive index, from the reflectivity measurements with a well-defined layer thickness. In this study, we will present the feasibility of determining the optical constants for candidate materials for EUV photomask absorbers using EUV reflectometry.

DS 9.3 Mon 15:30 CHE 91

Grazing incidence X-ray fluorescence measurement on nanostructures for element sensitive reconstruction — •Anna Andrle[1], Philipp Hönicke[1], Philipp-Immanuel Schneider[1], Yves Kayser[1], Martin Hammerschmidt[2], Sven Burger[2,3], Frank Scholze[1], Burkhard Beckhoff[1], and Victor Soltwisch[1] — [1]Physikalisch-Technische Bundesanstalt, Abbestrasse 2-12, 10587 Berlin, Germany — [2]JCMwave GmbH, Bolivarallee 22, 14050 Berlin, Germany — [3]Zuse Institute Berlin, Takustrasse 7, 14195 Berlin, Germany

The production of the current and next generation of semiconductor devices requires a reliable and non-destructive characterization of the material composition and dimensional parameters of the nanostructures is necessary. A method based on grazing incidence X-ray fluorescence measurements is applied to lamellar gratings made of Si3N4. This technique is based on the X-ray standing wave field, which is sensitive to both the elemental composition and dimensional parameters of the nanostructures. With a finite element Maxwell solver, the X-ray standing wave field can be calculated and used in conjunction with a parameterized nanostructure to model experimental data and thus, derive the spatial distribution of elements and the geometric shape with subnm resolution. This reconstruction is executed with a Bayesian optimization approach to minimize the computational effort.

DS 9.4 Mon 15:45 CHE 91

Ultrafast time-resolved spectroscopic ellipsometry user station at ELI-Beamlines — •Martin Zahradník — ELI Beamlines. Institute of Physics. Czech Academy of Science. Za Radnicí 835, 252 41 Dolní Břežany. Czech Republic

Time-resolved ellipsometry is based on a pump-probe approach. The pump pulse from a laser hits the sample first, triggering charge transfer processes that change the dielectric function. The sample response, the change in the dielectric function, is then measured by a probe pulse. By varying the time delay between the pump and the probe pulses (from few femtoseconds to nanoseconds), the complete picture of the ultrafast phenomenon is obtained.

Our time-resolved PSC(R)A ellipsometer at ELI Beamlines has a super continuum probe beam that covers from 350-750 nm generated on a CaF2 crystal by 1 KHz, 7 mJ, 35 fs, Ti-sapphire laser. Thanks to an optical parametrical amplifier, the pump beam could be any wavelength from 190 to 2000 nm. A new call will be open for users to carry on measurements at this ellipsometer. During the talk, the details of the setup will be explained and example data showing the dynamics of the dielectric function of model thin films will be presented.

Supported by the projects Structural dynamics of biomolecular systems (CZ.02.1.01/0.0/0.0/15-003/0000447) and Advanced research using high intensity laser produced photons and particles (CZ.02.1.01/0.0/0.0/16-019/0000789) from the European Regional Development Fund.

DS 9.5 Mon 16:00 CHE 91

Excitonic Wave Function Reconstruction from Near-Field Spectra Using Machine Learning Techniques — Fulu Zheng and •Alexander Eisfeld — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Strasse 38, D-01187 Dresden, Germany

A general problem in quantum mechanics is the reconstruction of eigenstate wave functions from measured data. Self-assembled molecular aggregates on dielectric surfaces are promising candidates for optoelectronic devices. Strong interactions between the transition dipoles of the molecules lead to delocalized excitonic eigenstates where an electronic excitation is coherently shared by many molecules [1]. Information about these states is vitally important to understand their optical and transport properties. Here we show that from spatially resolved near field spectra it is possible to reconstruct the underlying delocalized aggregate eigenfunctions [2, 3]. Although this high-dimensional nonlinear problem defies standard numerical or analytical approaches, we have found that it can be solved using a convolutional neural network. For both one-dimensional and two-dimensional aggregates we find that the reconstruction is robust to various types of disorder and noise.

[1] A. Eisfeld, C. Marquardt, A. Paulheim, and M. Sokolowski, Phys. Rev. Lett. 119, 097402 (2017). [2] X. Gao and A. Eisfeld, J. Phys. Chem. Lett. 9, 6003 (2018). [3] F. Zheng, X. Gao and A. Eisfeld, Phys. Rev. Lett. 123, 163202 (2019).

DS 10: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions II (joint session O/HL/CPP/DS)

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

DS 10.1 Mon 15:00 GER 38

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

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

DS 10.2 Mon 15:15 GER 38

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

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

[1] Braun, Rep. Prog. Phys. 59, 1267-1338 (1996), [2] H. Ebert, D. Ködderitzsch and J. Minár, Rep. on Prog. in Phys. 74, 096501 (2011), [3] L. Nicolaï and J. Minár, AIP Conf. Proc. 1996, 020033 (2018)

DS 10.3 Mon 15:30 GER 38

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

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

DS 10.4 Mon 15:45 GER 38

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

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

References

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

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

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

DS 10.5 Mon 16:00 GER 38

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

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

DS 10.6 Mon 16:15 GER 38

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

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

DS 10.7 Mon 16:30 GER 38

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

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

DS 10.8 Mon 16:45 GER 38

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

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

DS 10.9 Mon 17:00 GER 38

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

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

DS 10.10 Mon 17:15 GER 38

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

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

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

DS 11: 2D semiconductors and van der Waals heterostructures II (joint session HL/DS)

Time: Monday 15:00–18:30 Location: POT 81

Invited Talk DS 11.1 Mon 15:00 POT 81

Resonantly hybridized excitons in moiré superlattices in van der Waals heterostructures — •Alexander Tartakovskii — Department of Physics and Astronomy, University of Sheffield, Sheffield, S3 7RH, UK

Recent years have seen significant effort in exploration of monolayer semiconductors such as transition metal dichalcogenides (TMDs) MoS_2, WS_2, $MoSe_2$, WSe_2 etc. Atomically-thin layers of two-dimensional materials can be assembled in vertical stacks held together by relatively weak van der Waals forces, allowing for coupling between monolayer crystals with incommensurate lattices and arbitrary mutual rotation. The lattice constant difference and the mutual rotation angle present new degrees of freedom for the design of novel meta-materials.

A profound consequence of using these new degrees of freedom is the emergence of an overarching periodicity in the local atomic registry of the constituent crystal structures, known as a moiré superlattice. Here, we show that in semiconducting heterostructures built of incommensurate $MoSe_2$ and WS_2 monolayers, excitonic bands can hybridize, which results in the resonant enhancement of the moiré superlattice effects. $MoSe_2$ and WS_2 are specifically chosen for the near degeneracy of their conduction band edges to promote the hybridization of intra- and interlayer excitons. For $MoSe_2/WS_2$ heterostructures with almost aligned pairs of monolayer crystals, the resonant mixing of the electron states leads to amplified effects of the heterostructure's geometrical moiré pattern on the dispersion of the hybridised excitons.

DS 11.2 Mon 15:30 POT 81

Intralayer and interlayer exciton dynamics in WSe_2/WS_2 van-der-Waals heterostructure — •Manan Shah, Lorenz Maximilian Schneider, and Arash Rahimi-Iman — Department of Physics and Materials Sciences Center, Philipps-Universität, Marburg, 35032 Germany

The van-der-Waals heterostructures (vdW-HS) comprising atomically thin transition-metal dichalcogenides (TMDCs) provide an unprecedented level of freedom for bandgap engineering. However, the HSs give rise to more complex behaviour due to the change in effective dielectric screening, interlayer coupling strength, and moiré potential. The effectiveness of these parameters primarily depends upon the spacing, lattice constant mismatch, and the twist angle between the layers. The hybrid band structure of the vdW-HS system arising from the magnitude of these phenomena is not yet completely understood.

Here, we report a type-II WSe_2/WS_2 HS where the electrons accumulate in the WS_2 monolayer (ML) and the holes accumulate in the

WSe_2 ML owing to charge transfer, giving rise to interlayer excitons. This tungsten-based HS is of particular interest due to the presence of energetically favourable spin-forbidden dark A-excitonic states and a strong excitonic binding energy. Our optical-spectroscopy results exhibit the intralayer excitons, intralayer phonon-assisted dark excitons, and interlayer excitons along with the emergence of new excitonic states with a large oscillator strength between the optical bandgap of the constituting MLs [M. Shah et al., *Semiconductors* (in press)].

DS 11.3 Mon 15:45 POT 81

Enabling tailored 2D materials by introducing 1D organic-inorganic perovskites with supramolecular intra-layer interactions — •Philip Klement[1], Natalie Dehnhardt[2], Chuan-Ding Dong[3], Samuel Bayliff[4], Julius Winkler[2], Peter J. Klar[1], Stefan Schumacher[3,5], Sangam Chatterjee[1], and Johanna Heine[2] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Germany — [2]Department of Chemistry and Material Sciences Center, Philipps-Universität Marburg, Germany — [3]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn University, Germany — [4]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, USA — [5]College of Optical Sciences, The University of Arizona, Tucson, USA

One of the major current challenges in 2D materials* synthesis is the intentional design of building blocks to introducing superior chemical and physical properties. The limiting factor in this approach is the commonly-believed paradigm that in-plane covalent interactions are strictly necessary to form 2D materials, limiting the number of candidates. Here we show that individual single layers of 2D organic-inorganic perovskites with only 1D covalent intralayer-interactions exist. [BzA]3[BiCl5]Cl (BzA = benzylammonium) is exfoliated down to single layers and reveals extremely strong dimensional effects evidenced by a 0.4 eV shift of the photoluminescence between bulk and single layers. We demonstrate that already 1D covalent interactions render 2D materials possible.

DS 11.4 Mon 16:00 POT 81

Layer-dependent and time-resolved photoluminescence in hBN-encapsulated InSe — •Tommaso Venanzi[1,2], Himani Arora[1,2], Stephan Winnerl[1], Alexej Pashkin[1], Phanish Chava[1,2], Zahkar Kudrynskyi[3], Takashi Tanigushi[4], Kenji Watanabe[4], Artur Erbe[1], Amalia Patane[3], Manfred Helm[1,2], and Harald Schneider[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, UK — [4]National Institute for Material Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

In the last years van der Waals semiconductors have become a subject of intense research. Within this class of materials, InSe shows promising optical and electronic properties. Here we present the optical properties of thin flakes of InSe encapsulated in hBN. The encapsulation in hBN protects the InSe flakes from external contamination assuring long-term stability and reducing the disorder potential in the flake. We have studied the photoluminescence (PL) for different temperatures and number of InSe atomic layers. The relative weights of the exciton and electron-hole contributions to the PL emission are discussed using a lineshape analysis. Our model introduces a PL temperature to include the effects of the disorder potential on the PL emission. Furthermore, we observe a sharp increase of the PL lifetime while decreasing the number of layers. This is due to direct-to-indirect bandgap transition driven by the thickness of the InSe flake.

DS 11.5 Mon 16:15 POT 81

Optical Initialisation and Readout of Spin Defects in hBN — •A. Gottscholl[1], M. Kianinia[2], V. Soltamov[1], C. Bradac[2], C. Kasper[1], K. Krambrock[3], A. Sperlich[1], M. Toth[2], M. Dietz[1], I. Aharonovich[2], and V. Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]School of Mathematics and Physical Sciences, Iniverity of Technology Sydney, Ultimo, NSW 2007, Australia — [3]Departomento de Fisica, Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brazil

The concept of optically addressable spin states in solids is considered as a major building block of upcoming quantum technologies. While several candidates in 3D crystals including diamond and silicon carbide have been extensively studied, the identification of spin-dependent processes in 2D materials has remained elusive. Optically accessible spin states in hBN are already theoretically predicted, however, they have not been observed experimentally yet. We investigated a bright 850nm defect-related fluorescence in hBN with magnetic resonance techniques and identified it as a negatively charged boron vacancy V_B^-, possessing a spin triplet ground state and a zero field splitting of 3.5 GHz [1]. The defect shows an optically detected magnetic resonance signature at room temperature and can be optically spin polarized at lower temperatures. Our results constitute a leap forward in establishing two-dimensional hBN as a prime platform for scalable quantum technologies.

[1] Gottscholl et al., arXiv:1906.03774

DS 11.6 Mon 16:30 POT 81

Theory of optical absorption in monolayers of transition metal dichalcogenides — •Frank Lengers, Doris E. Reiter, and Tilmann Kuhn — Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm Str. 10, 48149 Münster

Monolayers of transition metal dichalcogenides are attractive materials for optoelectronics due to their strong exciton-light interaction. At the same time the interaction of excitons and phonons plays a crucial role in these systems leading to strong phonon-assisted processes in optical experiments.

In this contribution different theoretical methods for the computation of linear absorption spectra in monolayers of transition metal dichalcogenides are investigated. To be specific, we consider the spectra of $MoSe_2$ using either a correlation expansion in 2nd or 4th Born Approximation or an approximation closely related to the time convolution less master equation used in the theory of open quantum systems. We show that the 2nd Born Approximation gives poor results for elevated temperatures due to the exceptionally strong exciton-phonon interaction. On the other hand the time convolution less approach gives suprisingly good results despite its simplicity when compared to higher-order correlation expansion. This rather easy method can therefore be readily applied to the class of atomically thin solids where strong carrier-phonon interaction plays a vital role.

30 min. break.

DS 11.7 Mon 17:15 POT 81

Band filling and cross quantum capacitance in ion gated semiconducting transition metal dichalcogenide monolayers — •Haijing Zhang[1,2], Christophe Berthod[2], Helmuth Berger[3], Thierry Giamarchi[2], and Alberto Morpurgo[2] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [2]University of Geneva, Geneva, Switzerland — [3]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Ionic liquid gated field-effect transistors based on semiconducting transition metal dichalcogenides are used to study a rich variety of extremely interesting phenomena, while important aspects of how charge carriers are accumulated in these systems remain elusive. Here we present a thorough analysis of charge accumulation in MoSe_2 and WSe_2 monolayers. We identify the conditions when the chemical potential enters different valleys in the monolayer band structure and find that an independent electron picture describes the occupation of states well. Unexpectedly, however, the same analysis of the experiments shows that the total device capacitance cannot be simply described in terms of the series connection of a geometrical capacitance and of a quantum capacitance given by C_Q=e^2/(dμ/dn), as commonly assumed. This unexpected behavior occurs because a cross quantum capacitance contribution is present, which originates physically from mutual screening of the electric field generated by charges on one plate from charges sitting on the other plate. Our findings reveal an important contribution to the capacitance of physical systems that had been virtually neglected until now.

DS 11.8 Mon 17:30 POT 81

Theory of Exciton-Electron Coupling in Two-Dimensional Semiconductors — •Frederik Schirdewahn[1], Dominik Christiansen[1], Andreas Knorr[1], Tommaso Venanzi[2], Stephan Winnerl[2], and Malte Selig[1] — [1]Technische Universität Berlin, Germany — [2]Helmholtz Zentrum Dresden-Rossendorf, Germany

The strong Coulomb interaction in monolayers of doped transition metal dichalcogenides (TMDCs) leads to the formation of tightly bound excitons and electron gas assisted exciton transitions (trions)[1,2]. Here we present a microscopic approach within the Heisenberg equation of motion formalism for the excitonic absorption including trion signatures[3]. We discuss the impact of doping density and temperature on the absorption spectrum. Additionally we present a joint experiment theory study for THz pump VIS probe experiments of doped monolayer $MoSe_2$, where we find a red shift of exciton and trion lines which we trace back to a heating of the electrons due to the THz pulse finding a good comparison between theory and experiment.

[1] G. Plechinger et al., Nat. Commun. 7, 12715 (2016)
[2] T. C. Berkelbach et al., Phys. Rev. B 88, 045318 (2013)
[3] A. Esser et al., phys. stat. sol. (b) 2, 317 (2001)

DS 11.9 Mon 17:45 POT 81

Bosonic Condensation in a hybrid monolayer MoSe2-GaAs-microcavity — •Max Waldherr[1], Nils Lundt[1], Martin Klaas[1], Simon Betzold[1], Matthias Wurdack[2], Anton Nalitov[3], Sefaattin Tongay[4], Elena Ostrovskaya[2], Alexey Kavokin[3], Sven Höfling[1,5], and Christian Schneider[1] — [1]Technische Physik, Physikalisches Institut and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Germany — [2]Nonlinear Physics Centre, Research School of Physics and Engineering, Australian National University, Canberra, Australia — [3]Physics and Astronomy School, University of Southampton, Highfield, Southampton, UK — [4]School for Engineering of Matter, Transport, and Energy, Arizona State University, Tempe, Arizona, USA — [5]SUPA, School of Physics and Astronomy, St. Andrews, UK

We observe bosonic condensation in a hybrid exciton-polariton system in the strong-coupling regime, with monolayer MoSe2 and GaAs quantum well excitons collectively coupling to a Tamm-plasmon mode. The onset of condensation in the hybrid polariton branch manifests in a superlinear increase of its emission intensity, accompanied by a distinct collapse of the linewidth, a core sign of temporal coherence. At further increasing pumping powers, we observe a continuing blueshift of the resonance originating from particle interactions with uncondensed excitons in the reservoir states. The spin-polarized emission is a clear sign of valley-selective condensation.

DS 11.10 Mon 18:00 POT 81

Micro-photoluminescence studies of defects hosting localized excitons in single-layer MoS_2 — •Oleg Gridenco, Kathrin Sebald, Christian Tessarek, Martin Eickhoff, and Jürgen Gutowski — Institute of Solid State Physics, University of Bremen, D-28359 Bremen, Germany

Beside to free excitons, single-layer transition metal dichalcogenides (TMDs) can also host localized excitons that are bound to defect states and emit with energies smaller than the free-exciton energy. These localized emission centres often appear in as-prepared samples after exfoliation, but they can also be created or enhanced at specific positions by local engineering. In this talk, we will introduce our recent progress in the study of point defects in single-layer MoS_2. Defects were introduced by scanning a Ga^+ ion beam over a certain area of a single-layer using a focused ion beam (FIB) machine. The number of defects was controlled by varying the Ga^+ ion dose. By performing low-temperature micro-photoluminescence (μPL) spectroscopy we investigate the emission properties of localized excitons. Moreover, we found that the intentionally generated defect-related emission centres dominate the optical spectra of MoS_2 at low temperatures. Additionally, light emitted from free or localized excitons needs to be efficiently collected. Here we will discuss how plasmonic nanostructures on top of single-layers are particularly well suited for enhancing the quantum yield of single-layer TMDs.

DS 11.11 Mon 18:15 POT 81

On-demand exchange and spin-orbit in bilayer graphene sandwiched between TMDC and ferromagnet — •Klaus Zollner[1], Martin Gmitra[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute of Physics, P. J. Šafárik University in Košice, 04001 Košice, Slovakia

Van der Waals heterostructures offer great potential for future device applications. Bilayer graphene on a transition-metal dichalcogenide (TMDC) experiences strong proximity spin-orbit coupling (SOC) [1], and record spin lifetime anisotropies are achievable [2]. Moreover, one can turn ON and OFF the SOC in bilayer graphene with a gate voltage [3], and realize a spin-orbit valve [1]. Similarly, one can have on-demand proximity exchange in a bilayer graphene/ferromagnetic-insulator heterostructure [4],realizing an exchange valve. The logical next step is to combine both proximity effects, exchange and SOC in bilayer graphene sandwiched between TMDC and ferromagnet-insulator. In this talk, we will present our results of a time-reversal field effect valve in doubly proximitized bilayer graphene.

This work was supported by DFG SPP 1666, SFB 1277, the EU Horizon 2020 research and innovation program under Grant No. 785219, and by the reintegration scheme MSVVaS SR 90/CVTISR/2018 and VVGS-2019-1227.

[1] Gmitra et al., Phys. Rev. Lett. 119, 146401 (2017). [2] Omar et al., Phys. Rev. B 100, 155415 (2019). [3] Island et al., Nature 571, 85 (2019). [4] Zollner et al., N. J. Phys. 20, 073007 (2018).

DS 12: Thermoelectric and Phase Change Materials

Time: Monday 16:30–17:45 Location: CHE 91

DS 12.1 Mon 16:30 CHE 91

Atom Probe Investigation of Intermixing and Thermal stability in GeTe-Sb_2Te_3 Superlattices for Memory Applications — •Nikita Polin, Oana Cojocaru-Mirédin, Henning Hollerman, Alexander Meledin, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, Aachen, Germany

A chalcogenide superlattice is a periodic structure of layers of two (or more) chalcogenide materials with typical layer thickness of several nanometers. Devices based on GeTe-Sb_2Te_3-superlattices were found to switch with one order of magnitude lower power consumption compared to conventional bulk based $Ge_2Sb_2Te_5$ devices. However, the layers were found to be prone to intermix during deposition at elevated temperatures. Investigation of the thermal stability of the superlattices is thus of applicational and scientific interest.

For this purpose sputtered and annealed GeTe-Sb_2Te_3-superlattices are studied by Atom Probe Tomography (APT), Transmission Electron Microscopy and X-Ray-Diffraction in a correlative manner. Due to the 3D chemical information of the specimens arising from the APT some unexpected findings on the nanoscale could be made: Besides the conventional defects as grain boundaries more exotic nanostructural defects, such as layer splitting, layer dissolving and layer gluing, were found. Additionally heterointerfaces between Ge-rich phases and the surrounding $Ge_2Sb_2Te_5$ were found even at high annealing temperatures of 350°C. Such interfaces might be decisive for the electrical, magnetic, thermoelectric and optical properties of the superlattices.

DS 12.2 Mon 16:45 CHE 91

Impact of interfaces on bipolar resistive switching behavior in amorphous $Ge_2Sb_2Te_5$ thin films — •Hagen Bryja, Christoph Grüner, Jürgen W. Gerlach, Mario Behrens, Martin Ehrhardt, Bernd Rauschenbach, and Andriy Lotnyk — Leibniz Institute of Surface Engineering (IOM), Permoserstraße 15, 04318 Leipzig, Germany

Electrochemical metallization (ECM) memories have attracted much attention as candidates for next generation non-volatile memory applications due to their fast switching, simple structure, high scalability and low energy consumption. Chalcogenide compounds like Ge-Sb-Te-based materials are extensively studied solid electrolytes for such devices and considered within the most promising candidates. However, besides Cu, Ag and Te, the influence of different electrode materials in chalcogenide-based ECM cells has not been investigated and the origin of analog resistive switching, observed in some devices, is still under debate. To shed light on these questions, ECM cells were fabricated using various electrode materials (Al, Ti, Cr, Ta, Co, Cu, Ag, Au, Pt and Cr-CrO_x), a pulsed laser deposited amorphous $Ge_2Sb_2Te_5$ solid electrolyte and a Pt counter electrode. The devices were studied by electrical measurements, secondary ion mass spectrometry and transmission electron microscopy in conjunction with energy-dispersive X-ray spectroscopy. Depending on the utilized electrode material, analog switching, digital switching or no switching occurs. It is observed that the switching behavior is strongly affected by the GST/electrode interfacial interactions, i.e. diffusion and reaction layer formation.

DS 12.3 Mon 17:00 CHE 91

Nanoscale characterization of laser-switched $Ge_3Sb_2Te_6$ with scattering-type Scanning Near-field Optical Microscopy (s-SNOM) and Kelvin Probe Force Microscopy (KPFM) — •Julian Barnett[1], Lukas Wehmeier[2], Andreas Hessler[1], Konstantin Wirth[1], Susanne Kehr[2], Lukas Eng[2], and Thomas Taubner[1] — [1]Institute of Physics (IA), RWTH Aachen — [2]Institute of Applied Physics, TU Dresden

Laser-switching of phase-change materials (PCMs) has gathered renewed interest for (re-)writable nanophotonic applications, such as all-optical memory or metasurfaces [1], because their non-volatile transition between two states with distinctly different optical properties allows for local encoding of information. This application-oriented research is based on the development of PCMs with new optical functionalities, requiring a fundamental understanding of physical processes during local switching to optimize speed, cyclability and control over intermediate states.
Scattering-type Scanning Near-field Optical Microscopy (s-SNOM) is capable of non-destructive, nanoscale characterization of laser-switched PCM devices [2]. We use s-SNOM in combination with Kelvin Probe Force Microscopy (KPFM) to investigate the local electronic properties of laser-switched $Ge_3Sb_2Te_6$, where a single measurement clearly shows four distinctive states: as-deposited amorphous, crystallized, melt-quenched reamorphized, and recrystallized.
[1] M. Wuttig et al. (2017), Nat. Photon. 11, 465.
[2] M. Lewin et al. (2015), Appl. Phys. Lett. 107, 151902.

DS 12.4 Mon 17:15 CHE 91

Thermoelectricity of molecular junctions and their near-Carnot efficiency — •Matthias A. Popp and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Staudtstraße 7, 91058 Erlangen, Germany

We report on thermoelectric transport in molecular junctions, measured with the recently developed squeezable nanojunction technique [1]. A broad ensemble of resonant tunnel junctions with metallic electrodes is investigated. We find correlations between the electric conductance G and the Seebeck coefficient S with unexpected, rigid boundaries. A comparison with the resonant tunneling model shows excellent agreement with experimental data and exposes the generality of the findings. In this framework, measuring $I(V)$ and S for a given junction provides access to the full thermoelectric characterization of the electronic system. A rather unspecific resonant molecular junction displays significant thermoelectric conversion efficiencies. Design rules for optimized efficiency are given.

[1] M. A. Popp and H. B. Weber, Applied Physics Letters 115, 083108 (2019)

DS 12.5 Mon 17:30 CHE 91

Phonons and thermal conductivity in Si/SiO_2 rolled-up nanostructures — •Igor Bogush[1,2] and Vladimir Fomin[3,4] — [1]Scoala Doctorala de Stiinte Fizice si Ingineresti, Institutul de Cercetare si Inovare, Moldova State University, Chisinau MD-2009, Republic of Moldova — [2]Department of Theoretical Physics, Faculty of Physics, Moscow State University, 119899, Moscow, Russia — [3]Department of Theoretical Physics, Moldova State University, Chisinau MD-2009, Republic of Moldova — [4]Institute for Integrative Nanosciences, Leibniz IFW Dresden, Dresden D-01069, Germany

We have developed a differential-geometry formalism for elastodynamic equations applicable for analytical and numerical simulations of phonons in nanowires with arbitrary cross-section geometry and applied it for rolled-up nanostructures. Phonon spectrum for rolled-up Si/SiO_2 bilayer nano-structures with free boundaries is shown to have a similar form as that for unrolled flat nanostructures. Analytical calculations lead to the energy corrections proportional to the ratio of the bilayer width to the structure radius. Geometrical effects for rolled-up structures with small width/radius ratio are neglectable. Therefore realistic rolled-up structures with contacting boundaries can be simulated as flat structures preserving contacting boundary conditions in geometrically non-local sense. Phonon modes are denser for structures with more windings. On this basis we explain the experimentally observed thermal conductivity decrease with increasing number of windings. The present work is supported by the DFG grant no. FO 956/4-1.

DS 13: Layer Deposition II: Deposition Methods

Time: Monday 16:45–18:00 Location: CHE 89

DS 13.1 Mon 16:45 CHE 89

Real-Time Investigations during Sputter Deposition on Polymer Thin Films — •Matthias Schwartzkopf[1], Marc Gensch[1,2], Thomas Strunskus[3], Franz Faupel[3], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,4] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]TUM, James-Franck-Str. 1, D-85748 Garching — [3]CAU zu Kiel, Kaiserstr.2, D-24143 Kiel — [4]KTH, Teknikringen 56, SE-100 44 Stockholm

The reproducible low-cost fabrication of functional polymer-metal-nanocomposites remains a major issue in applied nanotechnology. In order to obtain full control over the nanostructural evolution at the metal-polymer interface, we employed time-resolved surface sensitive X-ray scattering during sputter deposition of gold on thin polystyrene films and silicon substrates [1,2]. We correlate the evolution of the metallic layer morphology with changes in the key scattering features. This enabled us to identify the impact of atomic deposition rate on the growth regimes with their specific thresholds [3]. Our study opens up the opportunity to improve nanofabrication of tailored metal-polymer nanostructures for organic electronics like photovoltaic applications and plasmonic-based technologies. [1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015); [2] Schwartzkopf et al., Nanoscale 5, 5053 (2013); [3] Schwartzkopf et al., ACS Appl. Mater. Interfaces 9, 5629 (2017).

DS 13.2 Mon 17:00 CHE 89

Real time video analysis of droplets in spray pyrolysis deposition process — •Jonas Köhling and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Spray pyrolysis is a cost-effective and scalable process used for deposition of thin functional films in areas of electronic, optics or even medicine. The properties of the thin films are influenced by the behavior of droplets with respect to the surface temperature of the substrate used for the deposition. Usually, smoother films were observed for temperatures higher than Leidenfrost temperature [1], which depends mainly on the solvent and the substrate.

In this work, we have developed a system to monitor the interaction of droplets smaller than 80 μm on a hot surface for a timescale below 1 ms. Such small droplets are produced by an ultrasonic atomizer and sprayed onto the substrate with controlled temperature. A high-speed camera with up to 10.000 frames per second is used to monitor the behavior of the droplets. Using a computer algorithm, the droplets are analyzed automatically and properties such as droplet size distribution and their lifetime have been determined. Analysis of the droplet lifetime allows for the systematic determination of Leidenfrost temperature and optimization of spray pyrolysis process for the thin film deposition.

[1] M. Ortel and V. Wagner, J. Cryst. Growth, 2013, 363, 185-189

DS 13.3 Mon 17:15 CHE 89

Atomic layer deposition of optical coatings on PMMA — •Pallabi Paul[1], Kristin Pfeiffer[2], and Adriana Szeghalmi[1,2] — [1]Institute of Applied Physics, Abbe Centre of Photonics, Friedrich Schiller University Jena, Germany — [2]Fraunhofer Institute for Applied Optics and Precision Engineering, Jena, Germany

Atomic layer deposition (ALD), based on self-saturating surface reactions, is a promising chemical coating technology due to its conformal film growth on complex shaped substrates. Thermoplastics like poly(methyl methacrylate) (PMMA) is an important alternative to glass optics and has widely been used in producing various optical components. However, precision coatings on plastics are rather challenging due to the tendency of crack formation and typically low adhesion of the dielectric coatings to the polymer surface. Thus, materials and processes need to be tuned to the particularities of specific polymer. In this work, optimization of ALD processes to develop uniform, homogeneous and dense optical thin films of Al2O3, TiO2 and SiO2 on

PMMA has been carried out and a five-layer antireflection coating is demonstrated. While uncoated PMMA substrates have a reflectance of nearly 8% in the visible spectral range, the reflectance of double-sided antireflection coating does not exceed 1.2% in the spectral range of 420 nm to 670 nm with a total average reflectance of only 0.7%. Microscopic analysis of cross-hatch areas on PMMA indicates superior adhesion and excellent environmental stability of ALD coatings. Furthermore, 3D conformal growth of ALD films is exploited on PMMA dome ensuring identical spectra on the entire dome surface.

DS 13.4 Mon 17:30 CHE 89

One-step Synthesis of Carbon-supported Electrocatalysts — •Sebastian Tigges[1], Nicolas Wöhrl[1], Ivan Radev[2], Ulrich Hagemann[1,3], Markus Heidelmann[1,3], Thai Binh Nguyen[1,3], Stanislav Gorelkov[2], Stefan Schulz[1], and Axel Lorke[1] — [1]University of Duisburg-Essen and CENIDE, 47057 Duisburg, Germany — [2]ZBT GmbH, 47057, Duisburg, Germany — [3]University of Duisburg-Essen and ICAN, 47057 Duisburg, Germany

Cost-efficiency, durability and reliability are the main challenges in the commercialization of fuel cells, thus research is focusing on development of new material systems for use in electrocatalysis. Especially long-term stability needs to be improved, since degradation mechanisms lead to a reduced lifetime of conventional catalyst materials. Here, we present a novel, one-step approach to synthesize a metal/carbon-hybrid material by plasma-enhanced chemical vapour deposition, demonstrated for the model electrocatalyst Pt/C. Platinum loading, oxidation state, and particle size distribution of the catalyst can be fully controlled. Highly monodisperse size distributions and small mean particle sizes of the Pt nanoparticles are achieved. Due to the one-step nature of the process, the Pt nanoparticles are embedded into the support (carbon nanowalls), which improves long-term stability, while maintaining good electrochemical surface area. By using different precursors, the versatile synthesis process can be easily adapted to deposit other metal/carbon-hybrids for a variety of potential applications. Control of the functionalization and doping of the catalyst is discussed briefly.

DS 13.5 Mon 17:45 CHE 89

Epitaxial growth of Cr_2AlC MAX phase thin films by pulsed laser deposition — •Marc Stevens, Alexander Jemiola, Michael Farle, and Ulf Wiedwald — Faculty of Physics and Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, Germany

MAX phases ($M_{n+1}AX_n$) are ternary or quaternary compounds of layered hexagonal structures, where M is an early transition metal, A is an A group element and X is either C or N [1]. Within the last years, much attention is put on magnetic MAX phases with Cr and/or Mn as two possible M elements. The magnetic properties of such $(M1_xM2_{1-x})_2AX$ phases are driven by competing ferromagnetic and antiferromagnetic correlations leading to complicated phase diagrams [2,3]. One parent compound of such MAX phases is Cr_2AlC. In this work, we show the first successful synthesis of epitaxial Cr_2AlC films on MgO (111) substrates by pulsed laser deposition (PLD) at film thicknesses of 10-50 nm. The epitaxial relation is Cr_2AlC (0001) || MgO (111) in the growth direction and Cr_2AlC $[11\bar{2}0]$ || MgO $[10\bar{1}]$ in the film plane. We compare the growth of Cr_2AlC on MgO(111) and Al_2O_3(0001) and discuss the impact on the magnetic properties. Funding by the Deutsche Forschungsgemeinschaft (DFG) within the CRC/TRR 270 is gratefully acknowledged.

[1] M. W. Barsoum, Prog. Solid State Chem. 28, 201 (2000). [2] A. S. Ingason, M. Dahlqvist, and J. Rosen, J. Phys.: Condens. Matter 28, 43 (2016). [3] Iu. Novoselova et al., Sci. Rep. 8, 2637 (2018).

DS 14: 2D Materials and their Heterostructures I (joint session DS/O/HL)

Time: Tuesday 9:30–11:30 Location: CHE 89

DS 14.1 Tue 9:30 CHE 89

Plasma-enhanced atomic layer deposition of AlN at 40°C for encapsulation and dielectric integration of 2D materials — •Michele Bissolo, Alex Henning, Theresa Grünleitner, and Ian D. Sharp — Walter Schottky Institute, 85748 Garching, Germany

To date, hexagonal boron nitride (h-BN) is the material of choice for the dielectric integration of 2D materials since it preserves the intrinsic photoluminescence yield, charge carrier mobility, and band gap of 2D semiconductors by reducing strain, effects of interfacial defects, and remote phonons. However, h-BN must be either mechanically transferred with a polymer stamp onto a bulk substrate, which introduces contamination, or grown by MBE at temperatures above 800°C, which is incompatible with BEOL, microlithography, and temperature-sensitive materials. Here, we demonstrate atomically flat aluminum nitride (AlN), grown by plasma-enhanced atomic layer deposition (PEALD) at 40°C, as a scalable alternative to h-BN. AlN has a similar band gap ($E_g = \sim 6$ eV) and a larger dielectric constant ($\epsilon = \sim 9$) in comparison to h-BN. Because ALD is conformal, it enables the full enclosure of the 2D material. In this work, we test PEALD AlN as a substrate and encapsulation layer for mono- and few-layer MoS_2. Raman spectroscopy suggests a strain-free integration of MoS_2 with AlN and photoluminescence shows a relatively stronger emission from the A and B excitons without emission from defects. We demonstrate the improved field-effect mobility with MoS_2 field-effect transistors enclosed by an AlN dielectric layer. This work provides a scalable route to the dielectric integration of 2D materials critical for future optoelectronics.

DS 14.2 Tue 9:45 CHE 89

Spin-Sensitive Readout of Two-Dimensional Wigner Crystals in Transition-Metal Dichalcogenides — •Johannes Knörzer[1,2], Martin Schuetz[3], Geza Giedke[4,5], Dominik Wild[3], Kristiaan de Greve[3], Richard Schmidt[1,2], Mikhail Lukin[3], and Ignacio Cirac[1,2] — [1]Max-Planck-Institut für Quantenoptik, Garching, Germany — [2]Munich Center for Quantum Science and Technology, München, Germany — [3]Physics Department, Harvard University, Cambridge, USA — [4]Donostia International Physics Center, San Sebastián, Spain — [5]Ikerbasque Foundation for Science, Bilbao, Spain

Wigner crystals are prime candidates for the realization of regular electron lattices under minimal requirements on external control and electronics. However, technical challenges have prevented their detailed experimental investigation to date. Here we propose an implementation of two-dimensional electron lattices for quantum simulation based on self-assembled Wigner crystals in transition-metal dichalcogenides. We show that these semiconductors allow for minimally invasive all-optical detection schemes of charge ordering and total spin. For incident light with optimally chosen beam parameters and polarization, we predict a strong dependence of the transmitted and reflected signals on the underlying lattice periodicity, thus revealing the charge order inherent in Wigner crystals. At the same time, the selection rules in transition-metal dichalcogenides provide direct access to the spin degree of freedom via Faraday rotation measurements.

DS 14.3 Tue 10:00 CHE 89

Growth of ultra-thin large sized 2D WS_2 flakes in at air-liquid interface — •Talha Nisar[1], Torsten Balster[1], Ali Haider[2], and Veit Wagner[1] — [1]Department of Physics and Earth Science, Jacobs University Bremen, Campus Ring 1, 28759, Bremen, Germany — [2]Department of Life Sciences and Chemistry, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

2D tungsten disulfide (WS_2) flakes were obtained at the air-liquid interface by a technique recently developed [1]. For this purpose, aqueous solution of ammonium tetrathiotungstate (ATTW) is used as precursor. The process exhibit a clear temperature dependence. At the room temperature, no flakes are observed. When the aqueous solution of ATTW is kept at 80°C, formation of flakes is observed. These flakes can be transferred from the air-liquid interface to a silicon substrate by a controlled dip-coating process. Large flakes with lateral size of up to 100μm were obtained. Thicknesses ranging from bilayer WS_2 to 5 MLs as measured by atomic force microscopy. Various spectroscopic techniques (FTIR, Raman, UV-Vis and XPS) are applied to investigate the chemical reaction mechanism for the formation of the flakes. These results show that the initial flakes are made of WO_3. The obtained flakes are converted to WS_2 by a post annealing step at 500-900 °C with an additional sulfur source in Ar/H_2 environment. The successful conversion to WS_2 after annealing is confirmed by Raman and XPS. This non-expensive growth technique can be used to produce large WS$_2$ flakes for various applications. [1] X. Zeng, et al, Nanoscale, 2017, 9, 6575-6580

DS 14.4 Tue 10:15 CHE 89

Electrical Properties and Doping effects of Chemical Vapor Deposition Growth Layered MoS2 Transistor on Different Back gate oxide Substrates — •Ying-Chun Shen and Yu-Lun Chueh — Department of Materials Science and Engineering National Tsing-Hua University 101, Sec. 2, Kuang-Fu Road, Hsinchu 30013, Taiwan, R. O. C

Recently, there have been many research evolvements in the transition-metal dichalcogenides (TMDCs) materials, which are featured by exotic properties of single or a few layers derivative in terms of direct or indirect bandgap, mechanical or electrochemical behavior. In addition to the pristine properties, the chemical and physical features of TMDCs can be controllably tuned by either nano-structure or dopants. Due to the nature of the TMDCs, they have been the promising candidates of the next-generation semiconductor devices. In our study, we have demonstrated the chemical vapor deposition growth layered MoS2 transistors on different back gate oxide substrates, such as SiO2, HfO*2 and Al2O3. Among these three substrates, HfO2 based MoS2 transistor exhibits the best performance, e.g., higher drain current up to 10 mA, on-off ratio about 106, stable mobility around 20 cm2/ V* s. Furthermore, we performed the doping effect by adding metal ions, and investigate the ion influence on the MoS2 transistor. Moreover, we also compared the electrical performance of distinct metal ions and the number of ions. Here, we provide not only the properties of back gate oxide selection but also a roadmap of ion doping effect to boost the electrical characteristics of the MoS2 transistors.

DS 14.5 Tue 10:30 CHE 89

Optical properties of TMDC monolayers interfaced with 2D metals — •Katharina Nisi[1], Shruti Subramanian[2,3], Florian Sigger[1], Margaux Lassaunière[4], David O. Tiede[4], Hendrik Lambers[4], Alexander Holleitner[1], Joshua Robinson[2,3], and Ursula Wurstbauer[4] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany — [2]Department of Materials Science and Engineering, The Pennsylvania State University, USA — [3]Center for 2-Dimensional and Layered Materials, The Pennsylvania State University, USA — [4]Institute of Physics, University of Münster, Münster, Germany

Two-dimensional metals such as 2D-Ga or 2D-In prepared by confinement epitaxy are an emerging class of materials with peculiar properties including superconductivity and strong plasmonic response [1]. The plasmon resonance of those 2D metals spectrally overlaps with the excitonic transition energies of semiconducting transition metal dichalcogenides. Hybrid structures of 2D metals with TMDCs are promising for enhancing the light matter interaction. We investigate the optical response of 2D metal-TMDC hybrid structure by a combination of spectroscopic imaging ellipsometry, photoluminescence and Raman spectroscopy.

[1] B. Bersch et al. arXiv:1905.09938 (2019).

DS 14.6 Tue 10:45 CHE 89

Rigid Band Shifts in Two-Dimensional Semiconductors through External Dielectric Screening — •Malte Rösner[1], Lutz Waldecker[2,3], Archana Raja[4,5], Christina Steinke[6], Aaron Bostwick[4], Roland J. Koch[4], Chris Jozwiak[4], Takashi Taniguchi[7], Kenji Watanabe[7], Eli Rotenberg[4], Tim O. Wehling[6], and Tony F. Heinz[2,3] — [1]Institute for Molecules and Materials, Radboud University, Netherlands — [2]Department of Applied Physics, Stanford University, USA — [3]SLAC National Accelerator Laboratory, USA — [4]Lawrence Berkeley National Laboratory, USA — [5]Kavli Energy NanoScience Institute, University of California Berkeley, USA — [6]Institute for Theoretical Physics, University of Bremen, Germany — [7]National Institute for Materials Science, Japan

We investigate the effects of external dielectric screening on the electronic dispersion and the band gap in the atomically thin, quasi-two-dimensional (2D) semiconductor WS2 using angle-resolved photoemission and optical spectroscopies, along with first-principles calculations. We find the main effect of increased external dielectric screening to be a reduction of the quasiparticle band gap, with rigid shifts to the bands themselves. Specifically, the band gap of monolayer WS2 is decreased by about 140 meV on a graphite substrate as compared to a hexagonal boron nitride substrate, while the electronic dispersion of WS2 remains unchanged within our experimental precision of 17 meV. These essentially rigid shifts of the valence and conduction bands result from the special spatial structure of the changes in the Coulomb potential induced by the dielectric environment of the monolayer.

DS 14.7 Tue 11:00 CHE 89

Unveiling valley lifetimes of free charge carriers in monolayer WSe$_2$ — •Manfred Ersfeld[1], Frank Volmer[1], Lars Rathmann[1], Luca Kotewitz[1], Maximilian Heithoff[1], Mark Lohmann[2], Bowen Yang[3], Kenji Watanabe[4], Takashi Taniguchi[4], Ludwig Bartels[3], Jing Shi[2], Christoph Stampfer[1,5], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany — [2]Department of Physics and Astronomy, University of California, Riverside, California 92521, USA — [3]Department of Chemistry and Materials Science & Engineering Program, University of California, Riverside, California 92521, USA — [4]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan — [5]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

We report on nanosecond long, gate-dependent valley lifetimes of free charge carriers in WSe$_2$, unambiguously identified by the combination of time-resolved Kerr rotation (TRKR) and electrical transport measurements. While the valley polarization increases when tuning the Fermi level into the conduction or valence band, there is a strong decrease of the respective valley lifetime consistent with both electron-phonon and spin-orbit scattering. The longest lifetimes are seen for spin-polarized bound excitons in the band gap region. We explain our findings via two distinct, Fermi level-dependent scattering channels of optically excited, valley polarized bright trions either via dark or bound states.

DS 14.8 Tue 11:15 CHE 89

Superconducting Properties of MXene Monolayers — •Cem Sevik[1], Jonas Bekaert[2], and Milorad Milosevic[2] — [1]Department of Mechanical Engineering, Eskisehir Technical University, Ankara, Turkey — [2]Department of Physics, University of Antwerp, Antwerpen, Belgium

MXenes are a new class of two-dimensional materials, consisting of a carbon or nitrogen layer sandwiched in between two transition metal layers. Various experimental studies have demonstrated that these crystals have broad and growing areas of application, such as Li-ion batteries, super-capacitors, fuel-cells, and hydrogen storage. Since most of the MXene monolayers are metals, they could also host superconductivity, depending on their electronic and vibrational properties. Therefore, we have systematically investigated the superconducting properties of monolayer MXenes of stoichiometry M2X (M being the transition metal and X either C or N), with a first-principles approach to Eliashberg theory. Due to the presence of the transition metal, we found the choice of the type of exchange-correlation and inclusion of spin-orbit interactions to be crucial to describe the vibrational and superconducting properties of these monolayers. Cautiously considering these, we have identified five new superconducting monolayer MXenes, out of which three carbides (Mo2C, W2C, and Sc2C) and two nitrides (Mo2N and Ta2N). The highest predicted critical temperature (Tc) of 17 K is found for Mo2N. Our first principle-based systematic analysis clearly has opened up a whole new class of superconductors with sizeable Tc in the monolayer limit.

DS 15: Organic Thin Films, Organic-Inorganic Interfaces I (joint session DS/CPP)

Time: Tuesday 9:30–11:00 Location: CHE 91

DS 15.1 Tue 9:30 CHE 91

Shape controlled assembly of carboxylic acids: intercalation into molecular nanotunnels — Rodrigo Ortiz de la Morena[1], Andika Asyuda[2], Hao Lu[2], Hannah Aitchison[1], Kelly Turner[1], Stephen M. Francis[1], •Michael Zharnikov[2], and Manfred Buck[1] — [1]EaStCHEM School of Chemistry, University of St Andrews, North Haugh, St Andrews KY16 9ST, United Kingdom — [2]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

Binary self-assembled monolayers (SAMs) combining a Y-shaped aromatic carboxylic acid (CA), 1,3,5-benzenetribenzoic acid (H3BTB), and a cage-type alicyclic CA, adamantane CA (AdCA), were prepared by molecular adsorption from solution on Au substrates modified by underpotential deposition of Ag. These SAMs exhibit a pronounced dependence of their structure on the assembly protocol. Exposing an AdCA SAM to H3BTB results in the disordered arrangements. In contrast, exposing an H3BTB SAM to AdCA doesn't seemingly affect the highly regular row structure of the native H3BTB layer, with no signs (STM) of AdCA adsorption. However, spectroscopic analysis reveals its presence, suggesting that the AdCA molecules are hidden in the nanotunnels of the H3BTB monolayer. Additional evidence for this hypothesis is provided by appearance of densely packed and highly ordered AdCA monolayer upon local removal of H3BTB. Formation of such a compact layer is explained by expulsion of AdCA from the H3BTB nanotunnels of the surrounding intact mixed SAM, driven by release of stress in the nanotunnels built up when AdCA is intercalated.

DS 15.2 Tue 9:45 CHE 91

Reestablishing odd-even effects in anthracene-derived monolayers by introduction of a proper symmetry — Christoph Partes[1], Eric Sauter[2], Michael Gärtner[1], Martin Kind[1], Andika Asyuda[2], Michael Bolte[1], Andreas Terfort[1], and •Michael Zharnikov[2] — [1]Institut für Anorganische und Analytische Chemie, Universität Frankfurt, 60438 Frankfurt, Germany — [2]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

A series of anthracene[2,3-d]oxazolyl-2-alkylthioacetates (AOxCnSAc) with n = 2-6 methylene groups in the alkyl chain were designed and synthesized to investigate the influence of the substitution along the long axis of the molecule on the structural behavior of the respective self-assembled monolayers (SAMs) on Au(111). While in previous work anthracene-terminated alkanethiols, in which the alkyl group was attached to the off-axis 2-position of the acene, showed an exceptionally small influence of the number of methylene groups (n) in the aliphatic linker, the new system exhibits a strong dependence of almost all monolayer properties on the length of the aliphatic linker, with the parity of n being the decisive parameter - so-called odd-even effects. The high quality and well-defined character of these SAMs, along with a low band gap of only 3.0 eV, make them relevant for application in organic and molecular electronics.

DS 15.3 Tue 10:00 CHE 91

Exploring Electron Beam Induced Processing on Porphyrin Multilayers for the Fabrication of Nanostructured Ultrathin Membranes — •Christian Preischl, Elif Bilgilsoy, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II Friedrich-Alexander Universität Erlangen-Nürnberg

We investigate two gas-assisted electron beam lithography methods, i.e. Electron-Beam-Induced-Deposition and Electron-Beam-Induced-Surface-Activation (EBISA) on porphyrin multilayers. In EBISA, a surface is irradiated by a focused electron beam, resulting in an activation of the exposed area. The activated areas can then lead to the decomposition of suitable precursor gases.[1] Here we show that EBISA on thin layers of a free-base porphyrin (2HTPP) is compatible with the precursors $Fe(CO)_5$ and $Co(CO)_3NO$[2]. Remarkably, the latter exhibited no EBISA-reactivity on other activated organic substrates like Self-Assembled-Monolayers or Surface-Anchored Metal-Organic Frameworks[3]. We also demonstrate that thin layers of 2HTPP can be cross-linked to form a 2D carbon membrane via low energetic electron irradiation. This membrane is stable enough to transfer the metallic nanostructures onto any desirable substrate.

[1] H. Marbach, Appl.Phys. A 117 (2014) 987 [2] M. Drost et al., Small Methods 1 (2017) 1700095 [3] M. Drost et al., ACS Nano 12 (2018) 3825

DS 15.4 Tue 10:15 CHE 91

Fabrication of metallic nanostructures via FEBIP on top of ultrathin organic membranes — •Alexander Wolfram, Christian Preischl, Elif Bilgilsoy, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, GER

We report a novel method to fabricate ultrathin organic membranes with metallic nanostructures. In a first step, clean iron nanostructures were prepared on a self-assembled-monolayer (SAM) of 1,1',4',1"-terphenyl-4-thiol (TPT) via Electron-Beam-Induced-Deposition (EBID) by using $Fe(CO)_5$ as precursor.[1] In a next step, the SAM is converted into a carbon nanomembrane (CNM) by using low energetic electron-induced crosslinking.[2] In a third step, the membrane was then transferred onto SiO_2 or a TEM grid. We demonstrate that the nanostructures maintain their shape and the membrane remains intact during the transfer. In this way, metallic nanostructures on a free-standing CNM can be fabricated. We also show the influence of the underlying substrate (Ag or Au) of the SAM and the associated wet chemical process on the appearance of the transferred nanostructures.

[1] M. Walz et al., *Angew. Chem. Int. Ed.*, 49 (2010) 4669 [2] A. Turchanin, A. Gölzhäuser, *Advanced Materials*, 28 (2016) 6075.

DS 15.5 Tue 10:30 CHE 91

Interfaces between Tetraphenylporphyrin and Low-Work Function Metals: Interphase Formation Studied with HAXPES — •Maik Schöniger, Stefan R. Kachel, Jan Herritsch, Philipp Schröder, Claudio K. Krug, Mark Hutter, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

Fabrication of organic electronic devices often involves the electrical contacting of organic semiconductors by vapor deposition of metals, resulting in the formation of metal-organic interfaces. These interfaces are crucial for the device's performance in terms of e.g. charge-carrier injection. However, especially metals with low work function can diffuse into and react with the organic material, leading to extended interphases consisting of the reaction products. The question then is: How thick is the formed interphase? As well-defined model systems, we investigated metalloporphyrin (M_xTPP) interphases formed through reaction of tetraphenylporphyrin (H_2TPP) with different vapor-deposited metals M, including earth alkalines (Mg, Ca) and the alkali metal Li. The non-destructive depth-profiling technique of choice is hard X-ray photoelectron spectroscopy (HAXPES), because H_2TPP and M_xTPP can be distinguished by their N 1s signals. Compared to earlier work with Fe and Co, Mg and Ca show increased reaction depths up to few nanometers. In the case of Li, complete reaction to Li_2TPP was observed in a 24 nm thick H_2TPP film. TPD-MS results showed that even thicker H_2TPP layers fully react.

DS 15.6 Tue 10:45 CHE 91

Extended Interphase Formation at a Metal/Organic Interface: Lithium on Tetraphenylporphyrin — •Stefan Renato Kachel, Maik Schöniger, Jan Herritsch, Philipp Schröder, Mark Hutter, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

Porphyrins are versatile model compounds for organic semiconductors (OSC) in application-related studies of metal/organic interfaces. The properties of such interfaces strongly influence the performance of organic electronic devices. To study processes at the interface between an OSC and a low work-function metal, lithium was deposited onto tetraphenylporphyrin (H2TPP) layers and the product composition was analyzed with temperature-programmed desorption mass spectrometry (TPD-MS) and X-ray photoelectron spectroscopy (XPS). With sufficient amounts of Li, we found complete conversion of H2TPP into dilithium tetraphenylporphyrin (Li2TPP). The depth range of this reaction exceeds several 10 nm, contrasting previous findings for transition metals. Even a 50 nm thick layer of H2TPP fully reacted with an excess of Li. For substoichiometric amounts of Li, singly metalated LiHTPP was found. This study shows that the metal/organic interface can be very diffuse with a thick reacted interphase layer separating the metal from the pristine OSC.

DS 16: 2D semiconductors and van der Waals heterostructures III (joint session HL/DS)

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

Invited Talk DS 16.1 Tue 9:30 POT 81

Radiative Lifetime and Fine Structure of Excitons in Transition Metal Dichalcogenide Monolayers — •Xavier Marie — Université de Toulouse, LPCNO, INSA-CNRS-UPS, Toulouse, France

Optical properties of atomically thin transition metal dichalcogenides are controlled by robust excitons characterized by a very large oscillator strength [1,2,3]. Encapsulation of monolayers such as MoSe2 in hexagonal boron nitride (hBN) yields narrow optical transitions approaching the homogeneous exciton linewidth [4,5]. We demonstrate that the exciton radiative rate in these van der Waals heterostructures can be tailored by a simple change of the hBN encapsulation layer thickness as a consequence of the Purcell effect [6].

The time-resolved photoluminescence measurements together with cw reflectivity and photoluminescence experiments show that the neutral exciton spontaneous emission time can be tuned by one order of magnitude depending on the thickness of the surrounding hBN layers.

I will also discuss recent results on the fine structure of excitons in MoSe2 and MoS2 monolayers.

[1] G. Wang et al, Rev. Mod. Phys. 90, 021001 (2018) [2] D. Lagarde et al, PRL 112, 047401 (2014) [3] C. Robert et al, PRB 93, 205423 (2016) [4] F. Cadiz et al, PRX 7, 021026 (2017) [5] G. Wang et al, PRL 119, 047401 (2017) [6] H.H. Fang et al, PRL 123, 067401 (2019)

DS 16.2 Tue 10:00 POT 81

Control of Excitons in Monolayer Transitionmetal Dichalcogenides via Extrinsic Dielectric Screening — •Frederik Otto, Philip Klement, and Sangam Chatterjee — Institute of Experimental Physics I, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany

Electric field lines between charges in freestanding monolayers of transition metal dichalcogenides (TMDs) can extend freely outside the material's perimeters due to the absence of screening carriers on top and on the bottom of the sample. Similarly, field lines extending into a close dielectric, *e.g.*, the substrate, are subject to extrinsic screening effects. This effectively weakens the Coulomb interaction of charge carriers and therefore, iduces changes to the exciton binding energy and electrical band gap.

In order to obtain knowledge about the interaction range and the effect of the static dielectric constant of the surrounding dielectric environment on A and B-excitons of the K-point, we investigated monolayer samples WSe$_2$ supported on either TiO$_2$ (high static dielectric constant) or SiO$_2$ (low static dielectric constant) and samples encapsulated between the two substrate materials.

DS 16.3 Tue 10:15 POT 81

Revealing the quantum nature of excitons in encapsulated monolayers by optical dispersion measurements — •Lorenz Maximilian Schneider[1], Shanece S. Esdaille[2], Daniel A. Rhodes[2], Katayun Barmak[3], James C. Hone[2], and Arash Rahimi-Iman[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Marburg, 35032, Germany — [2]Department of Mechanical Engineering, Columbia University, New York, NY 10027, USA — [3]Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027

The dispersion of excitons in TMDC monolayers has been a topic of several recent theoretical studies and is the base of a true understanding of the physics of such systems. Nonetheless, the theoretical papers have contradicting predictions ranging from the formation of Dirac cones or the formation of a second linear exciton branch around zero in-plane momentum to calculations that just expect ordinary degeneracy-lifted parabolic dispersions. Here, we employ Fourier-space spectroscopy to directly measure the dispersion of the A-exciton in a high-quality h-BN encapsulated monolayer system. A remarkably strong dispersion with 2 meV shifts in within the light cone, respectively an effective mass of 7E-4 m_e can be deduced. Models based on exchange interaction and exciton–polariton formation due to the large oscillator strength are discussed in order to understand the phenomenon clearly observed in PL and reflection spectra [1]. Futhermore, density and temperature dependent behaviour is presented.

[1] L.M. Schneider et al., Optics Express (in press)

DS 16.4 Tue 10:30 POT 81

Light-driven capacitive charge injection in 0D-2D hybrid nanostructures — •Ilka Kriegel[1], Michele Ghini[1], Liberato Manna[1], Nicholas J. Borys[2], and P. James Schuck[3] — [1]Department of Nanochemistry, Istituto Italiano di Tecnologia, Italy — [2]Department of Physics, Montana State University, Bozeman, MT, USA — [3]Department of Mechanical Engineering, Columbia University, New York, NY, USA

In this work we reveal that the coupling of indium tin oxide (ITO) nanocrystals to monolayer MoS2 results in a light-driven charge-injection scheme that quasi-permanently dopes monolayer MoS2 to extents competing with electrostatic doping. The cooperative electronic properties of such novel 0D 2D hybrids display efficient and permanent charge separation after light absorption. The electrons are stored in the nanocrystals, while the holes are transferred to the 2D material accumulating in regions of initially enhanced n-type doping and preferentially along edges and grain boundaries. Charge separation over distances up to 40 μm away from the local (micron sized) optical excitation spot are observed. Notably, carrier injection follows a capacitor-like behavior with capacitance values in the femto Farad range leading to the photo-charging of a model capacitor. An average optically induced photodoping of each nanocrystal with more than 40 carriers is extracted. These studies present a foundational building block for next-generation light-driven energy storage devices. Additionally, the remote-control of local charge density opens prospects for contactless and optically driven 2D material electronics.

30 min. break

DS 16.5 Tue 11:15 POT 81

Broken adiabaticity induced by Lifshitz transition in MoS$_2$ and WS$_2$ single layers — •Dino Novko — Institute of Physics, Zagreb, Croatia — Donostia International Physics Center (DIPC), San Sebastián, Spain

The breakdown of the adiabatic Born-Oppenheimer approximation is striking dynamical phenomenon, however, it occurs only in a handful of layered materials. Here I show that adiabaticity breaks down in doped single-layer transition metal dichalcogenides in a quite intriguing manner. Namely, significant nonadiabatic coupling, which acts on frequencies of the Raman-active modes, is prompted by a Lifshitz transition due to depopulation and population of multiple valence and conduction valleys, respectively. The outset of the latter event is shown to be dictated by the interplay of highly non-local electron-electron interaction and spin-orbit coupling. In addition, intense electron-hole pair scatterings due to electron-phonon coupling are inducing phonon linewidth modifications as a function of doping. Comprehending these intricate dynamical effects turns out to be a key for mastering characterization of electron doping in two-dimensional nano-devices by means of Raman spectroscopy.

DS 16.6 Tue 11:30 POT 81

Transient Valley Grating Spectroscopy on WSe$_2$ — •Julian Wagner, Henning Kuhn, Robin Bernhardt, Jingyi Zhu, and Paul van Loosdrecht — Universität zu Köln, II. Physikalisches Institut, D-50937 Köln, Germany

The absence of space inversion symmetry combined with strong spin-orbit interactions and time-reversal in monolayer transition metal dichalcogenides lead to the emergence of a new quantum degree of freedom, the valley pseudospin. This valley degree of freedom can be manipulated making use of the selection rules for light matter interaction, i.e. one can for instance create pure pseudospin up or down states. These states, however, will decay due to intervalley scattering of the excitonic states involved. The mechanisms leading to intervalley scattering are currently intensely debated, partially due to the lack of experiments directly addressing this.

A direct technique to address the intervalley scattering is Transient Valley Grating Spectroscopy, which is a novel 4-wave mixing approach similar to spin grating techniques. Using this approach, we investigated the valley pseudospin dynamics in monolayer WSe$_2$. This allows for a direct determination of the intervalley scattering rate. Its temperature dependence shows that the dominant valley depolarization process is optical-phonon mediated intervalley scattering.

DS 16.7 Tue 11:45 POT 81

Exciton diffusion in WS_2 monolayers with suppressed disorder — •Koloman Wagner[1], Jonas Zipfel[1], Marvin Kulig[1], Raül Perea-Causín[2], Samuel Brem[2], Jonas D. Ziegler[1], Roberto Rosati[2], Takashi Taniguchi[3], Kenji Watanabe[3], Mikhail M. Glazov[4], Ermin Malic[2], and Alexey Chernikov[1] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [3]National Institute for Materials Science, Tsukuba, Ibaraki, Japan — [4]Ioffe Institute, St. Petersburg, Russia

Excitons are known to dominate optical properties of semiconducting transition metal dichalcogenides (TMDCs) both for monolayers and heterostructures. While excitons can also propagate across large distances due to the two-dimensional nature of the system, their behavior remains highly sensitive to local environmental inhomogeneities. In our work, we take advantage of material encapsulation in high-quality hexagonal boron nitride to study inherent exciton propagation unobscured by disorder. Using spatially- and time-resolved photoluminescence microscopy we find highly efficient linear diffusion and pronounced non-linear phenomena. In order to explain our findings we employ a combination of numerical and analytical approaches, discuss the role of dark states as well as non-radiative exciton-exciton scattering and present a mechanism for rapid diffusion facilitated by free electron-hole plasma.

DS 16.8 Tue 12:00 POT 81

Chemical Trend of Transition-Metal Doping in WSe_2 — •Dan Han[1,2,3], Shiyou Chen[1], and Mao-Hua Du[2] — [1]East China Normal University, Shanghai, China — [2]Oak Ridge National Laboratory, Oak Ridge, USA — [3]Ludwig-Maximilians-Universität München, Munich, Germany

Transition-metal dichalcogenides (TMDs) are promising nanoscale materials with a wide range of applications. Chemical doping is a powerful tool for tailoring the physical and chemical properties of TMDs for targeted functionalities. As an important TMD, WSe_2 has great potential for applications in FET and CMOS technologies. However, precise control over the type and density of free carriers remains challenging. We performed first-principles calculations to study intrinsic defects and transition-metal (TM) dopants in WSe_2. Our results show that TM doping can effectively control the Fermi level in WSe_2 with no significant compensation by intrinsic defects. Nb and Ta are effective p-type dopants capable of generating a high free hole density in WSe_2. While n-type doping is possible by Re and Cu, the doping efficiency is reduced due to the lower attainable dopant concentration and higher ionization energies. The chemical trend in the attainable concentration of various substitutional TM dopants in WSe_2 is largely determined by the competition between the dopant incorporation in WSe_2 and the formation of the secondary phase $TMSe_2$. Such a competition is strongly affected by the different crystal environments of the TM ion in $TMSe_2$ and WSe_2.

DS 16.9 Tue 12:15 POT 81

Interlayer excitons in pristine bilayer MoS2 with strong oscillator strength — •Etienne Lorchat[1], Maximilian Waldherr[1], Sefaattin Tongay[2], Takashi Taniguchi[3], Kenji Watanabe[3], Christian Schneider[1], and Sven Höfling[1] — [1]Technische Physik and Wilhelm Conrad RöntgenResearch Center for Complex Material Systems, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, Arizona 85287, United States — [3]National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan

In the high density limit, the interaction between electrons in a 2D electron gas (2DEG) and excitons in Transition Metal Dichalcogenide (TMD) are predicted to yield a new, unconventional superconductive phase via excitonic cooper pairing. However, this interaction only gets notable if exciton aquires an out of plane dipole to interact with the 2DEG as well as an in-plane dipole to be easily excited with light. The commonly studied excitons in TMD monolayers or heterobilayers present solely one type of the dipole. Among the various approach, we will present here the hybrid interlayer exciton in MoS2. Using field-dependent photoluminescence spectroscopy as well as reflectivity we will demonstrate the emergence of an excitonic resonance, which combines a static dipole moment with a significant oscillator strength.

DS 16.10 Tue 12:30 POT 81

Optoelectronic transport in van der Waals heterostructures of Weyl semimetal $MoTe_2$ — •Maanwinder Partap Singh[1,2], Jonas Kiemle[1,2], Alexander Holleitner[1,2], and Christoph Kastl[1,2] — [1]Walter Schottky Institut, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstraße 4, D-80799 Munich, Germany

Unlike topological insulators which are topologically protected by the bulk band gap, Weyl semimetal's topological protection comes from the fact that their 3D Weyl nodes are separated in momentum space. $MoTe_2$ belongs to the family of transition metal dichalcogenides, and it crystallizes in several structures. At room temperature, it exists as either hexagonal (2H, a semiconducting phase) or monoclinic (1T', a metallic phase) structure. Upon cooling, the monoclinic phase undergoes a transition at 240 K into an orthorhombic phase known as T_d phase, which breaks inversion symmetry and results in a type II Weyl semimetal phase. Here, we study the optoelectronic properties of $MoTe_2$ as function of temperature and layer number using photocurrent and photoconductance spectroscopy. In particular, we investigate the ultrafast electron dynamics using an on-chip Terahertz spectroscopy to disentangle hot electron currents and photogalvanic effects.

DS 16.11 Tue 12:45 POT 81

Surface Ripplocations in van der Waals materials: Structural & Electronic Properties — •James McHugh[1], Pavlos Mouratidis[1], Kenny Jolley[1], and Patrick Briddon[2] — [1]Dept. of Chemistry, Loughborough University — [2]School of Engineering, Newcastle University

Ripplocations are a new class of defect, unique to layered solids, which are characterised by the accommodation of extra material at sharp, localised folds. Dislocations in three-dimensional materials arise from the balance of strain and disregistry. In contrast, anisotropic van der Waals materials may completely alleviate strain through out-of-plane buckling.

We have conducted first-principles and analytical investigation of the properties of surface ripplocations on van der Waals layers. Analytical expressions for the formation energy, height and width of ripplocations are derived and compared to ab-initio simulations, showing that surface ripplocations readily form epitaxially on van der Waals materials.

The accommodation of extra material across a ripple is considered in terms of a Frenkel-Kontorova model, where it is found that ripplocations exhibit a "double kink" structure owing to the interplay of curvature and disregistry across the defect. Additionally, it is found that ripplocations induce a reduction in the band gap of layered semiconductors, with PDOS simulations identifying this change with the transition metal atoms across the curved regions. In combination with their high mobility this suggests the possibility of using ripplocations as a defect engineering platform.

DS 17: Organic Thin Films, Organic-Inorganic Interfaces II (joint session DS/CPP)

Time: Tuesday 11:15–12:45 Location: CHE 91

DS 17.1 Tue 11:15 CHE 91

Strong coupling of exciton polaritons in laterally structured organic microcavities — •Tony Henseleit[1,2], Markas Sudzius[1,2], Harmut Fröb[1,2], and Karl Leo[1,2] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials — [2]Technische Universität Dresden

Strong coupling in inorganic semiconductor materials has been investigated for many years with rising interest in strong coupling in organic materials. The realization of strong coupling at room temperature leads to possible applications as for example polariton lasing and enables investigation of many other interesting physics such as polariton blockade effects.

A polariton is a quasi particle comprising of a photon coupled to an exciton. We are focusing on exciton polaritons in layered resonator structures with organic active materials. We investigate organic materials at room temperature in strong coupling regime and can report to see a reasonable large splitting of the cavity mode in our spectroscopic studies. Furthermore we are especially examining the influence of lateral periodic submicrometer structures on strongly coupled polaritons. This results in an additional confinement of the particles in the system and forms for example waveguide modes in the structure.

DS 17.2 Tue 11:30 CHE 91

Electrochemical Deposition of Polyelectrolytes — •Felix Plamper[1], Sabine Schneider[2], and Olga Mergel[2] — [1]TU Bergakademie Freiberg, Germany — [2]RWTH Aachen University, Germany

Charged polymers (polyelectrolytes) interact with oppositely charged counterions. In case of redox-active counterions, their charge can be changed by electrochemical means, allowing a solubility change of these complexes at the electrode (electrochemically-induced film formation). Hence, we address polycations of various architectures made of quaternized poly(dimethylaminoethyl methacrylate) and derivatives to assess their influence on the electrodeposition with help of hexacyanoferrates. A rotating ring disk electrode (RRDE) used during hydrodynamic voltammetry is a powerful method to learn about the interactions of polymers and electroactive species. The RRDE allows a quantification of the deposition efficiency DE. The DE assigns the ratio of charge which was used to produce the deposited electroactive species compared to the total charge. It complements Quartz Crystal Microbalance QCM measurements, which is sensitive to the deposited mass, providing information on the water contents in the films. Different linear polyelectrolytes are investigated and a comparison between other architectures, like star-shaped polymers and microgels, was obtained. The results demonstrate that linear polymers of moderate molar mass are most efficient in the deposition due to pronounced intermolecular physical crosslinking (by help of the hexacyanoferrates), while hydrophilic side groups weaken the deposition by water uptake.

DS 17.3 Tue 11:45 CHE 91

Tuning the electronic properties of graphene with periodically arranged metal-organic coordination networks — •Qiankun Wang, Brian D. Baker Cortés, Joris de la Rie, Mihaela Enache, and Meike Stöhr — Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

Here, we investigate by means of scanning tunneling microscopy and photoelectron spectroscopy how the electronic properties of graphene are modified upon deposition of 5,10,15,20-tetra(4-pyridyl)porphyrin (2HTPyP) with and without coordination to Co atoms. Graphene was prepared on two different substrates, namely Cu(111) and CuOx, and it has been reported to be n-type doped on Cu(111) and quasi-freestanding on CuOx. Thereby, a comparison how the molecular adsorption changes the electronic properties of doped/undoped graphene could be done. We will discuss (i) the transition of the H-bonded self-assembled 2HTPyP network into a long-range ordered metal-organic coordination network (MOCN) upon Co deposition and (ii) the electronic level alignment at the graphene/MOCN interface and how this is influenced by the underlying substrate. Our study provides a viable possibility for the usage of graphene as a charge and spin transport material in future electronic and spintronic applications.

DS 17.4 Tue 12:00 CHE 91

Growth of Extended DNTT Fibers on Metal Substrates by Suppression of Step-Induced Nucleation — •Maximilian Dreher, Dayeon Kang, Tobias Breuer, and Gregor Witte — Philipps-Universität Marburg, 35032 Marburg, Germany

Due to their anisotropic optoelectronic properties, crystalline organic fibers constitute an interesting class of nanoscale materials with great potential for integration into future optoelectronic devices based on organic-inorganic hybrid systems. While chemical synthesis allows for flexible tailoring of electronic molecular properties, structural control of hybrid structures is hampered by the incompatibility of traditional structuring methods. Here we examine the formation of crystalline fibers of dinaphthothienothiophene (DNTT), a recently synthesized organic semiconductor with high charge carrier mobility, upon film growth on noble metal substrates. Based on a comparison of the film growth on a regularly stepped, vicinal surface, we show by STM measurements that substrate steps affect the azimuthal molecular orientation in the seed layer. In particular, they induce a fiber orientation which competes with that of fibers formed on flat terraces and thereby strongly limits the fiber dimensions. We demonstrate a strategy to suppress this parasitical step-induced fiber nucleation by first exposing Ag(111) surfaces to oxygen, which causes a selective saturation of the active step sites, while subsequent deposition of DNTT yields strongly enlarged fibers that are epitaxially aligned on the (111) surface [1,2]. [1] M. Dreher et al., Adv. Mater. Interfaces 5, 1800920 (2018) [2] M. Dreher et al., Nanoscale Horiz. 4, 1353-1360 (2019)

DS 17.5 Tue 12:15 CHE 91

Epitaxial Growth of PEN and PFP Thin Films on hBN(0001) — •Darius Günder[1], Tobias Breuer[1], Takashi Taniguchi[2], and Gregor Witte[1] — [1]Philipps University, Marburg, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

Hexagonal boron nitride (hBN) has gained considerable attention because it is an insulating 2D material, which is frequently used as gate dielectric in transistor applications [1]. Combining XRD, AFM, UV/Vis spectroscopy and polarization resolved optical microscopy we demonstrate that pentacene (PEN) and perfluoropentacene (PFP) form epitaxial films on exfoliated hBN(0001) substrates where molecules adopt a lying orientation on highly ordered hBN surfaces, while they grow in an upright molecular fashion on defective surfaces. We demonstrate in particular that PEN does not crystallize in a new polymorph as reported by Zhang et al. [2]. Based on our azimuthal analyses, the epitaxial relation between PEN and PFP films and hBN substrates is resolved and compared to the similar growth behavior on graphite substrates [3,4].

[1] M. Kratzer et al., J. Journal of Physics D 52, 383001 (2019).
[2] Y. Zhang et al., Phys. Rev. Lett. 116, 016602 (2016).
[3] J. Götzen et al., Phys. Rev. B 81, 085440 (2010).
[4] R. Felix et al., Cryst. Growth Des 16, 6941 (2016).

DS 17.6 Tue 12:30 CHE 91

Organic light-emitting diodes for high-brightness operation: self-heating and switched-back regions — •Anton Kirch[1], Axel Fischer[1], Matthias Liero[2], Jürgen Fuhrmann[2], Annegret Glitzky[2], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden, Germany — [2]Weierstrass Institute Berlin, Germany

Nonlinear effects typically involve switching phenomena that can lead to abrupt catastrophic device failure. For example, organic light-emitting diodes (OLEDs) suffer from strong electrothermal feedback that arises upon Joule self-heating. The interaction between temperature-dependent conductivity and power dissipation results in a positive feedback loop that finally destroys the device by thermal runaway. The situation becomes more severe for large-area OLEDs where the operation regime can locally differ. Former modeling studies, using a network of thermistors, led to the proposal that a so-called *switched-back* region arises. In this area, the current density, as well as the brightness, decreases although the total device current still increases when running an IV scan.

Here, we experimentally prove the existence of a switched-back region. We demonstrate that its appearance agrees with the simulation that solely uses electrothermal modeling. Our study aims to improve the long-term stability of high brightness OLED lighting tiles e.g. as applied in the automotive sector.

DS 18: Transport Properties

Time: Tuesday 11:45–13:00 Location: CHE 89

DS 18.1 Tue 11:45 CHE 89

Magnetoconductance of Bi quantum films in parallel magnetic fields — •Doaa Abdelbarey[1], Christoph Tegenkamp[1,2], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Institut für Physik, TU Chemnitz

Bismuth has attracted a lot of interest because of its unique electronic properties such as low carrier concentrations and high carrier mobilities, In particular, strong Rashba splitting of the edge states appears in quantum films generated by epitaxial growth. Thus high-quality thin films open new pathways to tailor the electronic properties further. Magneto-conductance of films grown epitaxially on Si(111) with a thickness of 10 to 100 bilayers (BL) was measured at T= 9 K in parallel magnetic fields up to 4T. For B-fields in plane and parallel to the current direction only WAL is observed irrespective of thickness. However, if the B-fields are in plane, but perpendicular to the current, a crossover from weak anti-localization (WAL) to weak localization (WL) and back is seen for films up to 70 BL. For thicker films only WAL is observed. The observed coherent part of conductance in parallel B-fields perpendicular to current is characterized by an intriguing change from strong to weak coupling between edge states as a function of layer thickness and their hybridization with the quantized bulk states. For films thicker than 50 BL also incoherent scattering comes into play, which dominates above 80 BL.

DS 18.2 Tue 12:00 CHE 89

Layer by Layer Resistive Switching — •Jon-Olaf Krisponeit[1,3], Bernd Damaschke[2], Vasily Moshnyaga[2], and Konrad Samwer[2] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen, Germany — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [3]MAPEX Center for Materials and Processes, University of Bremen, 28359 Bremen, Germany

Beyond their complex magneto-resistive transport behavior, perovskite manganites have been shown to exhibit also memristive properties. Employing conductive atomic force microscopy (CAFM) on a $La_{0.85}Sr_{0.15}MnO_3$ thin film on MgO(100), we reveal a novel resistive switching mechanism which is based on the electric-field-induced healing of so-called "dead" layers.[1]

Under application of an electrical bias, these layers of highly resistive nature are switched to a bulk-like, conducting state. The switching process can be reversed by voltage pulses of the opposite polarity. Proceeding in a layer-by-layer fashion, the effect allows for multi-state functionality: The variable number of insulating layers, sandwiched between the conductive bulk and the cantilever tip, results in an electrically tunable tunnel barrier with multiple well-defined resistance states.

Financial support from the DFG via SFB 602, SFB 1073 and the Leibniz program, and by the Institutional Strategy of the University of Bremen, funded by the German Excellence Initiative, is acknowledged.

[1] Krisponeit et al., *Phys. Rev. Lett.* **122**, 136801 (2019).

DS 18.3 Tue 12:15 CHE 89

Ac conductivity of nano-granular metals prepared via FEBID — •Marc Hanefeld and Michael Huth — Physikalisches Institut, Goethe Universität, Max-von-Laue-Str. 1

Focused Electron Beam Induced Deposition (FEBID) is a versatile technique to create nano-granular metals with tunable electronic transport properties [1]. In granular metals metallic nanoparticles are surrounded by a dielectric matrix which leads to a transport mechanism based on thermally assisted tunnelling. This opens up promising possibilities for sensing applications [1] and has triggered ongoing research concerning their response to a time-dependent ac stimulus [2].

Current research focuses mainly on two different material properties, namely an apparent universal power law and a temperature-independent scaling behaviour in the real part of the complex ac conductivity, both present in many disordered solids and recently reported in granular metals of palladium in zirconia [2].

We present recent results on the ac conductance response of nano-granular Pt(C)-FEBID 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. The focus in this talk will lie on generating a deeper understanding of links between the dc and ac conductance behaviour of nano-granular materials.

[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 18.4 Tue 12:30 CHE 89

Quantum Corrections in Magnetotransport of $BaPbO_3$ thin films — •Robert Bartel, Patrick Seiler, Thilo Kopp, and German Hammerl — Experimental Physics VI, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany

Recently metallic $BaPbO_3$ attracted attention as two-dimensional superconductivity was observed in bilayers of insulating $BaBiO_3$ and $BaPbO_3$ [1]. Here a detailed study of the transport properties of $BaPbO_3$ will be presented. Low temperature and magnetic-field dependent measurements of the sheet resistance of $BaPbO_3$ can be understood in terms of quantum corrections based on disorder, spin-orbit coupling or electron-electron interaction [2].

[1] B. Meir, S. Gorol, T. Kopp, G. Hammerl, Phys. Rev. B 96, 100507(R) (2017)

[2] P. Seiler, R. Bartel, T. Kopp, G. Hammerl, Phys. Rev. B 100, 165402 (2019)

DS 18.5 Tue 12:45 CHE 89

Calculating DC Conductivity in Substitutionally Disordered Graphene using the Kubo-Greenwood Formula — •Jacob Robbins and Jorge Sofo — The Pennsylvania State University, University Park, USA

We develop a method for calculating the electronic transport in monolayer graphene with a small percentage of carbon atoms substituted for nitrogen impurities. The Hamiltonian is treated in the tight binding approximation, with only nearest neighbor hopping included. While many authors find DC conductivity in such systems using the adiabatic electric field of Kubo (1957), we apply the perturbation theory approach of Greenwood (1958). This distinction allows us to find the DC conductivity of finite systems, without equilibrating to infinite time, at which point all conduction has ceased.

DS 19: 2D semiconductors and van der Waals heterostructures IV (joint session HL/DS/O)

Time: Tuesday 14:00–16:00 Location: POT 81

DS 19.1 Tue 14:00 POT 81

Resolving the interlayer charge transfer in van der Waals heterostructures by ultrafast THz emission nanoscopy — •Markus Plankl[1], Martin Zizlsperger[1], Fabian Mooshammer[1], Felix Schiegl[1], Fabian Sandner[1], Markus A. Huber[1], Tom Siday[1], Jessica L. Boland[2], Tyler L. Cocker[3], and Rupert Huber[1] — [1]Department of Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Photon Science Institute, University of Manchester, Manchester M13 9PL, UK — [3]Department of Physics and Astronomy, Michigan State University, 48824 Michigan, USA

In van der Waals heterostructures composed of two transition metal dichalcogenide monolayers, photogenerated electron-hole pairs are spatially separated on ultrafast timescales, giving rise to the formation of interlayer excitons. Yet, the underlying interlayer charge transfer has only been investigated in a spatially averaged manner. Consequently, probing nanoscale transfer efficiencies and tunneling rates has so far remained elusive. Since the tunneling of photoexcited charge carriers between adjacent layers represents an ultrafast current along the out-of-plane direction, a concomitant electromagnetic pulse in the terahertz spectral range is emitted. By combining electro-optic time-domain spectroscopy with near-field microscopy, we resolve this characteristic fingerprint of the interlayer carrier dynamics on the nanoscale with subcycle temporal resolution. Thereby, we infer tunneling characteristics, which we relate with the nanoscale conductivity of the heterostructure.

DS 19.2 Tue 14:15 POT 81

Influence of dark states on excitonic spin relaxation in transition metal dichalcogenides — •Malte Selig, Dominik Christiansen, and Florian Katsch — Technische Universität Berlin, Berlin, Germany

Energetically low lying dark exciton states with momenta well above the radiative cone manifest a significant relaxation channel for optically pumped excitons in transition metal dichalcogenides (TMDCs). While they have been demonstrated to influence the optical linewidth [1], lineshape [2], relaxation and luminescence properties [3], they can also be expected to play a crucial role for the spin relaxation of excitons.

Here we present a Heisenberg equation of motion theory for the intervalley exchange coupling, mediating the spin relaxation, and exciton phonon coupling. We demonstrate that the interplay of both mechanisms leads to unintuitive signatures in pump probe experiments where the A transition is pumped and either A or B transition are probed [4]. Additionally we reveal that the presence of energetically low lying dark excitons significantly quenches the efficiency of intervalley exchange coupling [5]. Our theoretical results shine new light on existing experimental data.

[1] M. Selig et al.,Nature Commun. 7,13279 (2016)
[2] D. Christiansen et al., Phys. Rev. Lett. 119, 187402 (2017)
[3] M. Selig et al., 2D Mat. 5, 035017 (2018)
[4] M. Selig et al., Phys. Rev. Research 1, 022007(R) (2019)
[5] M. Selig et al., arXiv:1908.11178 (2019)

DS 19.3 Tue 14:30 POT 81

Kelvin probe force microscopy-based direct measurements of contact resistance in 2D semiconductor thin film transistors — •Aleksandar Matkovic[1], Andreas Petritz[2], Gerburg Schider[2], Markus Krammer[4], Markus Kratzer[1], Michael Gärtner[3], Andreas Terfort[3], Christian Teichert[1], Egbert Zojer[4], Karin Zojer[4], and Barbara Stadlober[2] — [1]Institute of Physics, Montanuniversität Leoben, Leoben, Austria. — [2]Joanneum Research MATERIALS, Institute for Surface Technologies and Photonics, Weiz, Austria. — [3]Institute of Solid State Physics, Graz University of Technology, Graz, Austria. — [4]Institut für Anorganische und Analytische Chemie, Goethe-University Frankfurt, Frankfurt am Main, Germany.

This study aims at direct determination of the contact resistance in MoS$_2$-based thin film transistors (TFTs). Exfoliated single-crystal flakes of MoS$_2$ have been used in a bottom-contact TFT configuration. Pyrimidine-containing self-assembled monolayers (SAMs) were employed to tune the work function of gold electrodes. Kelvin probe force microscopy measurements were carried out during operation of the devices in order to directly image potential drops across the channel and to study the influence of different SAM treatments on the contact resistance. By independently imaging potential drops at both, carrier injection and extraction points, we demonstrate the asymmetry of contact resistances in MoS$_2$-based TFTs, as well as their non-linear and bias-dependent behavior.

DS 19.4 Tue 14:45 POT 81

MOVPE of large-scale 2D-2D heterostructures for optoelectronic applications — Annika Grundmann[1], Clifford McAleese[2], Ben Richard Conran[2], Andrew Pakes[2], Dominik Andrzejewski[3], Tilmar Kümmel[3], Gerd Bacher[3], Kenneth Bo Khin Teo[2], •Michael Heuken[1,4], Holger Kalisch[1], and Andrei Vescan[1] — [1]Compound Semiconductor Technology, RWTH Aachen University, Aachen, Germany — [2]AIXTRON Ltd., Cambridge, United Kingdom — [3]Werkstoffe der Elektrotechnik and CENIDE, University Duisburg-Essen, Duisburg, Germany — [4]AIXTRON SE, Herzogenrath, Germany

Vertical heterostructures of two (or more) different 2D layer provide many fascinating opportunities by combining the unique intrinsic chemical, physical and (opto)electronic properties of 2D materials. Without the need of consideration of lattice matching, a nearly infinite number of potential combinations of 2D layers are possible. Transition metal dichalcogenide (TMDC) monolayers are the most widely studied 2D semiconductors beyond graphene and thus provide a strong basis for understanding the properties of 2D heterostructures. Unlike mechanical exfoliation, direct successive growth of 2D-2D heterostructures requires a controlled synthesis of the respective monolayers with pristine interlayer interfaces and no intermixing of disparate layers. Here, we report on direct successive MOCVD of vertical MoS$_2$-WS$_2$ and WS$_2$-MoS$_2$ heterostructures as well as MOCVD of WS$_2$ and MoS$_2$ onto graphene previously deposited in another MOCVD reactor.

DS 19.5 Tue 15:00 POT 81

Efficient Hot Electron Transfer at Graphene-WS2 van der Waals Bilayers — SHuai Fu and •Hai Wang — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Hybridization of (semi-)metallic and semiconducting monolayers, such as graphene and layered transition metal dichalcogenides (TMDs), enables efficient and sensitive photodetectors, by combing the synergetic properties of strong absorption at exciton resonances in TMDs, efficient charge transfer cross the interfaces and ultrahigh charge mobility in graphene. In spite of the great advance in devices, the fundamental understanding of the mechanism underlying the ultrafast charge flow across the heterostructures lags far behind, and effective means of controlling its efficiency have not been established.

Employing Terahertz spectroscopy, we shed light on the fundamentals of ultrafast interfacial nonequilibrium dynamics in graphene-WS2 van der Waals bilayers. We report an efficient and ultrafast hot electron injection from graphene to WS2, which competes with hot carrier heating process in graphene. We will discuss the mechanism underlying the hot electron charge transfer process, and factors governing its efficiency and lifetime of interfacial charge states, which are critical for efficient optoelectronics (i.e. photodetectors) based on van der Waals heterostructures.

DS 19.6 Tue 15:15 POT 81

Excitation Induced Dephasing in Monolayer Transition Metal Dichalcogenides — •Florian Katsch, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, 10623 Berlin, Germany

Exceptionally strong Coulomb interactions in atomically thin transition metal dichalcogenides lead to tightly bound electron-hole pairs (excitons) dominating their linear and nonlinear optical response. The latter involves bleaching [1], energy renormalizations [2], and higher-order Coulomb correlation effects like biexcitons [3] and excitation induced dephasing (EID) [4]. Whereas bleaching, energy renormalizations, and biexcitons are widely investigated, EID in exciton dominated semiconductors so far lacks microscopic calculations. Within a Heisenberg equations of motion formalism we identify the coupling between excitons and exciton-exciton scattering continua as the most prominent process causing EID and sideband formation. Evaluating the EID for single-layers of transition metal dichalcogenides, we find a good agreement with recent experiments [5,6].

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DS 19.7 Tue 15:30 POT 81

Dirac physics in honeycomb semiconductors — •Christiaan Post[1], Nathali Franchina Vergel[2], Tomas Meerwijk[1], Jesper Moes[1], Xavier Wallart[2], Guillaume Fleury[3], Ludovic Desplanque[2], Ingmar Swart[1], Christophe Delerue[2], Bruno Grandidier[2], and Daniel Vanmaekelbergh[1] — [1]Debye Institute for Nanomaterials Science, Utrecht, The Netherlands — [2]Institute of Electronics, Microelectronics and Nanotechnology (IEMN), Lille, France — [3]Laboratory for Chemistry of Organic Polymers (LCPO), Bordeaux, France

III-V semiconductor quantum wells have obtained a central place in advanced logics and opto-electronics. In more recent research, the effects of a nano scale geometry forming a periodic scattering potential in the lateral directions of the quantum well have been discussed and calculated. In case of a nano-scale honeycomb geometry, Dirac cones are formed similar as for graphene, creating massless fermions while the semiconductor quantum well band gap remains nearly unaltered.

In this research, we report on the electronic characterization of a modulated InGaAs quantum well with a honeycomb symmetry. The honeycomb symmetry is fabricated by perforating the quantum well with a triangular symmetry using nano-scale lithography. By performing scanning tunneling microscopy experiments, the electronic properties of the sample are intensively investigated, showing the combined electronic properties of a two-dimensional material and Dirac-like features. Muffin-tin calculations support the obtained experimental results, revealing the exciting properties of these novel materials.

DS 19.8 Tue 15:45 POT 81

Structural and electronic properties of twisted MoS_2 bilayers — •Somepalli Venkateswarlu, Andreas Honecker, and Guy Trambly de Laissardière — Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Université de Cergy-Pontoise, France

Vertically stacked transition metal dichalcogenides of multilayer structures have gained increasing attention because of their fascinating features in electronics and optical properties [1]. We performed calculations of structural and electronic properties of nontwisted and twisted MoS_2 bilayers using first-principle calculations [ABINIT][2] and the tight-binding (TB) method. Our results reveal significant differences in the band structures of twisted and nontwisted ones: the appearance of a crossover between direct and indirect band gap, gap variation, and atomic relaxations. For rather large angles, the band structures are very similar for different rotation angles [3]. For the smallest angles, TB calculations predict some flat bands in the valence band and conduction band. As in twisted bilayer graphene, the corresponding states are localized in the AA stacking region of the Moiré pattern.

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DS 20: Focus Session: Organic-based Hybrid Thermoelectrics I

Waste heat at moderate temperatures of around 100°C constitutes an energy source of enormous potential for recuperative technologies such as themoelectrics. By their inherently low thermal conductivity, possibility for p- and n-type doping, sustainability as well as low-cost processing, organic semiconductors have entered the focus of interests in recent years. In addition, the strong electron-phonon interaction in this material class results in a wealth of new phenomena ranging from phonon-drag effects to electronic correlations. However, a comprehensive picture of the microscopic mechanisms governing the thermoelectric properties as well as advanced hybrid material concepts are necessary to further enhance their thermoelectric figure-of-merit and, thereby, to pave the way towards first technologically relevant implementations.

This focus session aims for bringing together material scientists, chemists and physicists working in the fields of material synthesis, thin film preparation, doping of organic semiconductors, in-depth thermoelectrical characterizations as well as theoretical modelling. Only the concerted approach by the various disciplines will allow for a successful transformation of academic research into technologically relevant applications. Thus, this focus session will also provide a suited platform for an intense informational exchange as well as for initiating possible future collaborations between the participating groups.

Organizers: Manfred Albrecht (Universität Augsburg), Wolfgang Brütting (Universität Augsburg), Jens Pflaum (Universität Würzburg)

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

Invited Talk DS 20.1 Wed 9:30 CHE 89

Progress and challenges of organic and hybrid based thermoelectrics — •Mariano Campoy-Quiles — Institute of Materials Science of Barcelona (ICMAB-CSIC)

Heat is a ubiquitous source of energy. About half of the energy that the sun delivers to the Earth is in the form of infrared radiation. Moreover, two/thirds of the energy produced for human consumption is lost in the form of heat. In this scenario, solid state heat-to-electricity converters, i.e. thermoelectrics, have strong potential to harvest part of this untapped diluted energy source. Widespread use of thermoelectric generators has been thus far elusive due to the relatively high cost of the technology, and the fact that most thermoelectric materials operating at low temperatures are based on non-abundant or toxic materials. Solution processed carbon based materials are currently being investigated as a very promising alternative for low-cost, low temperature thermoelectrics. In this talk I will describe the progress and challenges for three carbon based systems: highly doped conjugated polymers, carbon nanotubes, and composites thereof. I will focus on our current understanding of what governs the main material thermoelectric properties, namely electrical conductivity, Seebeck coefficient and thermal conductivity.

DS 20.2 Wed 10:00 CHE 89

FFT-based Integrated Transient Thermoelectric Measurement Setup for Thin Films — •Karthikeyan Manga Loganathan[1,2,3], Guodong Li[1,2], Vineeth Kumar Bandari[1,2,3], Feng Zhu[1,2,3], and Oliver G. Schmidt[1,2,3] — [1]Material Systems for Nanoelectronics, Chemnitz University of Technology, Chemnitz, Germany — [2]Institute for Integrative Nanosciences, Leibniz IFW Dresden, Dresden, Germany — [3]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany

Characterization of thin films for their thermoelectric figures of merit (zT) has been constantly met with the challenges in effectively measuring their thermal conductivity (k), electrical conductivity (σ) & Seebeck coefficient (S) coherently along the same plane. The author's work introduces a novel FFT-based measurement technique that independently measures the above parameters coherently along cross-plane direction for thin films with thicknesses as low as 50 nm. The technique incorporates FFT into the traditional transient measurement strategies of recording second and third harmonic voltage drops from the material in response to AC heating, established by David Cahill et al. [Phys. Rev. B, 1994]. This allows for the simultaneous measurement of the thin film's k and S in the cross-plane direction. The merits of this technique include enhanced ease, efficiency and accuracy of measurement of k, σ & S. The technique has been further employed to characterize organic materials and 2D multilayers such as CuPc, PEDOT, MoS2 and SnS2 for their cross-plane thermoelectric parameters.

Invited Talk DS 20.3 Wed 10:15 CHE 89

Thermoelectric microdevices - challenges and perspectives — •Gabi Schierning — IFW Dresden, Dresden, Germany

Next generation electronic devices require intelligent thermal management strategies in order to remove high density heat fluxes from the active electronic components or to harvest small amounts of energy for low-power electronics. Hence, hardware solutions for a smart and efficient thermal management are sought for. Micro-scale thermoelectric coolers (TEC) are therefore developed as one part of the thermal management. To fabricate these micro-scale TECs, we developed a fabrication technology such that tellurium-based compound semiconductors with decent thermoelectric performance at room temperature are deposited by electrochemical deposition combined with structuring by photolithographic processing. Current and temperature dependent cooling performances, transient cooling response, cooling cycling, and long-term stability under constant current of these micro-devices will be shown. Challenges that will be discussed are i) to integrate high figure-of-merit materials into the fabrication process, ii) to integrate the devices into real electronic circuitry, iii) to operate and characterize such devices as thermoelectric micro-harvesting devices rather than as micro cooling devices.

DS 20.4 Wed 10:45 CHE 89

Orgaic/inorganic hybrid composites for near-room temperature thermoelectric applications — •Rodrigo Rubio-Govea[1,2], Katherine Mazzio[1,2], and Simone Raoux[1,2,3] — [1]Institute for Nanospectroscopy, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Straße 15, 12489, Berlin, Germany — [2]Energy Materials In-Situ Laboratory Berlin (EMIL), Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Straße 15, 12489, Berlin, Germany — [3]Department of Physics, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489, Berlin, Germany

Hybrid organic/inorganic materials for thermoelectric application have received great attention in the last two decades due to the possibility of enhancing their performance. This is done by combining the intrinsic low thermal conductivity of the organic constituents and the high Seebeck coefficient and electrical conductivity of inorganic materials, making it possible to achieve high power factors and thermoelectric figures of merit. In this work we report the synthesis of hybrid composites consisting of chalcogenide-based nanowires and poly(3,4-ethylenedioxythiophene):polystyrene sulfonate and investigate how to control the thermoelectric properties based on the synthetic conditions. We found that it is possible to change the characteristics of the composite, including changing the majority charge carrier from p-type to n-type by engineering the composition of the inorganic component. We demonstrate an n-type composite with a power factor of 21.47 uWm-1K-2 and a zT value of 0.06 at 200 °C

DS 21: Layer Properties I: Electronic Properties

Time: Wednesday 9:30–10:45 Location: CHE 91

DS 21.1 Wed 9:30 CHE 91

Band structures of HgTe films from the cyclotron resonance — •Jan Gospodaric[1], Alexey Shuvaev[1], Vlad Dziom[1], Alena Dobretsova[2], Nikolay Nikolaevich Mikhailov[2], Ze Don Kvon[2], Elena Novik[3,4], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Rzhanov Institute of Semiconductor Physics and Novosibirsk State University, Novosibirsk 630090, Russia — [3]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany — [4]Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

An essential part of understanding the properties of materials is knowing their band structure. One of the most standardized methods to acquire the band structure of solids is provided by angle-resolved photoemission spectroscopy (ARPES), which provides access to the electronic structures of the area close to the surface of the sample (typical depths in Ångström range). However, in 2D heterostructures, additional buffer and capping layers limit this procedure. Here we present the results of an alternative method to obtain the band dispersion of such samples by probing the cyclotron resonance of the free carriers in thin films based on the HgTe. With the presented technique we can map both the electron and hole part of the band structures of HgTe films in semimetallic and topological insulating phases. The resulting band pictures overlap well with the theoretical results, provided by the $\mathbf{k} \cdot \mathbf{p}$ model.

DS 21.2 Wed 9:45 CHE 91

In-situ probing of the thickness-dependent electronic properties of BaBiO3 — •Rosa Luca Bouwmeester, Kai Sotthewes, and Alexander Brinkman — University of Twente, Enschede, the Netherlands

Being the parent compound of the high-Tc superconductors BaPb1-xBixO3 and Ba1-xKxBiO3, single crystal BaBiO3 has been studied extensively. Its insulator band gap is thought to be due to a breathing distortion [1,2,3]. In recent years, the thickness of BaBiO3 thin films is taken as a new degree of freedom to study its influence on the electronic properties [4,5,6]. In the ultra-thin limit, metallicity is predicted because the breathing distortion is suppressed. Experimentally, no insulator-to-metal transition has yet been observed. Here, in-situ scanning tunneling microscopy (STM) studies are performed on BaBiO3 thin films with thicknesses in the range of 4 unit cells to 50 nm. For the first time, in the ultra-thin limit, metallic behavior is observed.

References

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DS 21.3 Wed 10:00 CHE 91

Magnetodielectric Effect and Interface Couplings in LaMnO3/LaNiO3 Superlattices — •Philipp Ksoll[1], Vladimir Roddatis[2], and Vasily Moshnyaga[1] — [1]1. Physikalisches Institut, Uni Göttingen — [2]Institut für Materialphysik, Uni Göttingen

Multifunctional double perovskites, e.g. ferromagnetic insulating La2NiMnO6, have recently gained strong interest because of their rich physics and prospects for technological applications due to the magnetodielectric (MD) effect. To study the origin of MD coupling, epitaxial superlattices of (LaMnO3)n/(LaNiO3)n (LMO/LNO) with n varying from 20 u.c. down to one monolayer (n=1 yields La2NiMnO6) have been grown on Nb-doped SrTiO3(111) at relatively low (Tlow~650°C) and high (Thight~900°C) T by metalorganic aerosol deposition (MAD) technique, equipped with in situ optical ellipsometry. SLs grown at Tlow show an enhanced exchange bias field, HEB~40 Oe, and large coercive fields, Hc~800 Oe, as well as a suppressed saturation magnetization (msat,650°C~1/2*msat,900°C) as compared to those measured for SLs grown at 900°C. This means that the structure of interfaces and interfacial LMO/LNO magnetic coupling may be influenced by growth conditions. A relatively slow growth kinetics at 650°C seems to suppress the charge transfer between Mn and Ni cations, resulting an enhanced antiferromagnetic coupling between Mn3+ and Ni3+. Taking into account the data of in situ ellipsometry, we further performed measurements of dielectric constant for SLs with n=2, 5 at T=5-400 K and for frequencies, f=10E-6 - 2*10E6 Hz, to elucidate the role of LMO/LNO interfaces in the MD effect.

DS 21.4 Wed 10:15 CHE 91

Orbital- and thickness dependent band engineering of $\mathbf{WSe_2}$ by potassium surface functionalization — •Tom Klaproth[1], Carsten Habenicht[1], Roman Schuster[1], Bernd Büchner[1,2], Martin Knupfer[1], and Andreas Koitzsch[1] — [1]Leibniz Institute for Solid State and Materials Research, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Institute of Solid State Physics, TU Dresden, 01069 Dresden, Germany

Atomically thin transition metal dichalcogenides (TMDC) are promising candidates for implementation in next generation semiconducting devices, for which effective methods of property engineering are urgently needed. Alkali metal deposition is an important tool to tune the electronic properties of TMDCs and 2D materials in general. Here, by applying angle-resolved photoemission, electron-energy loss spectroscopy and density functional theory, we monitor how exactly potassium deposition alters the electronic structure of WSe_2, a prototypical TMDC with large spin-orbit coupling. We find that the changes of the electronic structure are more complex than previously anticipated.

There are two main features: i) The bandstructure shifts down on a thickness dependent rate, implying effective electron delocalization. ii) The density of selenium *vs* tungsten states depends on the doping level, which leads to changes of the optical response beyond increased dielectric screening. Our work gives detailed insight into the effects of potassium deposition on WSe_2, provides microscopic understanding thereof and improves the basis for property engineering of 2D materials.

DS 21.5 Wed 10:30 CHE 91

Material selection and diffusion control for electrochemical metallization memory by using nano-pillar structure diffusion barrier — •Yen Kai Cheng — Department of Material Science and Engineering, National Tsing Hua University, Hsinchu 30013, Taiwan

Ag and Cu based electrodes with TiOx and HfOx based electrolytes electrochemical metallization (ECM) random access memory is a promising candidate for nonvolatile memory applications due to its simple structure and excellent performances. However, several challenges are needed to solve as the cell area is scaled down, especially for the device reliability and variability. Since the formation and rupture of the conductive filaments is stochastic, the injection of cations plays a critical role in improving the reliability and variability. In this study, two directions are considered, First, the combinations of different electrode/electrolyte cause the diffusivity differences, result in different degrees of cation injections and LRS retention failure times. Second, an Al2O3 layer with nano-pillar array architecture inserted between the electrode and switching layer is demonstrated. The width between the nano-pillar is tunable from 10 nm to 30 nm by changing the coverage of Al2O3 layer. The Al2O3 layer is served as the barrier that restrained the Ag and Cu atoms to diffuse into the electrolyte. With this architecture design, the resistive switching behaviors not only show different degrees of multi-level storage potential, but also provide a roadmap and show which kind of electrode/electrolyte has the potential in the neuron application.

DS 22: 2D semiconductors and van der Waals heterostructures V (joint session HL/DS/O)

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

DS 22.1 Wed 9:30 POT 81

Impurity effects in graphene: resonances, localized states and Mott-transitions — Yuriy G. Pogorelov[1], •Denis Kochan[2], and Vadim M. Loktev[3] — [1]1IFIMUP-IN, Departamento de Física, Universidade do Porto, Porto, Portugal — [2]Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany — [3]N.N. Bogolyubov Institute of Theoretical Physics, NAS of Ukraine, Kyiv, Ukraine

Impurities modify electronic spectrum of graphene in several ways. For example, they can shift charge neutrality point, tilt the Fermi level, open spectral (quasi)gaps, form resonances, and localized states.

In the presentation we discuss formation of resonances, and localized states in graphene for Anderson-like impurities (Hydrogen, Copper, Fluorine) in top, bridge and hollow positions. Particularly, we focus on spectral transition between resonant and localized states, and Mott mobility edges, tracing dependencies on graphene Fermi energy, concentration of impurities, their sub-lattices distribution, and impurity hybridization strength.

Employing the group expansion of the Green's functions we calculated reconstructed band structure of graphene hosting Anderson impurities. Applying Ioffe-Regel-Mott criterion, we obtained system-specific critical concentrations at which system undergoes resonance-to-bound-state transition.

DS 22.2 Wed 9:45 POT 81

Twisted Bilayer Graphene Produced by Atomic Force Microscopy Techniques — •Lina Bockhorn, Lucas Gnörich, Johannes C. Rode, Christopher Belke, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

The electronic properties of bilayer graphene strongly depend on relative orientation of the two atomic lattices. The rotational mismatch between both layers opens up a whole new field of rich physics, especially around the magic angle.

Twisted bilayer graphene can be obtained by different methods. Here, we use atomic force microscopy techniques to generate twisted bilayer graphene. A diagonal cut is applied at high contact force through a monolayer graphene. Several folds spread from the newly created edge. The self-assembled twisted bilayer graphene is separated in folds with one or two rips.

We estimate the relative orientation of twisted bilayer graphene which is prepared by folding monolayer graphene [1, 2, 3].

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DS 22.3 Wed 10:00 POT 81

Magneto-Raman Spectroscopy for Probing Electron-Phonon and Electron-Electron Interactions in Graphene — •Jens Sonntag[1,2], Sven Reichardt[1,3], Ludger Wirtz[3], Mikhail Katsnelson[4], Bernd Beschoten[1], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany — [3]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [4]Radboud University, Institute for Molecules and Materials, Nijmegen, Netherlands

We present charge carrier density-dependent magneto-Raman spectroscopy measurements on suspended graphene and hBN/graphene heterostructures to investigate electron-phonon and electron-electron interactions, both without applied magnetic field and within the quantum Hall regime. Strikingly, at $B = 0\,\mathrm{T}$ we do not observe the expected strong renormalization of the G-mode energy as a function of charge carrier density n. We identify Laser induced heating and a limited electron-hole lifetime as possible origins.

Utilizing gate-tunable magneto-phonon resonances, we extract the charge carrier density-dependence of the Landau level transition energies and the associated effective Fermi velocity v_F. In contrast to the logarithmic divergence of v_F at zero magnetic field, we find a piecewise linear scaling of v_F as a function of n, due to a magnetic field-induced suppression of the long-range Coulomb interaction. Furthermore, we can estimate the excitonic correction to the energies of the Landau level transistions to $\approx 6\,\mathrm{meV}$.

DS 22.4 Wed 10:15 POT 81

Tip-enhanced Raman spectroscopy combined with other Scanning Probe Microscopy Methods: Focus on 2D Materials — •Jana Kalbacova[1], Marc Chaigneau[2], and Andrey Krayev[3] — [1]HORIBA Jobin Yvon GmbH, Germany — [2]HORIBA Scientific, France — [3]HORIBA Scientific, USA

New two dimensional materials are on the rise. After the wonder material graphene, new materials such as MoS2, MoSe2, WSe2 have an intrinsic bandgap and as such are opening new doors for semiconductor applications. Raman spectroscopy offers information on the chemical structure of materials but cannot provide information on the electronic properties such as surface potential or photocurrent of our sample. Co-localized measurements combining scanning probe microscopy (SPM) with Raman spectroscopy can already bring a wealth of information; however, further improvements can be obtained by a tip that will act as an antenna and amplify the Raman signal and thus breaking the diffraction limit in a method called Tip-enhanced Raman spectroscopy (TERS). Typically spatial resolution of 10 - 20 nm can be achieved. In this contribution, we investigate different 2D materials by a combination of TERS, tip-enhanced photoluminescence, Kelvin probe microscopy, and other SPM methods to show very locally for example doping variations or defects that would otherwise go unnoticed with other macro- and microscopic techniques.

DS 22.5 Wed 10:30 POT 81

Edge photogalvanic effect driven by optical alignment in bilayer graphene — •Susanne Candussio[1], Mikhail V. Durnev[2], Jun Yin[3], Artem Mishchenko[3], Helene Plank[1], Vasily V. Bel'kov[2], Sergey A. Tarasenko[2], Vladimir Fal'ko[3], and Sergey D. Ganichev[1] — [1]University of Regensburg, 93040 Regensburg, Germany — [2]Ioffe Institute, 194021 St. Petersburg, Russia — [3]University of Manchester, Manchester M13 9PL, UK

We report on the observation of the edge electric current excited in bi-layer graphene by terahertz laser radiation. We show that the current generation belongs to the class of second order in electric field phenomena and is controlled by the orientation of the THz electric field polarization plane. Application of a magnetic field normal to the graphene plane leads to a phase shift in the polarization dependence. In strong magnetic field the current exhibit 1/B-magnetooscillations with a period consistent with that of the Shubnikov-de-Haas effect and amplitude by an order of magnitude large as compared to the current at zero field measured under the same conditions. The developed microscopic theory shows that the current is formed in the edges vicinity limited by the mean-free path and originates from optical alignment of free carriers and scattering at the edges, which naturally break the P-symmetry. The observed magnetooscillations of the photocurrent are attributed to the formation of the Landau levels.

DS 22.6 Wed 10:45 POT 81

Electronic Properties of Two-Dimensional ZrSe$_3$-Films — •Lars Thole[1], Christopher Belke[1], Sonja Locmelis[2], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

The family of 2d materials offers a big variety of different material classes [1]. This includes the transition metal trichalcogenides (TMTC) of the form MX$_3$, where M is a transition metal and X is a chalcogen [2, 3]. Here we exfoliated ZrSe$_3$ into thin films and contacted them with electron beam lithography. These thin flakes were investigated by means of optical microscopy, atomic force microscopy and electrical measurements. During this, it was shown that the material degrades in ambient condition. Furthermore, an activation energy of about 0.6 eV was measured. Inducing charge carriers showed the samples to be n-doped semiconductors. Finally, a mean free path for the bulk material was determined.

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30 min. break

DS 22.7 Wed 11:30 POT 81

ultraviolet photodetectors based on mechanically exfoliated few-layer FePS3 and ZnO quantum dots with high responsivity — •juanmei duan[1,2], liang hu[3], yujia zeng[3], manfred helm[1,2], shengqiang zhou[1], and slawomir prucnal[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany — [2]Technische Universität Dresden, D-01062 Dresden, Germany — [3]College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, P. R. China

Metal-phosphorus-trichalcogenides (MPTs), FePS3, are newly developed 2D wide-bandgap semiconductors and have been proposed as excellent candidates for ultraviolet (UV) optoelectronics. In this work, few-layer FePS3/ZnO quantum dots heterojunction were studied with Transmission electron microscopy (TEM), scanning electron microscope (SEM), X-ray photoelectron spectroscopy (XPS), and Raman measurement. The photoresponse characteristic of UV detectors based on FePS3/ZnO were investigated under 365nm, 405nm illumination and bias voltages. The high photoresponse property paves the way for the further development of 2D MPTs/ZnO quantum dots in high-performance UV photodetectors.

DS 22.8 Wed 11:45 POT 81

Selectively grown Topological Insulator Nanodevices — •Daniel Rosenbach[1], Abdur Rehman Jalil[1], Jonas Kölzer[1], Nico Oellers[1], Michael Schleenvoigt[1], Tobias Werner Schmitt[2], Peter Schüffelgen[1], Gregor Mussler[1], Hans Lüth[1], Detlev Grützmacher[1], and Thomas Schäpers[1] — [1]Peter Grünberg Institut (PGI-9) and JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich, 52425 Jülich, German — [2]JARA-FIT Institute Green IT, RWTH Aachen University, 52062 Aachen, Germany

1-dimensional topological insulator nanoribbons in close proximity to elemental superconductors can be utilized to create localized Majorana modes for topological quantum computation architectures. We employ a selective area growth method using molecular beam epitaxy in order to define topological insulator nanodevices without harmful post processing steps. Using the transmission line method the interface of Bi$_2$Te$_3$ nanorribons towards ex situ applied Ti/Au contacts is probed at low temperatures. Furthermore, magnetotransport measurements on nano-Hallbars of down to 50 nm wide Bi$_2$Te$_3$ nanoribbons show indications of highly mobile charge carriers originating from 2-dimensional, topological surfaces. Finally, making use of a stencil mask on-chip, elemental superconductors like Nb and Al are deposited to define in situ, lateral topological Josephson junctions. Superconducting properties of proximitized topological nanoribbons are presented and discussed.

DS 22.9 Wed 12:00 POT 81

Investigation of one-dimensional materials — •Hadeel Moustafa, Peter Larsen, Morten Gjerding, and Karsten Jacobsen — Technical University of Denmark (DTU), department of physics.

1D materials are an interesting subset of materials with promising applications in batteries, photonic crystals and as electronic interconnects. 1D materials also present the possibility of combining them with other 1D materials or higher dimensional materials to create new hetero-structures with novel physical properties. Another potential application could be in heterogeneous catalysis, where the restricted geometry of 1D materials might lead to new types of atomic sites with different chemical characteristics. We identify potential 1D materials through a screening procedure applied to the ICSD and the COD. We employ the dimensionality scoring parameter defined in ref [1], which is based exclusively on the atomic geometry. The algorithm extract one-dimensional components from periodic three-dimensional crystals. So far around 300 compounds have been studied. Their basic properties like atomic structure, stability (heat of formation and convex hull), band structure, density of states and work function have been calculated. They are furthermore characterized using symmetry and grouped together using a clustering algorithm based on the root-mean-square-distance. In the future we expect to construct new potential 1D materials by element substitution in the constructed database. [1] http://doi.org/10.1103/PhysRevMaterials.3.03400.

DS 22.10 Wed 12:15 POT 81

Proximity exchange effects in excitons of TMDC/ferromagnet van der Waals heterostructures — •Paulo E. Faria Junior, Klaus Zollner, and Jaroslav Fabian — Universität Regensburg, Germany

Proximity effects in two-dimensional van der Waals heterostructures are an efficient way to modify intrinsic electronic properties[1]. In particular, proximity exchange offers the possibility of inducing magnetic properties in nominally nonmagnetic materials. Furthermore, this induced synthetic Zeeman splting exhibits strong signatures in the optical spectra. Combining ab initio calculations with tight-binding modeling and the effective Bethe-Salpeter equation for excitons, we investigate the proximity exchange in TMDC/ferromagnet systems: (i) (Mo,W)Se2 on the ultrathin van der Waals ferromagnet CrI3[2] and (ii) (Mo,W)S2/hBN on ferromagnets Co and Ni[3]. Since stacking different 2D materials requires adjusting the lattice parameters to obtain commensurate supercells, we also discuss the impact of biaxial strain in monolayer TMDCs[4]. We show the evolution of different optical transitions and the role of excitonic effects in the direct transitions. [1] Zutic et al., Mater. Today 22, 85 (2019). [2] Zollner, Faria Junior, Fabian, PRB 100, 085128 (2019). [3] Zollner, Faria Junior, Fabian, arXiv:1910.13223 (2019). [4] Zollner, Faria Junior, Fabian, PRB 100, 195126 (2019). Supported by: Alexander von Humboldt Foundation, Capes, DPG SFB 1277.

DS 22.11 Wed 12:30 POT 81

Decreasing Activation Energies with Thickness of Thin HfTe$_5$ layers — •Christopher Belke[1], Sonja Locmelis[2], Lars Thole[1], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

Hafnium pentatelluride (HfTe$_5$) is a layered two dimensional material from the class of Transition Metal Penta Chalcogenide with the chemical formula MX$_5$, where M is a transition metal and X a chalcogenide [1]. HfTe$_5$ shows a resistivity anomaly and is expected to be a topological insulator [2] with a bulk band gap of about 22 meV [3]. In addition, theory predicts that a single layer should show a band gap of about 400 meV and should be a quantum spin hall insulator [1].

We present that the electronic properties of HfTe$_5$ drastically change with decreasing thickness. We prepared samples with different thicknesses under 100 nm and made temperature dependent measurements to determine the activation energy in an Arrhenius plot. We found that the band gap increases with decreasing thickness. Conductivity measurements also show an anomaly due to a mobility change at around 120 K.

[1] H. Weng et al., Phys. Rev. X 4, 011002 (2014)
[2] S. Liu et al., APL Materials 6, 121111 (2018)
[3] H. Wang et al., Phys. Rev. B 93, 165127 (2016)

DS 22.12 Wed 12:45 POT 81

Tailoring of electronic and magnetic properties of hematene: a computational study — •Yidan Wei, Mahdi Ghorbani, and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Exfoliation of non van der Waals materials has established new class of two dimensional materials, such as hematene btained from hematite. In order to exploit and design potential applications, understanding the electronic and magnetic properties is crucial. Using density functional theory calculations, the atomic structures, electronic and magnetic properties of hematene are systematically investigated. Bare hematene in the ferromagnetic states is less stable than that in the anti ferromagnetic states, and it has a direct band gap. The stability, electronic and magnetic properties of hematene can change significantly with different terminations. Hematene covered with OH is a semiconductor with surface states removed, while hematene covered with H changes from semiconductor to half metal. Further, changes in the electronic characteristics are possible under with mechanical deformation. Applying strain causes significant changes in the electronic properties of hematene. In case of non-terminated hematene, both compressive and tensile strain can result in a reduction of the band gap in the anti-ferromagnetic state under biaxial and uniaxial deformation, and the band gap increases in case of OH terminated hematene. The band gap also increases under tensile strain in the ferromagnetic states. The deformation can lead to the enhancement of polarization.

DS 23: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions III (joint session O/HL/CPP/DS)

Time: Wednesday 10:30–13:30 Location: GER 38

Invited Talk DS 23.1 Wed 10:30 GER 38

Hybrid Perovskites: polarons, excitons and phase diagrams — •Georg Kresse, Menno Bokdam, and Ryosuke Jinnouchi — University of Vienna, Faculty of Physics and Center for Computational Materials Sciences

Halide perovskites are very promising solar cell materials. The first part of this presentation studies the formation of polarons and excitons in MAPbI3. We show that both, polarons and excitons, possess about similar binding energies. To obtain accurate results, the calculations have to be carefully converged with respect to the k-point sampling, something that has been often "overlooked" in the past [1].

The second part of the talk presents studies on the finite temperature behavior of MAPbI3. To achieve the required long simulation time and large length scales, an on-the-fly machine learning scheme that generates force fields automatically during first principles molecular dynamics simulations is used. This force field opens up the required time and length scales, while retaining the distinctive chemical precision of first principles methods [2]. Using machine learned potentials, isothermal-isobaric simulations give direct insight into the underlying microscopic mechanisms of the phase transitions. We observe that MAPbI3 is an very dynamic material even at room temperature, putting some question marks on the hereto considered static models.

[1] M. Bokdam, T. Sander, A. Stroppa, S. Picozzi, D. D. Sarma, C. Franchini, G. Kresse, Scientific Rep. 6, 28618 (2016); [2] R. Jinnouchi, J. Lahnsteiner, F. Karsai, G. Kresse, M. Bokdam, PRL 122, 225701 (2019).

DS 23.2 Wed 11:00 GER 38

Assessing ab-initio methodology to compute electronic properties of organic-inorganic metal halide perovskites — •Cecilia Vona, Dmitrii Nabok, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Organic-inorganic metal halide perovskites (HaPs) are materials widely studied for their light-harvesting properties. Owing to the interplay between strong electron-electron interaction and spin-orbit coupling, their theoretical investigation is still a challenge. Here we evaluate the methodology to compute their electronic structure. To this extent, we explore several approaches, within density-functional theory and many body perturbation theory, to compute the electronic structure of PbI_2, which is the precursor of many HaPs. Spin-orbit coupling effects are taken into account, and the hybrid functionals PBE0 and HSE are at the center of the investigation. We first explore several methods to determine the mixing parameter α, which in PBE0 and HSE defines the amount of Hartree-Fock exchange mixed with the semi-local functional PBE. We then use the results obtained from HSE and PBE0 for different values of α as starting point of G_0W_0 calculations. All the calculations are performed with the full-potential all-electron computer package `exciting`, in which LAPW+lo bases are implemented. We observed that hybrid functionals with a proper α value are most suitable to compute the electronic structure of PbI_2. Moreover, we show that the methodology is transferable to $CsPbI_3$, and we expect the same behavior for the lead-iodine perovskites.

DS 23.3 Wed 11:15 GER 38

Rashba-Dresselhaus Effect in Two Dimensional Layered Halide Perovskites — •Benedikt Maurer[1,2], Claudia Draxl[1,2], and Christian Vorwerk[1,2] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin — [2]European Theoretical Spectroscopy Facility

It has been shown that huge spin-orbit coupling in bulk hybride organic inorganic perovskites in combination with broken inversion symmetry leads to Rashba-Dresselhaus splitting, which influences the optoelectronic properties. This indicates that such effects also affect the optoelectronic properties of their two dimensional layered relatives, which are promising candidates as new light emitting materials. In this work, we aim at understanding which inversion symmetry breaking can lead to the Rashba-Dresselhaus effect in those materials. For this purpose, we develop model structures, where we replace the organic compounds by Cs atoms and disregard possible distortions in the inorganic layers, resulting in the structural composition $Cs_{n+1}Pb_nI_{3n+1}$. Using the all-electron full-potential density-functional-theory code `exciting`, we systematically study how atomic distortions impact the band structure for n=1, 2 and ∞. We identify displacement patterns that yield Rashba-Dresselhaus splitting, and determine the size of the splitting as a function of the displacement. Furthermore, we analyze the spin textures in electronic states around the band gap to differentiate between Rashba and Dresselhaus effect. Our study reveals in-plane lead displacements as the origin of the Rashba-Dresselhaus splitting.

DS 23.4 Wed 11:30 GER 38

Intrinsic polarons on polar surfaces — •Michele Reticcioli[1,2], Zhichang Wang[2], Igor Sokolovic[2], Michael Schmid[2], Ulrike Diebold[2], Martin Setvin[2], and Cesare Franchini[2,3] — [1]University of Vienna, Center for Computational Materials Science, Vienna, Austria — [2]Institute of Applied Physics, Technische Universitaet Wien, Vienna, Austria — [3]University of Bologna, Department of Physics and Astronomy, Bologna, Italy

Uncompensated charge at the surface boundary of polar materials is conventionally expected to form a two dimensional electron gas (2DEG), as a result of the alternating charged-plane stacking in the ionic crystals, interrupted by the surface cut. By means of density-functional theory calculations and surface-sensitive experiments, we propose a different paradigm able to accommodate the uncompensated charge in a more effective way, establishing a more favorable ground state for the system, that is the polaron formation (local lattice distortions coupled with charge localization). In fact, the intrinsic uncompensated charge tends to spontaneously localize and form polarons, rather than a 2DEG. Only beyond the critical polaron density, excess charge arising from external doping or defects starts to build dispersed electronic states. Here, we show how polarons and 2DEG compete on the polar KTaO3(001) surface.

DS 23.5 Wed 11:45 GER 38

Polarons in extended p-conjugated systems: the role of electron correlation. — •Daniele Fazzi[1], Klaus Meerholz[1], and Fabrizia Negri[2] — [1]Institut für Physikalische Chemie, Universität zu Köln, Luxemburger str. 116, 50939 Köln, Germany — [2]Dipartimento di Chimica, Università di Bologna, via F. Selmi, 2, 40126 Bologna, Italy

Polarons play a crucial role in governing charge transfer in organic materials. An accurate description of their electronic structure and electron-phonon couplings is mandatory to understand their response and transport properties.

We report a comprehensive investigation of polarons in extended p-conjugated systems (ladder-type polymers, graphene nano-ribbons, and cyanine-based compounds [1-2]). We show how spin polarized DFT lead to solutions of the polarons wavefunction which are not the most stable ones. This aspect, can be traced back to the multireference character of polarons. Broken symmetry DFT can address the electronic and structural properties of polarons, providing a correct assessment of charge transport parameters, otherwise incorrectly computed [3]. Multi-reference wavefunction methods are also considered to take into account correlation effects in charged and excited states.

Our study calls for a careful assessment in the description of charged/excited states in conjugated materials.

[1] Wang, S., et al., Adv. Mater. 2018, 30, 1801898. [2] Medina, S. et al., Phys. Chem. Chem. Phys., 2019, 21, 7281-7288. [3] Fazzi, D. et al, J. Mat. Chem. C., 2019, 7, 12876-12885.

DS 23.6 Wed 12:00 GER 38

Optical and x-ray absorption spectra of MgO from first-principles including many-body effects — •Vijaya Begum, Markus E Gruner, and Rossitza Pentcheva — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, Germany

We discuss the optical and x-ray absorption (XAS) spectra of MgO – a wide band gap oxide with versatile applications – in the framework of density functional theory (DFT) including many-body and excitonic corrections. The quasi-particle band gap improves over DFT with PBEsol as the starting exchange-correlation functional (4.58 → 7.52 eV) and is overcorrected with the hybrid functional HSE06 (6.58 → 8.53 eV) when compared to experiment (7.7 eV). Including excitonic effects by solving the Bethe-Salpeter equation (BSE) leads to excellent agreement with the experimental spectrum both for the real and imaginary part of the dielectric function, when starting with the HSE06 functional. Furthermore, the x-ray absorption spectra of the O and Mg K-edge calculated with the Exciting code exhibit good agreement with experiment regarding the positions of the prominent peaks, underlining the importance of including the core-hole and electron interactions within the G_0W_0+BSE. Projection of the electron-hole coupling coefficients from the BSE eigenvectors on the band structure allows to explore the origin of the peaks and identify the orbital character of the relevant contributions.

Funding by DFG CRC1242, project C02 is gratefully acknowledged.

DS 23.7 Wed 12:15 GER 38

Strain effects on the lattice-dynamical properties of titanium dioxide — •Peter Weber, Sebastian Tillack, Pasquale Pavone, and Claudia Draxl — Humboldt-Univeristät zu Berlin, Physics Department and IRIS Adlershof, Germany

A fingerprint of temperature-related anharmonic effects in a crystal is the change of the phonon frequencies with the volume. For anisotropic crystals, this variation must be generalized by the introduction of the mode Grüneisen tensor, which expresses the change of the phonon frequencies with respect to any applied strain. In this work, we present the results of an *ab-initio* investigation of the strain effects on the lattice-dynamical properties of the rutile and anatase phases of TiO_2. In particular, we focus our attention to the determination of the generalized Grüneisen parameters at the Brillouin zone center. In order to obtain all independent components of the Grüneisen tensor for these phases, all polar and nonpolar phonon frequencies at the Γ point are calculated for several strained configurations. These calculations are performed using density-functional theory as implemented in the full-potential all-electron software package `exciting` [1]. The connection between the Grüneisen tensors of the acoustic branches and the elastic constants of these materials is analyzed and discussed. Our results are also compared with available Raman scattering data for strained TiO_2.

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

DS 23.8 Wed 12:30 GER 38

Ab-initio phonon self-energies and fluctuation diagnostics of phonon anomalies: lattice instabilities from Dirac pseudospin physics in transition-metal dichalcogenides — •Jan Berges[1], Erik van Loon[1], Arne Schobert[1], Malte Rösner[2], and Tim Wehling[1] — [1]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Germany — [2]Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands

We present an ab-initio approach for the calculation of phonon self-energies and their fluctuation diagnostics, which allows us to identify the electronic processes behind phonon anomalies. Application to the prototypical transition-metal dichalcogenide 1H-TaS_2 reveals that coupling between the longitudinal–acoustic phonons and the electrons from an isolated low-energy metallic band is entirely responsible for phonon anomalies like mode softening and associated charge-density waves observed in this material. Our analysis allows to distinguish between different mode-softening mechanisms including matrix-element effects, Fermi-surface nesting, and Van Hove scenarios. We find that matrix-element effects originating from a peculiar type of Dirac pseudospin textures control the charge-density-wave physics in 1H-TaS_2 and similar transition-metal dichalcogenides.

DS 23.9 Wed 12:45 GER 38

Toward a general non-local polarizability density functional for van der Waals dispersion interactions — •Szabolcs Góger, Dmitry Fedorov, Péter Szabó, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

Density functional theory (DFT), while being a workhorse for electronic structure calculations, struggles with describing long-range electron correlations including van der Waals (vdW) dispersion interactions. Various promising approaches have been developed to include vdW interactions in DFT, but a broadly applicable method is yet to be found [1,2]. The first key issue is developing a general density functional for non-local polarizability in molecules and solids. In this work, we use different known properties of atomic and molecular polarizabilites including the direct relation between the dipole polarizability and vdW radius unveiled recently [3]. Diverse methods starting with the Slater-Kirkwood approach [4] are applied to simple quantum mechanical systems like the Drude oscillator and the hydrogen atom under the effect of various electric fields. Our model studies along with prior work on semi-local polarizability functionals [5] pave the way toward developing a unified non-local polarizability functional for molecules and materials.

[1] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)
[2] Stöhr *et al.*, Chem. Soc. Rev. **48**, 4118 (2019)
[3] Fedorov *et al.*, Phys. Rev. Lett. **121**, 183401 (2018)
[4] Slater and Kirkwood, Phys. Rev. **37**, 682 (1931)
[5] Vydrov and Van Voorhis, Phys. Rev. Lett. **103**, 063004 (2009)

DS 23.10 Wed 13:00 GER 38

Insights into van der Waals interactions from the quantum Drude oscillator model — •Dmitry Fedorov, Martin Stöhr, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

The quantum Drude oscillator (QDO) model [1] represents the response of all valence electrons in an atom by a single Drude particle with its charge, mass, and characteristic frequency. Due to the simple form, this model serves as an insightful approach for the description of atomic response properties and van der Waals (vdW) interactions [2]. Recently, the QDO model helped to unveil a non-trivial relation between the dipole polarizability and the atomic volume, $\alpha_{\text{dip}} \propto V^{4/3}$, [3] as well as the surprising direct relation between the multipole polarizabilities and the equilibrium distances in vdW-bonded atomic dimers [4]. Here, we provide a detailed insight into the physical background of the aforementioned findings. The connection between different striking scaling laws obtained by diverse ways shows the inner consistency and power of this simple but efficient model. We discuss the importance of the revealed quantum-mechanical relations between response and geometric properties of atoms for computational models like the Tkatchenko-Scheffler [5] and the many-body dispersion [2] methods.

[1] Jones *et al.*, Phys. Rev. B **87**, 144103 (2013)
[2] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)
[3] Kleshchonok and Tkatchenko, Nat. Commun. **9**, 3017 (2018)
[4] Fedorov *et al.*, Phys. Rev. Lett. **121**, 183401 (2018)
[5] Tkatchenko and Scheffler, Phys. Rev. Lett. **102**, 073005 (2009)

DS 23.11 Wed 13:15 GER 38

Conical intersections in molecular systems: 3D vs 2D models — •Erik Pillon, Dmitry Fedorov, Péter Szabó, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg

The molecular Aharonov-Bohm effect [1], covering various phenomena caused by the Berry (geometric or topological) phase in molecular systems, is an important playground for understanding fundamental quantum physics as well as for building quantum electronic devices. The related non-adiabatic effects, stemming from the coupling between the electron and nuclear degrees of freedom, are especially pronounced in systems possessing conical intersections (CI) in potential energy surfaces, ubiquitous in condensed matter and molecular physics. Many toy models have been introduced to study the influence of CIs on the nuclear dynamics from a general point of view. However, most of them, including the linear vibronic coupling model [2, 3] widely used in literature, employ two-dimensional (2D) real Hamiltonians. In our work, we check whether such models capture all the important features of real molecular systems. To this end, we perform a comparison of the conventional approaches with the general treatment of a CI within the three-dimensional (3D) complex Hamiltonian possessing SU(2) symmetry [4]. The features present within the 3D model but missing in the 2D case are identified and discussed.

[1] Zygelman, J. Phys. B: At. Mol. Opt. Phys. **50**, 025102 (2017)
[2] Longuet-Higgins *et al.*, Proc. R. Soc. A **244**, 1 (1958)
[3] Jahn and Teller, Proc. R. Soc. A **161**, 220 (1937)
[4] Berry, Proc. R. Soc. A **392**, 45 (1984)

DS 24: Layer Properties II: Optical Properties

Time: Wednesday 11:00–12:15 Location: CHE 91

DS 24.1 Wed 11:00 CHE 91

Theoretical description of optical properties in thin film materials — •Christine Giorgetti[1,2] and Valérie Véniard[1,2] — [1]Laboratoire des Solides Irradiés, CNRS, EcolePolytechnique, CEA/DRF/IRAMIS, Institut Polytechnique de Paris, F-91128 Palaiseau — [2]European Theoretical Spectroscopy Facility

In the framework of periodic boundary codes, the standard way to describe surfaces, or more generally isolated objects, is to build a supercell with vacuum, to separate the artificial replicas. We have shown that this procedure gives an absorption spectrum which depends on the vacuum introduced in the supercell.

We have proposed a new method called Selected-G to solve this vacuum problem. In TDDFT, it consists to solve the Dyson equation on a reduced set of reciprocal lattice vectors defined according to the thickness of the matter. During this derivation, we have evidenced a non-diagonal expression for the Fourier transform of the Coulomb potential, called slab potential. In the limit of an infinite thickness of matter, we recover the standard 3D expression of the Coulomb potential, and it has been successfully applied to describe optical properties for silicon surfaces.

In the case of electron energy loss (EEL), the vacuum problem also affects the in-plane components and the full expression of the slab potential in the Selected-G formalism is crucial to describe slabs of finite thickness, as it will be illustrated for few layers graphene slabs. These results open the question of the relationship between EEL and absorption spectra for thin slabs of matter.

DS 24.2 Wed 11:15 CHE 91

Highly reflective, stable mirror coatings for NIR and MIR spectral range by Atomic Layer Deposition — •Paul Schenk[1,2] and Adriana Szeghalmi[1,2] — [1]Fraunhofer-Institute for Applied Optics and Precision Engineering IOF, Center of Excellence in Photonics, Albert-Einstein-Str. 7, D-07745 Jena, Germany — [2]Friedrich-Schiller-University Jena, Institute of Applied Physics, Albert-Einstein-Str. 15, D-07745 Jena, Germany

Thin and smooth mirror coatings are essential for numerous optical systems in spectroscopy, astronomy, sensing, and lightning. Metallic reflectors cover from the ultraviolet to infrared a very broad spectral range. Well-established materials for highly reflective mirrors in the near (NIR) and mid (MIR) infrared spectral range are aluminum, silver, and gold. However, these materials degrade due to mechanical stress on the surface or thermal exposure, which leads to a decrease in reflectivity.

Iridium is a noble metal that has a reflectivity in the NIR and MIR spectral range similar to the established materials. It is very hard, extremely dense, chemically very stable and can be deposited as a smooth metal thin film by atomic layer deposition (ALD). It is scratch-resistant, abrasion-stable and thermally stable. Due to its enormously high melting point of over 2400 °C, it can even resist the highest temperatures. In the presented work, we studied the mechanical and thermal stability of iridium mirrors with regard to their reflectivity in the NIR and MIR spectral range.

DS 24.3 Wed 11:30 CHE 91

High resistive $\mathbf{NbO_2}$ thin-films for phase-change switching applications — •Julian Stoever, Jos E. Boschker, Nazir Jaber, Saud Bin Anooz, Martin Schmidbauer, Jutta Schwarzkopf, Martin Albrecht, and Klaus Irmscher — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

Niobium dioxide has recently gained increased interest as it exhibits a semiconductor-metal transition together with a structural phase transition similar to that of vanadium dioxide. (VO_2). In contrast to VO_2, NbO_2 has phase transition temperature of 1080 K, which is well above room temperature and makes the material very interesting for resistive switching devices. We demonstrate the growth of single-crystalline NbO_2(001) by pulsed laser deposition on MgF_2(001) substrates. A subsequently performed annealing step results in a significantly sharper symmetric NbO_2(004) x-ray diffraction peak and in a change of surface morphology. Ellipsometry, absorption spectroscopy and temperature-dependent resistivity measurements (TDR) were performed on the epitaxial layers. A single-crystalline NbO_2 bandgap energy of 0.89 ± 0.03 eV was consistently measured. This is in good agreement with density functional theory calculations by O'Hara et al. [J. Appl. Phys. 116, 213705 (2014)]. Furthermore, TDR were performed to determine deep level defects in the material. Finally, we will demonstrate first NbO_2 epitaxial layers on sapphire (Al_2O_3) substrates. Sapphire appeared to be more stable during the annealing, resulting in promising NbO_2 epitaxial layers.

DS 24.4 Wed 11:45 CHE 91

Metastability in Kesterite solar cells and dominant recombination process at open circuit voltage. — •Mbafan Samantha Lyam — Photovoltaics group, Martin Luther University, Halle-Wittenberg, 06120 Halle (Saale), Germany. — Department of Physics, Benue state University, Makurdi, PMB 102119, Nigeria.

kesterite solar cells (Cu2ZnSn(S,Se)4) have been investigated with the aim of determining meta-stability response and the dominant recombination path of the cells via open circuit voltage transients, admittance spectroscopy, capacitance voltage profiling techniques and current-voltage analysis. Exposure to red light was used to induce meta-stability and thereafter, the resulting slopes of the open circuit voltage transients, in combination with the diode quality factor and activation energy of the saturation current density obtained from fits of measured current-voltage curves, give insight into which region of recombination limits the cells at open circuit voltage.

DS 24.5 Wed 12:00 CHE 91

Tuning of Optical Properties in Highly Conducting Perovskites — •Mahdad Mohammadi, Aldin Radetinac, Thorsten Schneider, Alexey Arzumanov, Philipp Komissinskiy, and Lambert Alff — Institute of Materials Science, Advanced Thin Film Technology, Technische Universität Darmstadt, Darmstadt

The demand for transparent, conducting materials (TCMs) has skyrocketed in the past decades and will further increase due to the development and commercial success of devices like LCDs, capacitive touchscreens and OLEDs. For most TCM applications, doped wide-bandgap semiconductors like ITO (In_2O_3:Sn) are used due to the very good transparency in the visible. However, the conductivity in doped semiconductors is limited by the solubility of dopant elements. Recently, a new type of material has gained attention for application as TCM. The perosvkites SrMO3 (M = V, Mo, Nb) are all highly conducting, with $SrMoO_3$ ($\rho = 5.1\ \mu\Omega$cm) even surpassing the electrode material platinum. In addition, a moderately enhanced electron correlation reduces the plasma frequency ω_p and therefore induces transparency in large parts of the visible spectrum[1]. The scope of this work is to investigate the materials $SrVO_3$, $SrMoO_3$ and $SrNbO_3$ and related compounds to evaluate how and to what extend the properties can be manipulated towards desired characteristics. For this purpose, epitaxial thin films were deposited via pulsed laser deposition and characterized regarding structural, chemical, optical and electrical properties.

[1] A. Radetinac *et al.*, J. Appl. Phys., 119, 055302 (2016)

DS 25: Focus Session: Organic-based Hybrid Thermoelectrics II

Time: Wednesday 11:15–12:45 Location: CHE 89

Invited Talk DS 25.1 Wed 11:15 CHE 89

Organic thermoelectrics: fundamentals, challenges and recent results — •Martijn Kemerink — Centre for Advanced Materials, Universität Heidelberg, Germany

The potential use in thermoelectric applications of heavily doped organic semiconductors has led to a dramatic increase in research on these materials. In this talk, I will use recent results by ourselves and others to highlight some of the potential and some of the challenges of organic thermoelectrics (OTE). Specifically, I will focus on three aspects, being the role of the material morphology, the influence of doping on the energy landscape experienced by the mobile charge and the formal description thereof.

The topic of morphology will be addressed for systems containing either one or two semiconductors. In the former, it will be shown how processing-induced structural anisotropy can lead to a non-trivial simultaneous increase in electrical conductivity and thermopower. For the latter, the degree of phase separation will be shown to play the key role in determining whether the semiconductor blend behaves as an effective medium or not, which gives the unique opportunity to reach record-high thermopowers, albeit at the cost of a reduced but still finite electrical conductivity. Experimental results are interpreted by semi-analytical and numerical modeling that allows to identify strategies for fundamental and application-oriented research.

DS 25.2 Wed 11:45 CHE 89

Electronic Transport in Polymer Thin Films for Thermoelectric Applications — •Marie Siegert[1], Mahima Goel[2], Mukundan Thelakkat[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, University of Würzburg — [2]Applied Functional Polymers, University of Bayreuth — [3]ZAE Bayern

The interest in thermoelectric materials has greatly gained traction over the last decades due to their immense potential in waste heat recovery. Recently, the focus has shifted towards organic materials as a sustainable, low-cost alternative to inorganic semiconductors. Especially polymers hold great promise, as they can be solution processed at large scales and display low thermal conductivities. However, the improvement of their electrical conductivity σ, while retaining their Seebeck coefficient S, imposes a major challenge upon implementation in efficient thermoelectrics. Hence, we compare two possible strategies on improving the charge carrier transport in such disordered systems. At first, σ of organic composite films has been investigated, combining the well studied polymer PEDOT:PSS with crystallites of the low-dimensional molecular metal TTT_2I_3, which shows superior charge carrier transport over a wide temperature range[1]. Secondly, doped polymer films utilizing an oxidized hole conductor as dopant have been electrically characterized by means of σ and S. Both approaches will be evaluated with respect to the enhancement in σ and the underlying transport mechanisms. First estimations of the resulting power factors indicate future strategies to further enhance the electronic properties and thus, the figure of merit. [1] Huewe et al. *Adv. Mat.* 29 (2017).

Invited Talk DS 25.3 Wed 12:00 CHE 89

Tuning the Thermoelectric Performance of Hybrid Polymer/Nanoparticle Composites via Stoichiometric Control — •Katherine A. Mazzio[1], Danny Kojda[1], Britta Ryll[1], Jens Niederhausen[1], Rodrigo Rubio-Govea[1,2], Klaus Habicht[1,3], and Simone Raoux[1,4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Institut für Chemie, Humboldt Universität zu Berlin, Berlin, Germany — [3]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [4]Institut für Physik, Humboldt Universität zu Berlin, Berlin, Germany

Hybrid materials consisting of inorganic nanostructures embedded in conducting polymer matrices have emerged as promising systems for room temperature thermoelectric applications. They are attractive due to their intrinsic low thermal conductivities, the ability to engineer interfaces for energy filtering effects and phonon scattering, and their ability to take advantage of high-throughput and solution processable manufacturing. When synthesizing hybrid materials, one can think of them as a three phase system consisting of the organic material, the inorganic material, and the interface. Our goals revolve around controlling each of these components independently, and in this contribution, I will detail our recent efforts towards this end. Ultimately, we aim to develop an understanding of how to use solution-based synthesis to influence thermoelectric device properties.

DS 25.4 Wed 12:30 CHE 89

Radical Ion Doped Organic Single Crystals for Thermoelectric Applications — •Maximilian Frank[1] and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern eV), 97074 Würzburg

The successful application of organic semiconductors in lighting or photovoltaics would not have been possible without doping. Motivated by this, we will deal with the implementation of doped molecular crystals in thermoelectrics (TE) which promise the recovery of substantial amounts of waste heat generated upon primary energy consumption [1]. It is desirable to use materials with large Seebeck coefficient S, high electrical conductivity σ, and low thermal conductivity κ, which can be summarized in the dimensionless figure of merit at given temperature $zT = \frac{\sigma S^2}{\kappa} T$. In this sense, long-range ordered molecular crystals offer an interesting approach by their low thermal conductivities generic to van-der-Waals bound systems combined with moderate mobilities for electrons and holes. We use high quality polyaromatic single crystals to systematically alter their bandfilling and, thus, their electrical transport properties by electrochemical doping. The variations in electrical conductivity as well as Seebeck coefficient will be discussed as function of doping. The results will be critically evaluated in regard of the independent optimization of the thermoelectric parameters and, thus, of the implementation of doped single crystals and thin films in TE applications.

[1] C. Forman, et al., Renew. Sust. Energ. Rev. 2015, 57, 1568

DS 26: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions IV (joint session O/CPP/DS/HL)

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

Invited Talk DS 26.1 Wed 15:00 GER 38

Electron-phonon interactions in realistic materials — •Fabio Caruso — Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Functional materials used in actual devices are typically doped, they operate at finite temperature, and they may be subject to perturbations such as, *e.g.*, external fields and light pulses. These aspects may alter profoundly the electron-phonon interaction (EPI), its influence on the electronic properties of solids, and even lead to the manifestation of novel emergent phenomena absent in perfect crystals.

We conducted a first-principles investigation of the EPI in functional materials at realistic operational conditions based on many-body perturbation theory. Our work reveals that: (i) n-type doping of polar oxides, such as EuO and TiO_2, allows one to trigger and control the formation of polarons (electrons dressed by a phonon cloud) [1]; (ii) in the record-breaking thermoelectric material SnSe, temperature may lead to a five-fold suppression of carrier lifetimes due to enhanced phonon emission [2]. Overall, the striking sensitivity to doping, temperature, and external fields, makes the EPI a powerful tool to tailor the optoelectronic properties of quantum materials. Possible strategies to extend the many-body theory of the EPI to the study of time-dependent phenomena will further be discussed [3].

[1] J. Riley, F. Caruso, C. Verdi, *et al.*, Nature Commun. **9** (1), 2305 (2018). [2] F. Caruso, M. Troppenz, S. Rigamonti, C. Draxl, Phys. Rev. B **99** (8), 081104 (2019). [3] F. Caruso, D. Novko, C. Draxl, arXiv:1909.06549v (2019).

DS 26.2 Wed 15:30 GER 38

Fully Anharmonic, Non-Perturbative First-Principles Theory of Electronic-Vibrational Coupling in Solids — Marios Zacharias, Matthias Scheffler, and •Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

The coupling between nuclear vibrations and the electronic structure plays a pivotal role for many material properties, including optical absorption and electronic transport. In this regard, however, today's state-of-the-art methodologies rely on two approximations [1]: the harmonic (phonon) approximation for the nuclear motion and the linear response description of the electronic structure with respect to harmonic displacements. In this work, we overcome ***both*** these approximations by performing fully anharmonic *ab initio* molecular dynamics (*ai*MD) calculations and by accounting for the non-perturbative, self-consistent response of the wave functions along the *ai*MD trajectory. By this means, we obtain fully anharmonic, vibronically renormalized spectral functions, from which macroscopic material properties like temperature-dependent band gaps and electronic transport coefficients are obtained. We validate our approach using silicon as an example, for which the traditional electron-phonon coupling formalism is recovered. Using cubic $SrTiO_3$ as example, we further demonstrate that anharmonic electronic-vibrational coupling effects are not captured in traditional formalisms, but they play a decisive role here and in other complex materials like perovskites.
[1] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).

DS 26.3 Wed 15:45 GER 38

Thermal conductivity of highly-doped Si: Role of electron-phonon and point-defect phonon scattering — •Bonny Dongre[1], Jesús Carrete[1], Shihao Wen[2], Jinlong Ma[2], Wu Li[2], Natalio Mingo[3], and Georg KH Madsen[1] — [1]Institute of Materials Chemistry, TU Wien, A-1060 Vienna, Austria. — [2]Institute for Advanced Study, Shenzhen University, Shenzhen 518060, China — [3]LITEN, CEA-Grenoble, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France.

Theoretical investigation of the thermal conductivity reduction in highly-doped Si is an area of active research. Recently, first-principles electron-phonon scattering was found to produce a significant reduction in the thermal conductivity of highly-doped Si. However, the study could not reproduce the experimental results.

In the present work, we calculate the first-principles phonon scattering rates by electrons and point defects, and use them to calculate the thermal conductivity of highly-P- and B-doped Si for a range of temperatures and concentrations. We find that the phonon scattering by electrons dominates at carrier concentrations below 10^{19} cm^{-3} and is enough to reproduce the experimental thermal conductivity reduction at all temperatures. However, at higher defect concentrations point-defect phonon scattering contributes substantially to the thermal conductivity reduction even at room temperature. With a combined treatment of the phonon scattering by electrons as well as phonons, an excellent agreement is obtained with the experimental values at all temperatures.

DS 26.4 Wed 16:00 GER 38

Precise yet Fast High-Throughput Search for Thermal Insulators — •Florian Knoop, Thomas A.R. Purcell, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft

We present a systematic and numerically precise computational search for thermal insulators in material space performed with the *FHI-vibes* high-throughput framework [1]. *FHI-vibes* employs a robust metric that quantifies the degree of anharmonicity in the nuclear dynamics via the statistical comparison of first-principles forces with those forces that would act in the harmonic approximation. This enables us to efficiently scan over many materials, including complex oxides and chalcogenides as well as ternary structures like perovskites. By this means, we single out strongly anharmonic systems, for which we perform *ab initio* Green-Kubo simulations to assess their thermal conductivities, thereby naturally including all anharmonic effects [2]. Our strategy allows to avoid redundant calculations and to achieve a much higher quality of information than traditional high-thoughput studies. Besides validating the performed search and analyzing its results, we discuss how big-data analytics techniques can be utilized to further accelerate and guide this search.
[1] https://vibes.fhi-berlin.mpg.de
[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017)

DS 26.5 Wed 16:15 GER 38

Ambivalent Impact of Electron-Phonon Interaction on Electronic and Transport Properties of Organic Semiconductors — •Frank Ortmann — Center for Advancing Electronics Dresden, Technische Universität Dresden, Germany

Vibrations are omnipresent in molecules and of great importance in Organic Semiconductors due to the softness of the materials and the strong electron-phonon coupling. One possibility to investigate this interaction is to study the low-energy edge of optical absorption spectra, which lacks an in-depth understanding for organic materials. We have recently observed a strong dependence of low-energy excitonic features on the molecular building blocks in organic films, which we associated to molecular flexibility and polaron deformation. We will discuss implications of low-frequency molecular vibrations on the polaronic and excitonic density of states in donor-acceptor mixtures featuring charge-transfer excitons. We will also discuss how a distinguished treatment of strong-coupling molecular vibrations of different energies leads to an improved description of charge carrier transport in organic materials.

DS 26.6 Wed 16:30 GER 38

Quantum Nuclear Effects in Thermal Transport of Semiconductors and Insulators — •Hagen-Henrik Kowalski[1], Mariana Rossi[1,2], Matthias Scheffler[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]MPI for Structure and Dynamics of Matter, Hamburg, Germany

To date, the computation of thermal conductivities relies on either perturbation theory or (*ab initio*) molecular dynamics (MD) [1]. While perturbative approaches include quantum-nuclear effects (QNE), they typically neglect higher orders of anharmonicity. Conversely, classical MD includes all orders of anharmonicity, but neglects QNEs. To overcome these limitations, we have developed a formalism that accounts for ***both*** quantum-nuclear effects and all orders of anharmonicity. For this purpose, the nuclear dynamics are assessed via Thermostatted Ring Polymer MD (TRPMD) [2] and the thermal conductivity is obtained via the Green-Kubo formalism using a newly proposed TRPMD based heat-flux estimator. Using solid Argon and Silicon as model systems, we discuss the influence of QNEs on thermal transport by comparing velocity, energy, and heat-flux autocorrelation spectra. This allows to rationalize the impact of QNEs on vibrational frequencies, lifetimes, and on the thermal conductivity in different temperature regimes.
[1] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901, (2017).
[2] M. Rossi, M. Ceriotti, D. Manolopoulos, *J. Chem. Phys.* **140**, 234116 (2014).

DS 26.7 Wed 16:45 GER 38

Speeding-up *ab initio* molecular dynamics with hybrid functionals using adaptively compressed exchange operator based multiple time stepping — •Sagarmoy Mandal and Nisanth N. Nair — Department of Chemistry, Indian Institute of Technology Kanpur, India

Ab initio molecular dynamics (AIMD) with hybrid density functionals and a plane wave basis is known to predict the structural and dynamical properties of condensed matter systems accurately. However, such hybrid functional based AIMD simulations are not routinely used due to the high computational cost associated with the application of the Hartree-Fock exchange operator. We propose a strategy [1] to combine the Adaptively Compressed Exchange (ACE) operator formulation [2] and a multiple time step integration scheme to reduce the computational cost significantly. We also show that computing the

ACE operator with localized orbitals can further improve the computational efficiency. Finally, we use this method in combination with the Well-Sliced Metadynamics approach to compute the free energy barrier of chemical reactions in systems containing hundreds of atoms.

[1] S. Mandal, N.N. Nair, J. Chem. Phys. **151** (2019) 151102.
[2] Lin Lin, J. Chem. Theory Comput. **12** (2016) 2242.

DS 26.8 Wed 17:00 GER 38

Calculation of current-induced heating and vibrational instabilities in single molecule circuits — Giuseppe Foti and •Hector Vazquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

Current-induced heating in molecular wires arises from the interaction between tunneling electrons and localized vibrations. Vibrational instabilities occur when excitation of molecular vibrations is not balanced by dissipation mechanisms, and can lead to the breakdown of the junction. In this talk I will address predictions for vibrational instabilities in single molecule junctions with separated unoccupied resonances. We use DFT-NEGF to study the electronic structure of the junction under an applied bias, while rates of absorption and emission of vibrations are calculated using kinetic equations [1,2]. We find and characterize several unstable modes. These results are then generalized using model calculations to generate a stability diagram of the junction under bias [3]. The talk will discuss the effect of a self-consistent treatment of electron-vibration interaction, and highlight the role played by the structure of the electron-vibration coupling matrix. Our work reveals the interplay of electronic structure and electron-vibration coupling in a broad class of molecular wires.

[1] J-T Lü, P. Hedegaard and M. Brandbyge, Phys. Rev. Lett. 107, 046801 (2011).
[2] G. Foti and H. Vázquez, J. Phys. Chem. C 121, 1082 (2017).
[3] G. Foti and H. Vázquez, J. Phys. Chem. Lett. 9, 2791 (2018).

DS 26.9 Wed 17:15 GER 38

***Ab Initio* Green-Kubo Approach of Charge Transport in Crystalline Solids** — •Zhen-Kun Yuan, Marios Zacharias, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

State-of-the-art approaches for calculating the charge transport coefficients in crystalline materials rely on a harmonic description of the lattice vibrations and a perturbative treatment of electron-phonon couplings (EPCs) [1]. For materials featuring sizable anharmonic lattice vibrations and/or strong EPCs, such approaches are, however, not applicable. Here, we present an *ab initio* approach based on the Green-Kubo theory of linear response [2] that does neither rely on the harmonic approximation nor on a perturbative treatment of EPCs, thus overcoming these issues. The electrical conductivity is obtained from the time correlations of the electric charge flux, which is computed along fully anharmonic *ab initio* molecular dynamics trajectories. We demonstrate our approach by calculating the electrical conductivity of the harmonic material Si and the anharmonic $SrTiO_3$. We carefully check the convergence behavior of the calculated results with respect to supercell size and examine possible strategies to overcome finite-size effects [3].

[1] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).
[2] R. Kubo, M. Yokota, and S. Nakajima, *J. Phys. Soc. Jpn.* **12**, 1203 (1957).
[3] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).

DS 27: Focus Session: Functional Metal Oxides for Novel Applications and Devices I (joint session HL/DS)

Metal oxides exhibit a myriad of fascinating physical properties that enable a large variety of potential applications such as sensors and detectors, solar energy harvesting, transparent and potentially bendable electronics, power electronics, high-electron-mobility transisitors, memristors, topological quantum computation and so on. These functionalities typically require homo- or heteroepitaxial layers of high crystallinity with bendable amorphous semiconducting oxides as an exception. This session sets a focus on growth of bulk and thin films, experimental and theoretical investigation of their physical properties as well as fabrication and characterization of demonstrator devices.

Organizers: Oliver Bierwagen (Paul-Drude-Institut für Festkörperelektronik, Berlin), Holger Eisele (TU Berlin), Jutta Schwarzkopf (Leibniz-Institut für Kristallzüchtung, Berlin) and Holger von Wenckstern (Universität Leipzig).

Time: Wednesday 15:00–18:15 Location: POT 81

Invited Talk DS 27.1 Wed 15:00 POT 81

Modulation Doping in High-Mobility Alkaline-Earth Stannates — •Bharat Jalan — Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455, U.S.A.

Interfaces between perovskite oxides have created tremendous excitement because of the potential for emergent phenomena and novel field-effect devices. The vast majority of these papers focus on the $LaAlO_3/SrTiO_3$ (LAO/STO) interfaces including some on Al_2O_3/STO and $ReTiO_3$/STO (Re refers to the rare-earth elements) interfaces among others. Amazingly, all these heterostructures involve the use of STO as an active layer where electron transport occurs. Attempts to synthesize non-STO based *modulation-doped* heterostructure have been unsuccessful so far despite theoretical predictions. Nor has any appreciable level of control been gained over the electron density at the interface, which is critical to device applications.

In this talk, we will report the *first* demonstration of true *modulation doping in a wider bandgap perovskite oxides without the use of STO.* We show that the La-doped $SrSnO_3/BaSnO_3$ system precisely fulfills the theoretical criteria for electron doping in $BaSnO_3$ using electrons from La-doped $SrSnO_3$, and we demonstrate how rearrangement of electrons can be used to control the insulator-to-metal transition in these heterostructure. We further show the use of angle-resolved HAXPES as a non-destructive approach to not only determine the location of electrons at the interface but also to quantify the width of electron distribution in $BaSnO_3$. The transport results are in good agreement with the results of self-consistent solution to one-dimensional Poisson and Schrödinger equations.

DS 27.2 Wed 15:30 POT 81

Two-dimensional electron (hole) gas in $BaSnO_3/LaInO_3$ heterostructures: A first-principles study — •Wahib Aggoune, Dmitrii Nabok, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

We investigate the structural and electronic properties of heterostructures formed by the nonpolar $BaSnO_3$ (BSO) and polar $LaInO_3$ (LIO) perovskites, employing density functional theory. Focusing on the impact of thickness and surface termination of the LIO side, we analyze the electronic properties of the interface. For the stoichiometric LIO film, an internal electric field is induced due to the different terminations of its two sides. Increasing the LIO thickness, this field causes an upward shift of the valence band maximum (VBM). Reaching a thickness of 6 LIO unit cells, the VBM crosses the Fermi level, leading to partial occupation of the conduction band minimum (CBM). Consequently, a two-dimensional electron gas (2DEG) forms at the BSO side of the interface, confined within three unit cells. A high electron mobility is expected due to the *s*-character of the CBM. The corresponding hole gas (2DHG) forms at the LIO side, confined within one unit cell. As a result, this combination gives rise to the formation of a conducting interface starting from the insulating BSO and LIO components. We also present its results for interfaces with non-stoichiometric LIO. Depending on the surface termination, either a 2DEG or a 2DHG forms at the interface. In this case, the 2D charge confinement is mainly attributed to the spontaneous polarization induced at the interface.

DS 27.3 Wed 15:45 POT 81

Epitaxial growth of Lanthanum doped BaSnO3 thin films by PLD — •Reshma Ravindran, Daniel Pfützenreuter, Julian Stöver, Klaus Irmscher, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2 12489 Berlin

Barium stannate (BaSnO3) has gained a lot of attention during the last few years due to its high charge carrier mobility, which is higher than for most transparent conducting oxides and the highest reported for perovskite materials [1]. This makes BaSnO3 especially interesting for the use in electronic applications, e.g. field effect transistors. For single crystals, a mobility of 320 cm2/Vs at room temperature has been published. However, the mobility in epitaxial films is in the range of 70-100 cm2/Vs. This has initiated research efforts to improve structural and electrical properties of BaSnO3 thin films.

In our study, we report on epitaxially grown La-doped BaSnO3 (La concentration was 4 wt.-%) thin films on SrTiO3 substrates by pulsed laser deposition (PLD). We will show that PLD parameters like substrate temperature, target-to-substrate distance and laser spot size have to be carefully adjusted in order to obtain the formation of phase pure BaSnO3 thin films. Hall measurements will indicate that the charge carrier mobility is critically correlated with the structural quality of the epitaxial films analyzed by atomic force microscopy and x-ray diffraction. [1] H. J. Kim et al. Phys. Rev. B 86, 165205 (2012)

DS 27.4 Wed 16:00 POT 81

Epitaxial growth of La doped BaSnO$_3$ thin films by Plasma-assisted molecular beam epitaxy — •Georg Hoffmann[1], Martina Zupancic[2], Martin Albrecht[2], Zbigniew Galazka[2], and Oliver Bierwagen[1] — [1]Paul-Drude-Institut für Festkörperelektronik Leibniz-Institut im Forschungsverbund Berlin e.V. — [2]Leibniz-Institut für Kristallzüchtung

For oxide molecular beam epitaxy (MBE), the use of suboxides is an essential part for the growth of complex oxides, e.g. SnO for BaSnO$_3$ (BSO). However, the conventional approach of BSO growth using SnO suboxide from a SnO$_2$ charge (SnO + Ba + 2O → BaSnO$_3$) requires high cell temperatures and adds a parasitic oxygen background due to the reaction SnO$_2$ → SnO + 1/2 O$_2$. Using a SnO$_2$ + Sn mixture as a charge can address both issues, first: the suppression of the parasitic oxygen due to the reaction SnO$_2$ + Sn → 2 SnO and second: providing higher fluxes at lower temperatures.

Using this new approach, smooth BSO films were grown by plasma-assisted MBE on SrTiO$_3$ (STO) substrates. The crystal quality was analyzed in-situ by reflective high energy electron diffraction. Ex-situ, morphology and structural parameters were determined by atomic force microscopy, X-ray diffraction, and high resolution transmission electron microscopy images.

The results reveal an increased BSO growth-temperature window with decreasing SnO/Ba flux ratio. Further, the influence of the STO miscut angle, as well as the STO orientation will be discussed, and electrical properties of La doped BSO films are pointed out.

30 min. break

Invited Talk DS 27.5 Wed 16:45 POT 81

Engineering of LiNbO3 films for next generation acoustic and energy harvesting applications — •Ausrine Bartasyte, Samuel Margueron, Vincent Astié, Giacomo Clementi, Mihaea Ivan, and Merieme Oubahaz — FEMTO-ST Institute, University of Franche-Comté, Besançon, France

The next generation of high frequency wide-band RF filters or frequency-agile filters are urgently needed for the development of 5G infrastructures/networks/communications. Today, LiNbO3 and LiTaO3 single crystals are key materials in electro-optics and RF acoustic filters. This motivates further development of acoustic wave devices based on highly electromechanically coupled LiNbO3 thin films, adapted to the high-frequency applications. The challenges and the achievements in the epitaxial growth of LiNbO3 films and their integration with Si technology and to acoustic devices will be discussed in detail. The deposition techniques enabling the control of film composition/ nonstoichiometry of volatile alkali metal oxides & the methods of compositional analysis will be presented. We have demonstrated an extremely high acoustical performance compatible with filter applications for SAW devices, based on epitaxial LiNbO3 films, operating in the frequency range around 5 GHz. Moreover, it was demonstrated that the power density of 9.62 mW .cm-3 (comparable to present performance of lead-based piezoelectric harvester) can be harvested by vibrational energy transducer based on thick LiNbO3 films.

Invited Talk DS 27.6 Wed 17:15 POT 81

Oxide Memristors for unified data storage and data processing — •Heidemarie Schmidt — Leibniz-IPHT Jena — IFK, FSU Jena — Fraunhofer ENAS Chemnitz

In the future, new hardware components will determine the power and strength of artificial intelligence and manchine learning. These components are called memristors [1]. The first memristor with unified analog data storage and information processing is the BiFeO3 (BFO) memristor. BFO is an electroforming-free, bipolar memristor and its potential has been shown in in-memory information processing [2], neuromorphic computing [3], and hardware cryptography [4]. Another electroforming-free memristor is the unipolar memristor YMnO3 (YMO). In order to develop memristor technology and applications further, it is more than ever necessary to understand the underlying resistive switching mechanisms when a write voltage is applied. We discuss results from quasi-static test measurements on BFO [5] and from temperature dependent transport measurements on YMO [6]. [1] Leon Chua, IEEE Transactions on Circuit Theory 18, 507, 1971 [2] T. You et al., Adv. Funct. Mat. 24, 3357-3365, 2014. [3] N. Du et al., Front. Neurosci. 9, 227, 2015. [4] N. Du et al., J. Appl. Phys. 115, 124501, 2014. [5] N. Du et al., Phys. Rev. Applied 10, 054025, 2018. [6] V.R. Rayapati et al., J. Appl. Phys. 124, 144102, 2018

DS 27.7 Wed 17:45 POT 81

Investigations on leakage current in epitaxial K0.5Na0.5NbO3 thin films grown by PLD — •Daniel Pfützenreuter, Julian Stöver, Klaus Irmscher, Jens Martin, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin

KxNa1-xNbO3 is a lead-free, ferro- and piezoelectric compound, which offers a high potential for memory applications and sensors in thin films form. However, KxNa1-xNbO3 thin films often suffer from a high leakage current. This is assumed to be mainly attributed to the high volatility of the alkaline components at high temperatures, but also interface effects have to be regarded. Pulsed laser deposition (PLD) represents a suitable method for the epitaxial growth of K0.5Na0.5NbO3 films. In this study the impact of strain, film thickness and bottom electrode on vertical electric behaviour of epitaxially grown K0.5Na0.5NbO3 films is investigated. For this purpose, K0.5Na0.5NbO3 films were grown on SrRuO3 and La0.67Sr0.33MnO3 covered SrTiO3 and DyScO3 substrates as well as directly on SrTiO3:Nb substrates with a film thickness between 20 and 200 nm. While for small film thicknesses Ohmic charge transport is observed in I-V-measurements, the charge transport mechanism changes to pronounced Schottky like behaviour at thicker films. This transition is investigated in more detail by comparing the measured I-V curves with calculated ones for different mechanisms of current flow. Furthermore, we find a strong correlation between the lattice strain in the films and the kind of charge transport mechanism.

DS 27.8 Wed 18:00 POT 81

Tuning the composition properties of SrTiO3 thin films grown by metal-organic vapor phase epitaxy (MOVPE) — •Aykut Baki, Julian Stöver, Toni Markurt, Carsten Richter, Klaus Irmscher, Martin Albrecht, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2 12489 Berlin

SrTiO3 represents a prototype cubic perovskite and has several of interesting physical properties as for instance a high dielectric constant at room temperature and resistive switching behavior. MOVPE is employed as deposition method since it provides film growth close to the thermodynamic equilibrium and thus stoichiometric, defect-poor thin films with smooth surfaces and interfaces. In this study, epitaxial SrTiO3 films were successfully grown on 0.5 wt.% Nb-doped SrTiO3 substrates by using the metal-organic precursors Sr(tmdh)2-tetraglyme and Ti(iso-propoxid)2(tmdh)2 solved in dry toluene. It has been shown that the phase formation of phase-pure SrTiO3 is achieved by adjusting the substrate temperature to a range of 675 °C < TC < 725 °C. By varying the Sr/Ti ratio in the gas phase, the cation ratio in the SrTiO3 thin films has been precisely controlled. The structural quality of the grown films has been proved by high-resolution x-ray diffraction, atomic force microscopy and transmission electron microscopy. The insulating films have been tested for their dielectric properties by a Pt/SrTiO3/SrTiO3:Nb test-structure for temperatures between 20 K and 300 K. IV-curves have shown strong forming-less resistive switching.

DS 28: Poster: Thin Film Properties: Structure, Morphology and Composition

Time: Wednesday 15:00–18:00 Location: P1A

DS 28.1 Wed 15:00 P1A

Long-time stability of swift-heavy ion irradiated $LiNbO_3$ — •Veronica Lopez Marcos[1], Elke Wendler[1], Liang-Ling Wang[1,2], Alma Dauletbekova[3], Maxim Zdorovets[3], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Germany — [2]School of Physics and Technology, University of Jinan, P. R. China — [3]L. N. Gumilyov Eurasian National University, Nur-Sultan, Kazakhstan

Lithium niobate ($LiNbO_3$) has been a material of interest in optics for many years. For the production of photonic devices, ion-beam induced amorphisation can be applied, which is connected with a reduced refractive index. In order to satisfy optical application requirements, thick layers of amorphous material may be needed, which can be achieved by implantation of swift heavy ions. However, the long-term stability of the amorphous structure must be guaranteed, which is investigated in this presentation. $LiNbO_3$ samples were irradiated with 66 MeV Xe-ions at ion fluences from 5×10^{10} to 3×10^{13} cm^{-2}. Later the samples were analyzed with Rutherford backscattering spectrometry in channeling mode using 1.4 MeV He-ions. It was found that the fluence-dependent increase of damage is well represented by the direct impact model. The obtained radius of the amorphous tracks produced by individual ions is in agreement with previous results which were measured right after ion irradiation. This indicates that no annealing of amorphous tracks in a crystalline surrounding occurred. In order to understand the damage structure obtained when the tracks overlap forming a complete amorphous layer, further studies are in progress.

DS 28.2 Wed 15:00 P1A

Characterization of photochromic diarylethene films produced via spin-coating — •Viktor Udachin[1], Sven Nagorny[2], Sebastian Dahle[1], Jörg Adams[3], Andreas Schmidt[2], and Wolfgang Maus-Friedrichs[1] — [1]TU Clausthal, Institut für Energieforschung und Physikalische Technologien, Deutschland — [2]TU Clausthal, Institut für Organische Chemie — [3]TU Clausthal, Institut für Physikalische Chemie

Thin photochromic films that can reversibly change physico-chemical properties under suitable electromagnetic radiation have received considerable attention. Such functional coatings are crucial in development of novel optical imaging and lithography applications using photochromism [1, 2]. A promising photochromic substance is 4,4"-(perfluorocyclopent-1-ene-1,2-diyl)bis(5,5'-dimethyl-2,2'-bithiophene) (BTE-1) due to its comparatively high thermal- and photo-stability [2]. However, specifications of a spin-coating procedure to obtain homogeneous BTE-1 films with different optical properties are not well defined. In this study, we investigated the behaviour of BTE-1 during spin-coating and determined a set of parameters for the production of defect-free BTE1/PMMA coatings with different thicknesses. The films were produced on quartz substrates by changing spin-coating conditions and properties of solutions. The optical parameters, morphology and thickness of the films as well as the structure of the dye were studied via spectroscopic and microscopic techniques. [1] Kowarsch R. et al. Optics express 26.5 (2018): 5327-5341. [2] Andrew T. L., Tsai H. Y., Menon R. Science 324.5929 (2009): 917-921.

DS 28.3 Wed 15:00 P1A

Shaping silver nanoparticles using low energy ion irradiation — •Shiva Choupanian[1], Alessandro Nagel[2], Claudia Pacholski[2], and Carsten Ronning[1] — [1]Institute for Solid State Physics, Friedrich Schiller University Jena, Germany — [2]Institute of Chemistry, University of Potsdam, Germany

Ion irradiation of surfaces always comes up with other effects such as sputtering or/and ion beam mixing. When nanoparticles are irradiated with ions having an ion range comparable to the size of the object, strong deviation from the behavior of surfaces occurs. In this work, the morphology changes of silver nanoparticles on top of silicon substrates irradiated with Ga^+ ions with energies ranging from 1 to 30 keV were investigated. For higher energies, the morphology change of the nanoparticles occurs dominantly due to enhanced sputtering. However, by decreasing the energy to 8 and 5 keV, a combination of sputtering, ion beam mixing and Ostwald ripening results in the reforming of new particles on top of the surface.

DS 28.4 Wed 15:00 P1A

XPS characterization of ZnO thin films prepared by TALD — •Christoph Janowitz[1], Ali Mahmoodinezhad[1], Franziska Naumann[2], Paul Plate[2], Hassan Gargouri[2], Karsten Henkel[1], and Jan Ingo Flege[1] — [1]Brandenburg University of Technology Cottbus-Senftenberg, K.-Zuse-Str. 1, 03046 Cottbus, Germany — [2]SENTECH Instruments GmbH, Schwarzschildstraße 2, 12489 Berlin, Germany

Among the transparent conducting oxides (TCO's) like SnO_2 and In_2O_3 respectively In_2O_3:Sn (ITO), zinc oxide (ZnO) with comparable electronic and optical properties has attracted interest as an alternative due to its low cost, non-toxicity and high durability. Advances in the production of high quality films of ZnO, foster the realization of TCO based devices in optoelectronics and photovoltaics. Several approaches have been pursued for the deposition of ZnO films in which thermal atomic layer deposition (TALD) facilitates low temperature layer by layer growth for high-quality thin films. Zinc oxide films were deposited on Si (100) substrates using diethyl zinc (DEZn) as a zinc precursor and H_2O as an oxidizing co-reactant within a temperature window of 80 °C to 200 °C. The chemical composition and bonding states of the films were quantitatively determined using X-ray photoelectron spectroscopy (XPS) by decomposition of Zn2p and O1s core-level spectra. The films exhibited only a slight deviation from ideal stoichiometry with a small excess of oxygen. Also the carbon contamination dependence on the growth temperature was studied. The lowest carbon concentration was found for the sample grown at 150 °C.

DS 28.5 Wed 15:00 P1A

2D Extended crystalline films for organic electronics applications — •Fabian Streller, Tim Hawly, and Rainer Fink — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg

Excelling in applications where large area coverage, low cost and flexibility are limiting factors of device fabrication, organic semiconductors are of high interest as alternative functional layers in modern electronic devices. While well-established preparation methods for organic thin films such as physical vapor deposition (PVD) offer good process control via parameters, such as deposition rate, they suffer from intrinsic limitations, namely the formation of polycrystalline layers, leading to charge trapping at grain boundaries and hence, reduced charge carrier mobilities. Herein, we report on the formation of highly oriented, long range-ordered thin films created in a novel approach via surfactant assisted self-assembly at the liquid-liquid interface.[1] Thin films with thicknesses of only few monolayers crystallized out of solution, utilizing a surfactant-modified water surface as a substrate. Thus prepared film were characterized by microscopic (AFM, SAED) and spectroscopic (NEXAFS, STXM) methods. To further investigate their suitability in organic electronics (OFETs, OLEDs), charge transfer characteristics were measured, exceeding those of reference devices by at least an order of magnitude.

[1] Q. Wang, F. Yang, Y. Zhang, M. Chen, X. Zhang, S. Lei, R. Li, W. Hu J Am Chem Soc. 2018, 140, 5339-5342

DS 28.6 Wed 15:00 P1A

Light element analysis using an external proton beam — •Felix Junge[1], Masahiro Saito[1,3], Kim Holm[1,2], Felipe Lipp Bregolin[1], and Hans Hofsäss[1] — [1]II. Institute of Physics, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [2]Institut für Physik, 06120 Halle, Germany — [3]Toray Research Center Inc., 3-3-7, Sonoyama, Otsu, Shiga 520-0842, Japan

In this work, we describe the new setup for light element depth profiling using a 2.7 MeV external proton beam and helium gas atmospheric pressure conditions. This setup is used to simultaneously perform backscattering spectrometry (BS) and H-H coincidence elastic recoil detection analysis (C-ERDA) in transmission. The beam is extracted through a 170 nm diamond membrane of 1 mm^2 size. Polyamide and Mylar foils were used as reference samples. In addition, thin titanium layers were deposited on 100 nm to 500 nm thick Si_3N_4 membranes by magnetron sputtering and loaded with hydrogen using an inductively coupled plasma. H concentration profiles were investigated as a function of film preparation and plasma loading conditions. Furthermore, thin amorphous carbon layers with hydrogen content were produced by magnetron sputter deposition and examined with simultaneous BS and C-ERDA measurements. In order to investigate the possibility of detecting all light elements, samples of lithium manganese oxide were examined and the lithium was measured by NRA. The aim of our research is the development of an efficient method for the quantitative analysis and depth profiling of all light elements of a sample.

DS 28.7 Wed 15:00 P1A

GTSAXS measurements on resistively switching strontium titanate thin film structures — •Richard Valenta, Kilian Wilden, Christoph Boehnke, and Uwe Klemradt — 2. Physikalisches Institut, RWTH Aachen, Deutschland

We present an application of a novel variant of small angle x-ray scattering (Granzing incidence transmission small angle x-ray scattering (GTSAXS)) for structural analysis of resistively switching thin oxide films. Resistive Random Access Memory is a promising candidate for novel data storage techniques. Our samples consist of a thin strontium titanate layer sandwiched between a bottom electrode and a structured top electrode. By means of voltage pulses the devices can be switched reversely between different resistive states distinguished by creation and rupture of conductive filaments. Using GTSAXS we were able to detect a strong signal sensitive to the different resistive states which can be related to the shape of the filaments.

DS 28.8 Wed 15:00 P1A

The new Neutron Depth Profiling Instrument N4DP at the FRM2 — •Lukas Werner[1], Markus Trunk[1], Roman Gernhäuser[1], Ralph Gilles[2], Bastian Märkisch[1], and Zsolt Revay[2] — [1]Technische Universität München — [2]Heinz Maier-Leibnitz Zentrum

Neutron Depth Profiling (NDP) is a non-destructive nuclear analytical technique. It uses charged particles produced in neutron capture reactions (for example the neutron capture on ^{6}Li) to map isotope depth distributions in thin film samples. At the Forschungsneutronenquelle München 2 (FRM2) the new Neutron Depth Profiling instrument N4DP has been set up. The high neutron flux available at the experimental site allows for ex-situ as well as for *operando* studies of thin film samples (e.g. battery anodes during cycling). We will present the capabilities of the instrument alongside several application examples.

DS 28.9 Wed 15:00 P1A

Electron beam induced defect formation and evolution in single-layer WSe_2 — •Robert Leiter, Yueliang Li, and Ute Kaiser — Electron Microscopy Group of Materials Science, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany

Lattice defects in two-dimensional TMD monolayers, such as tungsten diselenide (WSe_2) can alter the electronic properties of the material [1]. Artificially creating such defects by means of an electron beam may be used to tailor the structure and properties of these monolayers for use in future devices [2].

Here, we use the C_c/C_s - corrected SALVE (Sub Ångström Low Voltage Electron microscopy) instrument to observe the dynamics of the formation and evolution of defects in WSe_2 atom by atom [3]. Single point defects are highly mobile and accumulate fast to more extended defects. With continued electron beam irradiation, inversion domains form, which contain several types of mirror twin boundaries (MTBs), previously reported to possess interesting electrical and magnetic properties. We also observe MTBs that were previously unreported for tungsten diselenide as well as a completely new type of boundary, not reported in any TMD so far. We show that with further increased electron dose, highly defective W-rich regions within the WSe_2 matrix form, paving interesting ways towards device engineering.

[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 28.10 Wed 15:00 P1A

Electron-beam-stimulated structure evolution of single-layer $MoTe_2$: From point to extended defects — •Janis Köster[1], Tibor Lehnert[1], Mahdi Ghorbani-Asl[2], Zhongbo Lee[1], Arkady Krasheninnikov[2], 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

The SALVE instrument is equipped with a Cc/Cs-corrector and operates between 20-80kV at atomic resolution. It enables the investigation of electron-beam-stimulated structural transformations in 2D materials on an atomic level. Here, we report the electron-beam-induced atom-by-atom evolution of single Te vacancies and Te divacancies in single-layer 2H-$MoTe_2$. At 40kV electron accelerating voltage, defect creation due to elastic interaction can be excluded because of the high mass of Te and Mo, and the observed defects originate from more complex interactions as a combination of inelastic and elastic events. We found different types of tetravacancies and trefoil-like defect structures as well as line defects in zigzag direction. Additionally, electron-beam-driven dynamics of defects were observed and their kinetic pathways were proven with DFT calculations. Our results may allow one-dimensional magnetic quantum systems in single-layer 2H-$MoTe_2$, by creating locally metallic quantum dots consisting of T' phase.

DS 28.11 Wed 15:00 P1A

Benefits of Ion-beam-assisted Sputtering on Chalcogenides — •Kai Scheuvens[1], Peter Kerres[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University — [2]JARA-FIT, RWTH Aachen University

Chalcogenide phase change materials (PCM) have been of great interest for research as well as application in fast switching data storages. Our sputter chamber, which is part of an UHV cluster, allows producing high quality textured thin films with a broad range of deposition parameters while keeping the oxygen contamination at a minimum. However, due to the chamber design, the fabrication of dense amorphous layers has been proven difficult. XRR Measurements on amorphous thin films show roughly 10% less density compared to other sputtered films of the same material, hinting at voids in the thin film. The formation of voids can be suppressed by applying additional energy to the film during deposition in the form of an ion beam. The influence of this ion beam assisted deposition (IBAD), specifically in terms of film density and stoichiometry, will be investigated in this study. Samples with varying ion fluxes will be produced and characterized via XRD, XRR, XPS and AFM.

DS 28.12 Wed 15:00 P1A

Interface effects in the electronic structure of chalcogenide heterostructures — •Peter Kerres[1], Matthias Dück[1], Kai Scheuvens[1], and Matthias Wuttig[1,2] — [1]1st Institute of Physics "new Materials", RWTH Aachen University, 52066 Aachen, Germany — [2]JARA-FIT, RWTH Aachen University, Germany

While thin film devices containing homogenous films of GeSbTe based phase change materials (PCM) have already found their way into applications, heterostructure applications of phase change materials, i.e. chalcogenide superlattices are still topic of ongoing research. In the heterostructures, the focus of study lies in the interface region between the two constituents. In this study, we focus on the GeTe/Sb_2Te_3 Interface and employ X-ray photoelectron spectroscopy (XPS) to find differences in the electronic structure of the heterostructure compared to single films of GeTe, Sb_2Te_3 and an alloyed GeSbTe compound. Several thin film stacks of textured crystalline films were prepared with heated sputter deposition in an UHV cluster and afterwards transferred to the analysis chamber for in-situ XPS measurements. Angle dependent core level spectroscopy (ARXPS) is employed to extract depth dependent data and attribute parts of the spectra to interface effects. The structure of the thin films is additionally verified with X-ray diffraction (XRD) and reflectometry (XRR) measurements.

DS 28.13 Wed 15:00 P1A

Investigation of in-plane texture of GeTe thin films — Marc Pohlmann[1], Marvin Kaminski[1], •Maria Häser[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen Germany — [2]JARAFIT Institute Green-IT, RWTH Aachen University and Forschungszentrum Jülich, 52056 Aachen, Germany

Chalcogenide-based Phase Change Materials (PCM) are a prominent candidate for energy efficient memory devices. This material class shows a strong difference in its electrical and optical properties between the amorphous and crystalline state. To understand the crystalline state in thin film devices the preparation of highly textured films for structural characterization is crucial. In this study, Molecular beam epitaxy is employed to grow GeTe thin films on two different Si(111) surfaces: A 7x7 Reconstruction and a R30°-$\sqrt{3} \times \sqrt{3}$-Sb-termination. Using X-Ray Diffraction methods (Θ-2Θ-Scans, Reciprocal space maps and Φ-Scans) two very different in-plane textures for the two surfaces were investigated. Additionally, a simulation of the mismatch between the 7x7 reconstructed Si(111) surface and thin film was performed and compared to the XRD results.

DS 28.14 Wed 15:00 P1A

Ultrathin $(SrO)_2$ buffer layer actuates strain relaxation in $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3(100)$ — •Vitaly Bruchmann-Bamberg[1], Alexandr Belenchuk[2], Yury Khaydukov[3,4], Vladimir Roddatis[5], and Vasily Moshnyaga[1] — [1]I. Physik. Inst., G.-A.-Universität Göttingen, Germany — [2]IIEN, Academy of Sciences of Moldova, Kishinev, Republic of Moldova — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany — [4]Max Planck Society Outstation at the Heinz Maier-Leibnitz Zentrum, Garching, Germany — [5]GFZ German Research Centre for Geosciences, Potsdam, Germany

Strain and oxygen octahedral distortions imposed by the substrate play a crucial role in epitaxially grown perovskites, e.g. they strongly affect electrical transport and magnetic properties of the double exchange manganite $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) films. Instead of changing the substrate, a buffer layer can also be used to structurally decouple the film from the substrate. We report on the in-plane strain relaxation of an LSMO film grown on a $(SrO)_2$ buffered $SrTiO_3$(100). The buffer layer manifests itself as the Ruddlesden-Popper defect at the interface which disrupts the integrity of the octahedral network imposed by the epitaxy. Strain relaxation as well as the structural decoupling of perovskites through a rock-salt interface, directly visualized by TEM, significantly improves electric and magnetic properties of LSMO (e.g. the Curie and metal-insulator transition temperatures were increased by 30 K). The financial support from DFG via the SFB 1073 (TP A02) and the FRM II at the MLZ Garching are acknowledged.

DS 28.15 Wed 15:00 P1A

Investigation and Deposition of Methylammonium Lead Iodide Thin Films for Perovskite Solar Cell — •Young Un Jin[1], Niels Benson[2], and Doru C. Lupascu[1] — [1]Institut für Materialwissenschaft, Universität Duisburg-Essen und Center for Nanointegration Duisburg-Essen (CENIDE) — [2]Institut für Nanostrukturtechnik, Universität Duisburg-Essen und Center for Nanointegration Duisburg-Essen (CENIDE)

The organic-inorganic lead halide perovskites have been getting the limelight due to their excellent performance in photovoltaic devices which contain charge transport and hole transfer materials. Recently, methylammonium lead iodide (CH3NH3PbI3, MAPI) light harvester has contributed to be recorded in the highest power conversion efficiency, over 23% of perovskite solar cell by NREL. A thin film of MAPI is demonstrated that it has broad light absorption, high carrier mobility and leads to be therefore appropriate to engineering of direct bandgap structure of interlayers in a photovoltaic device expected.

In this study, we focus on a progressive method to deposit a clean MAPI thin film for the surface quality and its material properties to figure out the key how these properties affect charge transport and the relationship with its defect density. On the overall proeprties to understand the fundamental physical properties and their influence we characterize the morphology of the surface and local defect densities in MAPI and investigate how morphological problems are associated with charge mobility and what defects can impact on the electrical and optical features.

DS 28.16 Wed 15:00 P1A

Comparison of surface preparation techniques for topological materials — AI Hamodi[1], T Hökelek[1], Yaser Hamodi[2], O. Abdulkareem[3], •Nami Nakamori[4], Omar Isam[2], N.Basheer Mahmood[5], Karam Naji[6], Ward Sheiko[7], and Ali Jihad[8] — [1]1Hacettepe University, Ankara, Turkey — [2]2Minstry of higher education and scientific research, Baghdad, Iraq — [3]3 Central Piedmont Community College, Texas, USA — [4]4Shanghai Institute of Ceramics, China — [5]5Ministry of education, Baghdad, Iraq — [6]6Lafargeholcim Company, France — [7]7Siemens Company, Oman — [8]8Thermoplastics company GmbH, Germany

The surface state of this type of material are heavily oxide at atmosphere pressure, to avoid the oxidation, grown of capping layer (Te or Se) is necessary directly after fowh of the films in ultra-high vacuum. Surface treatment can be classified in to i) Sputtering and annealing method which is really powerful technique for all type of materials ii) Top boost method, which is work only on some of these Topological material. Here we shows x-ray photoemission (XPS), low energy electron diffraction (LEED) and Angle-resolved photoemission spectroscopy (ARPES) results in detailed that prove our samples getting fresh surface after treatment. Additionally, we did overview surface treatment measurements for non-capped materials.

DS 28.17 Wed 15:00 P1A

Functionalization of Metal Oxid Surfaces with Porphyrins — •Klaus Götz[1,2], Annemarie Prihoda[1,2], and Tobias Unruh[1,2] — [1]Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen — [2]Interdisziplinäres Zentrum für Nanostrukturierte Filme, Universität Erlangen-Nürnberg, Cauerstr. 3, 91058 Erlangen

Porphyrins are widely studied for their use as catalysts and in dye sensitized solar cells. In these systems the porphyrins are bound to metal oxide surfaces as a functionalizing layer.

We study the binding mechanism in the porphyrin - metal oxide interface on TiO_2 and Co_3O_4. Special emphasis of our work is focused on the exchange process of organic stabilizing molecules with porphyrins.

One method is the combination of small angle x-ray and neutron scattering (SAXS and SANS) experiments. These are well suited to study core/shell systems. X-rays interact mainly with electrons and therefore SAXS yields information about the inorganic core of the nanoparticles. Neutrons on the other hand are very sensitive to hydrogen and therefore SANS is well suited to get information about the organic stabilizer shell.

Additionally, X-ray reflectivity (XRR) measurements can be used to study layered systems on flat substrates. This offers the possibility to study the exchange of oleic acid with porphyrins on TiO_2 Wafers as a test system.

The poster will show the complementary methods, focusing on the XRR measurements.

DS 28.18 Wed 15:00 P1A

Miniaturization of patterns formed in graded thin elastic film — •Sunita Singh[1] and Jayati Sarkar[2] — [1]Indian Institute of technology, Delhi,India — [2]Indian Institute of technology, Delhi,India

We study the instability and morphology of a thin incompressible, inhomogeneous elastic soft film, whose shear modulus is exponential function or arbitrary function of film thickness. An LSA (linear stability analysis) has been done to obtain the minimum stress or force required to perturb the top surface of the film. In our study, we obtained the smaller length scale features can be formed at the interface in these anisotropic (non-homogeneous) materials where the anisotropy exists only in the normal direction. The present work constituted the range of length scale of instability is $0.3h<\lambda<2.96$, lower critical stiffness from LSA and total energy minimization, to look out the evolved morphology with high aspect ratio at the interface of film and contactor. The similar length scale of instability can be obtained using different techniques like patterned substrates and bilayers where it was possible to decrease the length scale by about an order of magnitude than those formed in simple elastic thin films because of antagonistic energies (elastic and interaction) present. These techniques are also cost-effective than the existing techniques of lithography suitable for hard materials. The LSA gives a 4th order ordinary differential equation, which cannot be solved analytically, so we discretized it using finite difference method with 2nd order accuracy throughout the process. The studies involved numerical techniques for energy minimization, and also finite element schemes to tackle non-linearities.

DS 29: Poster: 2D Materials and their Heterostructures

Time: Wednesday 15:00–18:00 Location: P1A

DS 29.1 Wed 15:00 P1A

On the detection of hydrogenated cyclo[18]carbon by a graphene sheet — •Dominguez Gutierrez Francisco Javier[1], Martinez-Flores Cesar[2], Krstic Predrag[3], and Cabrera-Trujillo Remigio[4] — [1]Max-Planck-Institut für Plasmaphysik, Boltzmannstrasse 2, 85748 Garching, Germany — [2]Departamento de Quimica, Division de Ciencias Basicas e Ingenieria, Universidad Autonoma Metropolitana-Iztapalapa, Mexico City, Mexico — [3]Institute for Advanced Computational Science, Stony Brook University, Stony Brook, NY 11749, USA — [4]Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca, Mexico

In this work, we carry out a theoretical and computational study of the hydrogenated cyclo[18]carbon molecule adsorption by a graphene sheet. We utilize the self-consistent-charge density-functional tight-binding method and the electron-nuclear-dynamics approach to model the hydrogenation of a C18 by atomic and molecular hydrogen irradiation in an impact energy range of 0.5*25 eV. Quantum Classical Molecular dynamics simulations are performed to compute the probability of C18H molecules formation as a function of the impact energy. The carbon ring is previously thermalized to 5 and 300 K, which is deformed by the hydrogen bound after hydrogen irradiation at energies below 5 eV. Cx fragmentation rates cases after collision are also reported. Therefore, we investigate the adsorption rates of pristine and C18H molecules by a graphene sheet at 1 and 2 eV to explore electronic properties of a 2D carbon material.

DS 29.2 Wed 15:00 P1A

Charge signals in non-local spin measurements and how to avoid them — Frank Volmer, •Anne Schmidt, Timo Bisswanger, Christoph Stampfer, and Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

For spin-sensitive measurements a non-local device geometry is often used to avoid spurious signals due to the flow of charges. Nevertheless, in the vast majority of reported spin valve and Hanle measurements a background signal is observed which is not related to spins. This is especially true for lock-in based measurement techniques in which a charge signal, which is shifted in phase by 90° in regard to the spin signal, can show amplitudes several orders of magnitude higher than the actual spin signal. We discuss the origin of such charge signals and present a custom-made current source which is able to minimize their effects on spin measurements. By using this current source we are able to increase both the sensitivity and the speed in the measurement of graphene-based spin-valve devices with ferromagnetic Co electrodes and MgO tunnel barriers.

DS 29.3 Wed 15:00 P1A

Spatially resolved Raman spectroscopy of twisted bilayer graphene — •Aaron Johannes Schäpers[1], Robin Joey Dolleman[1], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany

Twisted bilayer graphene (tBLG) is attracting increasing attention mainly because of the possibility to observe highly interesting many body phenomena such as interaction driven insulating states, ferromagnetism or even superconductivity. All this phenomena depend crucially on the twist angle between the individual graphene layers. Although the overall twist angle can be adjusted when assembling tBLG structures, it is known that the twist angle can vary over the sample and thus making the twist angle homogeneity a key parameter for device quality. In our work, we present spatially resolved confocal Raman spectroscopy measurements as a non-destructive and fast way to provide detailed information about the twist angle homogeneity in artificially made tBLG samples. In particular, we present detailed Raman maps on tBLG samples of 4°, 6° and 8° twist angle, allowing extracting information of the twist angle variation, with the long-term aim to improve this method so that it can be applied for twist angles from 1° to 12°. Moreover, we show some Raman measurements on graphene/hBN heterostructures with different twist angles.

DS 29.4 Wed 15:00 P1A

Tunable spin-orbit coupling in bilayer graphene / WSe2 Heterostructures — •Julia Amann[1], Tobias Völkl[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]NIMS, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

Heterostructures of graphene and TMDCs are predicted to show strong spin-orbit coupling due to proximity effects. The built-in electric field in bilayer graphene opens an orbital band gap. In addition, applying an external electric field leads to a controllable switching of the spin-orbit splitting.

By van der Waals pickup technique, we fabricated stacks of bilayer graphene and WSe2 on top. We used hBN as an insulator for a Cr/Au topgate. With this dual gated device, it is possible to change the applied transverse electric field and the charge carrier concentration independently. The magnetoconductivity curves show a sharp peak from weak antilocalization as a sign of spin-orbit coupling, which decreases with increasing temperature. Further, we observed a clear dependence of the peak height on the displacement field. This indicates a tunability of the induced spin-orbit coupling.

The peaks were fitted using theory by McCann / Fal'ko, and the resulting spin relaxation times show a giant anisotropy (ratio between the out-of-plane and in-plane time) of ~40. The estimated Rashba- and valley-Zeeman spin-orbit coupling strengths are on the order of 1meV and show a strong dependence on the applied electric field.

DS 29.5 Wed 15:00 P1A

spectroscopy of 2D-metals hosted by epitaxial graphene — •Lassaunière Margaux[1], Nisi Katharina[2], Subramanian Shruti[3], Lambers Hendrik[1], Sigger Florian[2], Tiede David[1], Robinson Joshua[3], and Wurstbauer Ursula[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany — [3]Department of Materials Science and Engineering, The Pennsylvania State University, Pennsylvania, USA

Two-dimensional metal films show distinctly different behaviour compared to their three-dimensional cousins. Metals are no van der Waals materials, however, 2D films can be prepared via confinement epitaxy by intercalating metals between epitaxial graphene and the hosting SiC crystal. Here, we explore the fascinating properties of D gallium and indium that include plasmonic resonances and superconducting behaviour by a combination of spectroscopic imaging ellipsometry, scanning probe methods and Raman spectroscopy.

DS 29.6 Wed 15:00 P1A

Impact of disorder and imperfections on the optical properties of TMDCs — •Hendrik Lambers[1], Julian Klein[2], Margaux Lassaunière[1], David O. Tiede[1], Katharina Nisi[2], Alexander Holleitner[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany

Interfacial imperfections induced by substrate and environment are known to potentially reduce the electronic and optical properties of semiconducting transition metal dichalcogenides [1]. On the other hand, deterministically induced point defects induced by focused ion beams are promising candidates to serve as quantum emitters with well controlled energies that can be positioned with nm resolution [2]. Here, we investigate signature of disorder, imperfections and lattice defects one the properties of semiconducting 2D materials by a combination of scanning probe methods, optical and Raman spectroscopy.

[1] J. Klein et al. arXiv:1905.01242 (2019). [2] J. Klein et al. Nature Commun. 10, 10, 2755 (2019).

DS 29.7 Wed 15:00 P1A

Electron and exciton phonon interaction in gate tunable TMDC layers — •David O. Tiede[1], Hendrik Lambers[1], Margaux Lassaunière[1], Katharina Nisi[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Germany — [2]Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany

Semiconducting transition metal dichalcogenides are a class of 2D materials of great interest because of their unique properties such as valley selective optical excitation or phonon-mediated multi-valley superconductivity. Phonons are a significant mechanism for valley depolarization at elevated temperatures. We observe a significant coupling between the long-range oscillating electric field induced by the longitudinal optical (LO) phonon. This Fröhlich exciton LO-phonon interaction [1] is suppressed by doping and correlates with a distinct increase of the degree of valley polarization of up to 60 % even at elevated temperatures of 220 K [1]. Higher-doping is expected to turn the system to superconducting phase at low temperatures [2]. We study the electrical and optical response of gate tunable TMDC flakes by combined spectroscopic imaging ellipsometer, charge transport and Raman measurements.

[1] B. Miller et al. Nature Commun. 10, 807 (2019). [2] E. Piatti et al. Nano Lett. 18, 8, 4821-4830 (2018).

DS 29.8 Wed 15:00 P1A

Scanning-probe-induced assembling of gold striations on mono- and bi-layered MoS2 on SiO2 — Felix Trillitzsch[1], Arkadiusz Janas[2], Alper Özogul[1], Christof Neumann[1], Antony George[1], Benedykt R. Jany[2], Franciszek Krok[2], Andrey Turchanin[1], and •Enrico Gnecco[1] — [1]Friedrich Schiller University Jena, Jena, Germany — [2]Jagiellonian University, Krakow, Poland

Single crystal Au clusters have been collectively manipulated on mono- and bi-layered MoS2 islands grown on SiO2 using AFM. On the monolayer the clusters tend to move in a direction corresponding to the zigzag alignment of the Mo and S atoms, and to assemble into long stripes parallel to the scan direction. A detailed observation based on SEM shows that within each stripe the clusters remain separated by gaps of few nm in width possibly caused by electrostatic repulsion and/or the substrate roughness. The stripes also proved to be thermally stable, preserving their superstructures up to 823 K. On the bilayer gold clusters are less prone to move and assemble. Our results suggest that the formation of nanostructures from collective manipulation of metal clusters can be guided by a properly chosen scan path in a rather straightforward way.

DS 29.9 Wed 15:00 P1A

Dry-transfer of graphene and h-BN heterostructures onto hydrogen-terminated diamond — •Vasilis Dergianlis, Martin Geller, Dennis Oing, Nicolas Wöhrl, and Axel Lorke — Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057, Duisburg, Germany

Graphene is a 2D carbon allotrope that exhibits exceptional mechanical strength and electron mobility. Due to its high electron conductivity, graphene is considered one of the best conductors and can be also used as gate electrode in transistor-type devices. A second very important carbon allotrope is diamond, which is a wide-bandgap semiconductor in its bulk form. Chemical vapor deposition (CVD) grown, hydrogen-terminated diamond exhibits surface conductivity by a two-dimensional hole-gas (2DHG).

In our work, we are combining the two aforementioned carbon allotropes. We implement a dry transfer method to position graphene onto diamond in a transistor-like structure, where h-BN serves as the gate-dielectric and graphene as a top gate.The sample consists of bulk CVD grown diamond, where the H-termination of the surface induces a 2DHG as a conductive surface layer [1]. Graphene and h-BN flakes are exfoliated and transferred from SiO_2 substrates onto the functionalized diamond surface. We show device characterization such as IV-characteristics and gate-dependent photoluminescence.

[1] Oing, D., et al. Diamond and Related Materials (2019): **107450**.

DS 29.10 Wed 15:00 P1A

Optical characterization and transport measurements on 2D Films with the squeezable nanojunction technique — •Alexander Fuchs, Matthias A. Popp, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Staudtstraße 7, 91058 Erlangen, Germany

We use the recently developed Squeezable Nanojunction techique [1] for simultaneous optical characterization and transport measurements on vertically contacted 2D-Materials. With our technique we can adjust the distance between two chip surfaces on the atomic scale. Due to the optically transparent nature of our silicon carbide substrate material the technique allows for investigations of the interplay between optical properties and electrical transport phenomena of distance controlled tunneling contacts between Graphene-Graphene, Graphene-MoS_2-Graphene, $\mathrm{MoS}_2 - \mathrm{MoS}_2$ ... structures. On this poster we present concepts and capabilities of our setup along with first results.

[1] M. A. Popp and H. B. Weber, Applied Physics Letters 115, 083108 (2019)

DS 30: Poster: Organic Thin Films and Thin Oxides

Time: Wednesday 15:00–18:00 Location: P1A

DS 30.1 Wed 15:00 P1A

Optical and excitonic properties of molecular aggregates on dielectric surfaces — Fulu Zheng[1], Xing Gao[1,2], •Sidharta Nayak[1], and Alexander Eisfeld[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Strasse 38, D-01187 Dresden, Germany — [2]Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109-1055, USA

Aggregates of fluorescent dye molecules on dielectric surfaces are of great interest for various technological applications. Due to strong interactions between the molecular transition dipoles, the excitonic eigenstates are coherently delocalized over many molecules [1]. These eigenstates and the corresponding optical transitions are determined by the molecular arrangement. We discuss the dependence of dark and bright states on the molecular arrangement and the spatial shape of the electromagnetic radiation used to probe the aggregate [2]. Strongly inhomogeneous fields can be generated via radiation from the apex of a metallic tip, which allows also scanning across the aggregate. Resulting spatially resolved spectra provide extensive information on the eigenenergies and wave functions [2, 3]. We also found that these delocalized eigenfunctions can be directly reconstructed from spatially resolved near field spectra using convolutional neural networks [3].

[1] A. Eisfeld, C. Marquardt, A. Paulheim, and M. Sokolowski, Phys. Rev. Lett. 119, 097402 (2017).

[2] X. Gao and A. Eisfeld, J. Phys. Chem. Lett. 9, 6003 (2018).

[3] F. Zheng, X. Gao and A. Eisfeld, Phys. Rev. Lett. 123, 163202 (2019).

DS 30.2 Wed 15:00 P1A

Exploring charge transfer in a Protoporphyrin IX - Semiconductor Model System — •Ken Lim, Felix Eckmann, and Martin Stutzmann — Walter Schottky Institut, Technische Universität München, 85748, Garching, Germany

Photocatalytic reduction of CO_2 into carbon neutral solar fuels that can be easily stored are to date typically achieved by either homogeneous (in solution) or heterogeneous (on metal and semiconductors) catalysis techniques. This work investigates a simple model system of semiconductor substrates covered with Protoporphyrin IX (PPIX) monolayers in order to explore the possibility of combining heterogeneous and homogeneous catalysis approaches, benefiting from the advantages of both. To that end, PPIX monolayers were deposited onto various semiconductor substrates via the Langmuir-Blodgett process. Monolayer morphology was studied using atomic force microscopy revealing closely packed molecules on the surface with a tilted orientation. Fluorescence spectroscopy was used to evaluate the model system whereby quenching of monolayer fluorescence due to charge transport to the substrate suggests a decrease in efficiency for a photocatalytically reducing device. Our data shows a dependence of fluorescence peak position and intensity on the excitation wavelength and underlying substrate, especially when exciting at the Soret Band for AlN and GaN. Additionally, experiments with AlGaN substrates demonstrate a positive correlation between substrate bandgap and PL intensity, indicating fluorescence quenching due to electron transfer between excited S2 states and conduction band of the semiconductor.

DS 30.3 Wed 15:00 P1A

Photoelectron spectroscopy on characterisation and phosphonic — •Adriana Salazar[1,2], Valentina Rohnacher[1,2], Markus Frericks[2,4], Wolfram Jaegermann[4], and Wolfgang

Kowalsky[1,2,3] — [1]Kirchhoff Institute for Physics, Uni Heidelberg, Germany — [2]InnovationLab, Heidelberg, Germany — [3]Institute for High-Frequency Technology, TU Braunschweig, Germany — [4]Materials Science Department, TU Darmstadt, Germany

Hole and electron transport layers (HTL /ETL) are necessary for stable and efficient perovskite solar cells (PSCs). Tin Oxide (SnOx) is a promising candidate as ETL due to its suiting electron affinity which leads to an excellent interface with the perovskite absorber material. Further, SnOx owns a high electron mobility, high transmittance and high chemical stability, essential criteria for efficient PSCs.

In these studies, solution processed tin oxide thin films were investigated. Using photoelectron spectroscopy different states of the thin film preparation could be investigated. Here, this surface sensitive technique allows for a chemical analysis while also providing information about the electronic structure. To tune the work function and to reduce the surface reactivity, SnOx thin films were modified by self-assembled monolayers (SAMs) of 4'-(Dimethylamino)-3,5-difluoro-[1,1'-biphenyl]-4-yl)phosphonic acid (XFPA). Together with results from contact angle measurement, atomic force microscopy and infrared spectroscopy, a better understanding about the SAM formation and surface modification was achieved.

DS 30.4 Wed 15:00 P1A

Nanoscale Polarization-Resolved Surface Photovoltage of a Pleochroic Squaraine Thin Film — •Frank Balzer[1], Oliya S. Abdullaeva[2], Angelika Maderitsch[2], Matthias Schulz[3], Arne Lützen[3], and Manuela Schiek[2] — [1]University of Southern Denmark, Sønderborg, Denmark — [2]University of Oldenburg, Germany — [3]University of Bonn, Germany

Local polarized surface photovoltage (SPV) and UV-vis spectroscopy are used to characterize a squaraine:fullerene (SQIB:PCBM) photovoltaic layer blend, which has shown potential to act as neurostimulating platform. The molecular model squaraine donor material SQIB is known to crystallize into two polymorphs upon thermal annealing with distinct polycrystalline thin film texture. For the orthorhombic polymorph, the anisotropic optical response is dominated by the Davydov-split J-type absorption into an upper (UDC) and lower (LDC) Davydov component within the deep red. Kelvin probe force microscopy (KPFM) maps the differential SPV of the active layer on the nanoscale without complications by interfaces, which is spatially correlated with the pleochroic optical response of the thin film. The SPV shows a wavelength-dependent, bichromatic change upon rotating the polarization axis of the illuminating light. With that, subtler nanoscaled optoelectronic sensing platforms become possible.

DS 30.5 Wed 15:00 P1A

Analyzing the Influence of Doped Organic Semiconductor Interlayers on the Electronic Structure of Intrinsic Hole Transport Materials — •Markus Frericks[1,2], Christof Pflumm[3], Eric Mankel[1,2], Thomas Mayer[1], and Wolfram Jaegermann[1,2] — [1]Technische Universität Darmstadt, Darmstadt — [2]InnovationLab GmbH, Heidelberg — [3]Merck KGaA, Darmstadt

The electronic structure at the interfaces of layered electronic devices plays an important role in understanding and improving device properties. In organic light emitting diodes, often a doped layer is placed between the contact and the transport layer to improve the charge injection. While the interface towards the contact is widely studied, less focus is laid on the influence on the intrinsic transport layer. We examined layer systems of doped and undoped hole transport materials. To analyze the electronic structure of the organic semiconductors, photoelectron spectroscopy is used. The organic layers are stepwise deposited by thermal evaporation in an ultra-high vacuum system. In between each deposition step the sample is measured. This allows for the study of the energy level evolution with increasing distance from the interface. The rather difficult interpretation of these organic-organic interfaces is supported by computer modeling. It is found, that the Fermi level position in the intrinsic layer is strongly influenced by the doped layer below. It lies about 1 eV lower compared to a sample without doped layer.

DS 30.6 Wed 15:00 P1A

Sum-frequency generation vibrational spectroscopy of nHexadencanethiol on oxidised zinc — •Robert Rameker, Detlef Diesing, and Eckart Hasselbrink — Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen, Germany

Due to its interesting electronic properties, self-assembled organic monolayers are frequently investigated in semiconductor technology for the production of electrodes with tailor made electronic properties. Vibrational sum frequency spectroscopy (vSFS) is a powerful method for characterization of interfaces. From 2800 cm^{-1} to 3100 cm^{-1}, symmetric and antisymmetric vibrational modes of the methyl- and methylene groups were observed. Thermal and electrochemical methods were tried to make zinc oxide, which is a semiconductor with a band gap of 3.3 eV, from zinc by oxidation. A better vibronic signature of the adsorbed molecule is obtained for highly oxidised zinc substrates. X-ray photoelectron spectroscopy was used to quantify the coverage with organic molecules and to gain information about the binding between the organic molecules and the metal oxide surface. For characterisation, electrochemical impedance spectroscopy (EIS) is an important method to analyze anticorrosion effects in different electrolytes.

DS 30.7 Wed 15:00 P1A

Predicting Organic Thin-Film Structures with DFT and Machine Learning — •Fabio Calcinelli and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

The properties of a material depend on its structure, which for organic thin films often substantially differs from the bulk structure. A theoretical prediction of the most stable thin film structures through traditional, exhaustive first-principle studies is unfeasible due to the combinatorial explosion in the number of possible polymorphs.

The machine-learning based SAMPLE approach [1] can already circumvent this problem for monolayers, by using a few hundred DFT calculations to evaluate the energy of millions of polymorphs through Bayesian Linear Regression. It is our intention to extend the applicability of SAMPLE from monolayers to (meta)stable thin films.

As first step, we predict the best monolayers of a simple organic molecule on graphene, to verify SAMPLE's effectiveness in describing adsorption on organic substrates. Subsequently, we study thin film structures of pentacenequinone or -tetrone, for which experimental results are available. On this basis we develop a representation for intermolecular interactions in three dimensions and improve our methodologies for local optimization. With this functionality SAMPLE will provide valuable insight into the packing geometries of thin films and into the forces that drive their formation.

[1] Hörmann et al., Computer Physics Communications 244, 143-155, 2019

DS 30.8 Wed 15:00 P1A

Self-assembled monolayers of triptycene tripods — Fumitaka Ishiwari[1], Eric Sauter[2], Giulia Nascimbeni[3], Hiromu Tago[1], Yoshiaki Shoji[1], Shintaro Fujii[4], Manabu Kiguchi[4], Tomofumi Tada[1], Egbert Zojer[3], •Michael Zharnikov[2], and Takanori Fukushima[1] — [1]Laboratory for Chemistry and Life Science, Tokyo Institute of Technology, Yokohama 226-8503, Japan — [2]Applied Physical Chemistry, Heidelberg University, Heidelberg 69120, Germany — [3]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz 8010, Austria — [4]Department of Chemistry, Tokyo Institute of Technology, Meguro, Tokyo 152-8551, Japan

We designed 1,8,13-trimercaptomethyltriptycene (T1) and 1,8,13-trimercaptotriptycene (T2) as potential tripodal precursors for self-assembled monolayers (SAMs) and investigated their adsorption behavior on Au(111). Both SAMs adopt dense, nested hexagonal structures but differ in their adsorption configurations and structural uniformity. While the T2 SAM exhibits a low degree of order and noticeable deviation from the desired tripodal anchoring, all three anchoring groups of T1 are equally bonded to the surface as thiolates, resulting in an almost upright orientation of the benzene rings and large-area structural uniformity. These superior properties are attributed to the effect of conformationally flexible methylene linkers at the anchoring groups, absent in the case of T2. Since the triptycene framework can be functionalized by tail groups in various positions and with high degree of alignment, especially T1 appears as an ideal docking platform for complex and highly functional molecular films.

DS 30.9 Wed 15:00 P1A

A novel approach for fabrication of photochromic organic thin films via initiated Chemical Vapor Deposition (iCVD) — •Maximilian Heiko Burk[1], Stefan Schröder[1], Daniel Langbehn[2], Widukind Moormann[2], Thomas Strunskus[1], Stefan Rehders[1], Rainer Herges[2], and Franz Faupel[1] — [1]Christian-Albrechts University Kiel, Institute for Materials Science, Kaiserstr. 2, 24143 Kiel, Germany. — [2]Christian-Albrechts University Kiel, Otto-Diels-Institute for Organic Chemistry, Otto-Hahn-Platz 4, 24118 Kiel, Germany.

Initiated Chemical Vapor Deposition (iCVD) is a solvent-free, cost efficient technique to synthesize highly conformal organic thin films from the vapor phase. The underlying free radical polymerization can be specifically tuned by the deposition parameters and enables furthermore co-polymerization of manifold functional monomers.

In this work we demonstrate the first synthesis of photochromic organic thin films via iCVD deposition. The underlying concept is represented by sublimation of a solid photoswitchable styrenediazocine in a tailor-made steel unit and transportation into the reactor chamber via an inert carrier gas. The photochromic compound was co-polymerized with V3D3, a triple-functional cyclic compound to guarantee maximum rotational freedom of the azo-group after covalent bonding. Due to a high controllability of the uniform film formation, topography preservation and manifold choice of potential substrates it is possible to equip surfaces with photoswitchable properties in the nano-range without losing the characteristic properties of the material.

DS 30.10 Wed 15:00 P1A

Preparation and characterisation of spin-coated TiO2 thin films — •Anurag Pandey, Sandra Omoragbon, Lu He, Teresa Madeira, and Dietrich R.T. Zahn — Chemnitz University of Technology, Chemnitz, Germany

TiO2 thin films were synthesized by the sol-gel method using titanium tetraisopropoxide (TTIP) as a precursor under basic conditions to promote formation of thin nanoparticle films. After preparation, the solutions were dried and aged by stirring for 24 hours at room temperature. The thin films were deposited by the spin coating technique with 500/1000/2000/3000/4000 rpm for t=30 seconds on intrinsic, n-doped, and p-doped silicon substrates. The various spin-coated samples were annealed for 2h each at different temperatures of 200, 300, 400, 500, 600, 700, and 800°C.

The TiO2 thin films were characterised using mainly Raman and SEM for crystal phase determination, film thickness, surface and cross section homogeneity, and porosity. In this work we present and discuss the preliminary results obtained and conclude about the conditions that lead to the best photocatalytic performances of the prepared thin films.

DS 30.11 Wed 15:00 P1A

Preparation of thin TiO2 films by DC magnetron sputtering for photocatalytic applications — •Osadebamwen Sandra Omoragbon, Anurag Pandey, Lu He, Teresa I. Madeira, and Dietrich R. T. Zahn — Semiconductor Physics, Chemnitz University of Technology, Reichenhainer Str. 70, 09126,Chemnitz, Germany

Fossil fuels have been massively burnt in order to keep up to the augmenting energy demands of the world. This has triggered the ever-increasing carbon dioxide (CO2) emission. Photocatalytic reduction of CO2 into solar fuels and chemicals is a promising technology to contemporaneously curb the global warming and partially fulfill the energy requirements. Therefore, significant efforts are being put into the design and development of visible-responsive photocatalysts. Also TiO2 thin films are promising in this application even though they harvest light only in the ultraviolet range of the solar spectrum [1].

Here we report on preliminary studies of TiO2 thin films deposited on intrinsic, n-type and p-type silicon substrates by DC pulsed magnetron sputtering using a titanium metal target at room temperature and Ar and O2 as working gases. Thin films were deposited with different O2 gas flow rates (1, 3, 9, 12, 20 sccm) while keeping the Ar gas flow rate constant at 30 sccm. X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), and Raman Spectroscopy techniques were used to characterize the films. The main goal is to determine the conditions that lead to the best photocatalytic performance. [1] N. Shehzad, M. Tahir, K. Johari, T. Murugesan, A critical review on TiO2 based photocatalytic CO2, J. CO2 Util. 26 (2018) 98-122

DS 30.12 Wed 15:00 P1A

Magnetism and Phonon Transport in (La$_{0.6}$Pr$_{0.4}$)$_{0.7}$Ca$_{0.3}$MnO$_3$ Thin Films — •Karen P. Stroh, Vitaly Bruchmann-Bamberg, Daniel Metternich, Henning Ulrichs, and Vasily Moshnyaga — I. Physikalisches Institut, Georg-August-Universität Göttingen

Perovskite oxides represent an excellent example of correlated electron systems with strong coupling of electron, spin, and lattice degrees of freedom. They possess rich magnetic, electric, and structural phase diagrams. An example for this intriguing class of materials is the bandwidth-controlled and A-site-substituted manganite (La$_{1\text{-}y}$Pr$_y$)$_{1\text{-}x}$Ca$_x$MnO$_3$ (LPCMO). Heteroepitaxial LPCMO thin films were prepared by metalorganic aerosol deposition (MAD) on MgO(100) substrates and were investigated by various local and global techniques with a focus on the magnetic properties.

LPCMO is characterised by relatively strong electron-phonon coupling (EPC) and is well known as a classical colossal magnetoresistance (CMR) material. Not only magnetism but also thermal transport in manganites is substantially influenced by contributions of the lattice including Jahn-Teller distortions mediating EPC. This involves the question whether it may be used to manipulate thermal transport. Thermal conductivity in LPCMO films was studied by the 3ω technique and by means of transient thermal reflectance (TTR).

Financial support by the DFG via Project 399572199 and within the SFB 1073 (Project A02) is acknowledged.

DS 30.13 Wed 15:00 P1A

Multiscale modeling of VCM-based ReRAMs — •Nils Sommer[1], Kristof Lange[2], Soekki Son[1], Alexander Zurhelle[2], Rainer Waser[1,2], and Stephan Menzel[1] — [1]Peter Grünberg Institute (PGI-7), Forschungszentrum Jülich, Jülich, Germany — [2]Institute for Materials in Electrical Engineering II (IWE2), RWTH Aachen University, Aachen, Germany

Memristive elements enable the development of special, completely new hardware for neuromorphic systems. A promising class of memristive elements are redox-based resistive cells (ReRAMs), e.g. based on the valence change mechanism (VCM). In VCM cells, the primary switching mechanism is based on the movement of oxygen vacancies. However, the details of the switching process remain unclear. Our goal is to gain a deeper understanding of switching dynamics and limitations with a multiscale modeling approach. Using atomistic and continuous model simulations, we investigate the formation and dynamics of oxygen vacancies in the VCM cells as a function of the voltage, time, temperature and boundary effects such as oxygen exchange at the electrodes. Our results are the basis for physics based compact models that can be used for circuit designs.

DS 30.14 Wed 15:00 P1A

Emergence of a surface 2DEG in Anatase (001) thin films — •Marius Fuchs[1], Chiara Bigi[2,3], Alessandro Troglia[2,3], Pasquale Orgiani[2], Jun Jujii[2], Ivana Vobornik[2], Giancarlo Panaccione[2], Giorgio Rossi[2,3], Domenico Di Sante[1], and Giorgio Sangiovanni[1] — [1]Institut für Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [2]CNR-ION TASC laboratory, c/o Area Science Park - Basovizza, Strada Statale 14 km 163,5 - 34149 Trieste, Italy — [3]University of Milano, 20133 Milano, Italy

We report the emergence of a surface 2DEG in Anatase (001) thin films above a threshold thickness. DFT reveals the subsurface Ti dxy orbitals to nourish the 2DEG. The mechanism of formation is further analyzed by using Wannier functions. Additionally we investigate the phononic influence on the electronic dispersion.

DS 31: Poster: Layer Deposition and Layer Properties

Time: Wednesday 15:00–18:00 Location: P1A

DS 31.1 Wed 15:00 P1A

Influence of Stoichiometry on the properties of Mn$_2$Au thin films — •Daragh Mullarkey, Daniel Casey, and Igor V. Shvets — School of Physics, Trinity College Dublin, The University of Dublin, Dublin 2, Ireland

Mn$_2$Au is a bimetallic antiferromagnet with a Néel temperature of approximately 1500 K. Here, we deposit (110) Mn$_2$Au thin films onto Pt (111)/Al$_2$O$_3$ via molecular beam epitaxy. By varying the ratio of the Mn and Au atomic fluxes from separate Knudsen cells, precise control over the stoichiometry of the films can be obtained. We investigate how modifying the stoichiometry away from the ideal 2:1 Mn:Au ratio effects the crystallographic, electrical, and magnetic properties of the Mn_2Au thin films.

DS 31.2 Wed 15:00 P1A

Improvement of TiO_2 VO_2 multi-layers for application in thermochromic window-glazing — •Lukas Frommel, Martin Becker, Philip Klement, Florian Kuhl, Sebastian Benz, Jonas Hauptmann, Jörg Schörmann, and Sangam Chatterjee — Institute of Experimental Physics I and Center for Materials Research, Heinrich-Buff-Ring 16, Justus Liebig University Giessen, D-35392 Giessen, Germany

Thermochromic window glazing is a possible innovation to optimize the heat exchange in buildings. Vanadiumdioxid is a promising material for this application, because of a reversible insulator-to-metal transition at 68°C. To modify the characteristic temperature of this transition, a TiO_2 buffer layer can be used. While conventional preparation methods fail in terms of lateral upscaling, a new synthesis route for larger scales needs to be established.

Here, we prepare TiO_2 thin films by atomic layer deposition. Under variation of the process parameters, reactor temperature and precursor pulse times among others, different types and phases of TiO_2 are deposited and examined via X-Ray Reflectometry, Atomic Force Microscopy and Raman Spectroscopy. A VO_2 layer on top is prepared by rf-sputtering and the resulting multi-layer structure examined via UV-NIR Spectroscopy. The thickness and different structures of the TiO_2 buffer layer were found to significantly affect the switching properties of the VO_2.

DS 31.3 Wed 15:00 P1A

Compositionally Modulated $La_{1-x(t)}Sr_{x(t)}MnO_3$ Superlattices — •Yannik Sievers, Robert Gruhl, Vitaly Bruchmann-Bamberg, and Vasily Moshnyaga — Erstes Physikalisches Institut, Georg-August-Universität Göttingen

Bulk perovskite manganites $La_{1-x}Sr_xMnO_3$ (LSMO) possess a rich phase diagram, depending on the Sr-doping level, x. Usually, one examines only few special doping levels depending on the desired properties. Instead of a fixed doping level we studied LSMO films in a form of artificial lattices, consisting of layers with a different and alternating doping levels, yielding compositionally modulated $La_{1-x(t)}Sr_{x(t)}MnO_3$ superlattices with controllable doping level x(t) (x = t/d with t = [0,d]: time and d: transition-layer width). To grow such gradient lattices we further developed our metal-organic aerosol deposition (MAD), making possible the simultaneous usage of LMO and SMO precursor channels, which can be supplied by controllable feeding rates. The resulting artificial LSMO superlattices have been grown on $SrTiO_3(100)$ and characterized by AFM, XRD, XRR, SQUID, Raman-Spectroscopy as well as by in-situ ellipsometry. Financial support by DFG via SFB 1073 is acknowledged.

DS 31.4 Wed 15:00 P1A

Broadband antireflection coatings on polymethylmethacrylate prepared by Atomic Layer Deposition — •Lukas Gümbel, Philip Klement, Jörg Schörmann, and Sangam Chatterjee — Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Giessen, Germany

Transparent plastic optics are lighter than glass and easy to manufacture. They require surface functionalities such as antireflection and scratch-resistant coatings to enable their applications which is typically done by plasma-assisted processes that can damage the polymer substrate. Atomic Layer Deposition (ALD) offers precise thickness and composition control without thermally or plasma-stressing the underlying substrate.

Here we present broadband antireflection coatings on polymethylmethacrylate prepared by Atomic Layer Deposition. A thin Al_2O_3 film acting as adhesion layer is deposited from the trimethylaluminum-H_2O-process, and the processing parameters are optimized yielding a high GPC and ultra-smooth surfaces. Combining this with ALD-grown ZnO and SiO_2 facilitates antireflection coatings in the visible range that perfectly match precalculated antireflection designs. Our results enable precise conformal antireflection coatings of plastic optics.

DS 31.5 Wed 15:00 P1A

Exploring fragmentation processes in FXBID nanofabrication — •Andreas Späth[1], Kim Thomann[1], Benedikt Wolz[1], Kevin C. Prince[2], Robert Richter[2], Wolfgang Hieringer[3], and Rainer H. Fink[1] — [1]Physikalische Chemie II, FAU Erlangen-Nürnberg, Germany — [2]Elettra Sincrotrone Trieste, Basovizza, Italy — [3]Theoretische Chemie, FAU Erlangen-Nürnberg, Germany

Focused X-ray beam induced deposition (FXBID) is a novel technique for the additive fabrication of metallic nanostructures by illuminating metal organic precursor molecules with focused soft X-rays in a Fresnel zone plate based scanning transmission X-ray microscope (STXM) [1]. Fragmentation in FXBID is mainly caused by low-energy secondary electrons and, therefore, the fundamental processes of nanofabrication are very similar to such in electron beam induced deposition. However, FXBID provides tuning of deposition rate and potentially also fragment formation by variation of incident photon energy. For a detailed analysis of this aspect we have performed photon energy dependent mass spectrometry and secondary electron spectroscopy studies for several metal organic precursor molecules. The results are correlated with TD-DFT calculations of the molecular orbitals involved in soft X-ray absorption for a correlation of electron density localization and fragmentation. The project is funded by DFG grant SP 1775/1-1.

[1] A. Späth, Micromachines, 2019, 10, 834.

DS 31.6 Wed 15:00 P1A

Cesium-intercalated bulk $HfSe_2$ investigated by electron spectroscopy — •Jochen Simon, Martin Knupfer, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research, Dresden, Germany

We studied cesium-intercalated bulk $HfSe_2$ by combining electron energy loss spectroscopy and angle-resolved photoemission spectroscopy. The strong anisotropy, the band gap and the predicted electron mobilities make $HfSe_2$ a promising candidate for optical and electrical devices. Intercalation leads to a degree of disorder in the crystalline structure while superstructures emerge for higher doping levels. The change of the lattice parameters is less than 1% (in-plane) and 70% (out-of-plane), respectively. Loss spectra reveal features we consider to be charge carrier plasmons, in agreement with the semiconductor-to-metal transition indicated by angle-resolved photoemission spectroscopy. As expected for an ideal electron gas, the plasmon shows a quadratic momentum dispersion.

DS 31.7 Wed 15:00 P1A

Structure and Ferroelectricity in Strain-Stabilized Hexagonal TbMnO3 Thin Films — •Moritz Hirsbrunner[1], Rajesh Mandal[2], Daniel Steil[1], Karen Stroh[1], and Vasily Moshnyaga[1] — [1]Erstes Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077, Göttingen, Germany — [2]SRF, Department of Physics, Indian Institute of Science Education and Research, Pune, India-411008

Rare-earth-manganite-based multiferroic materials are of great interest because of their strong coupling of magnetic and electronic systems, resulting in cross-controlled magnetoelectric properties. Hexagonal TbMnO3 (h-TMO) films with room temperature ferroelectricity (FE) is of particular importance. Bulk TMO displays orthorhombic structure and exhibits FE with low polarization 0.06 μC/cm2 and ferromagnetism (FM) well below 100K. However, stabilization of hexagonal structure in TMO thin films by epitaxy strain was shown to result in a much larger room temperature polarization (8 μC/cm2). We optimized the growth of h-TMO thin films on YSZ(111) substrates by Metalorganic Aerosol Deposition (MAD) by varying the precursor ratio, substrate temperature, growth and cooling rate. X-ray diffraction (XRD) confirms the hexagonal structure of the films, showing a smooth surface with RMS ~0.3nm (AFM). Furthermore, optical spectroscopy and second harmonic generation (SHG) were measured to characterize the ferroelectricity of h-TbMnO3. The financial support of DFG via SFB1073 (A02, A06) is acknowledged.

DS 31.8 Wed 15:00 P1A

Strain Engineering of Antiferroelectric Thin Films — •Thorsten Schneider, Mahdad Mohammadi, Juliette Cardoletti, Maohua Zhang, Philipp Komissinskiy, and Lambert Alff — TU Darmstadt, Darmstadt, Germany

The demand for smaller and more efficient energy storage devices is ever-present in modern society. Within these, capacitors play an important role for short-time energy storage and conversion with high power density. However, to reduce the space consumption of these capacitors, the necessity for larger energy densities is of significant importance.

Antiferroelectric (AFE) Materials have the opportunity to overcome the problem of low energy density while maintaining a large power den-

sity due to a high polarization with no remnant polarization. Of the few known, lead-free AFE materials, $NaNbO_3$ offers a good opportunity to investigate the interplay between the polar and antipolar phase, since the energy barrier between these two phases is very small.
Here we present investigations of $NaNbO_3$ thin films. By utilizing epitaxial strain, a property closely linked with ferroelectricity, we manipulate the energy difference between the AFE and FE state in an attempt to stabilize the AFE double-hysteresis behaviour. As shown by X-Ray Diffraction measurements, the $NaNbO_3$ thin films grown on various perovskite single-crystals like $SrTiO_3$, LSAT and $DyScO_3$, are epitaxially strained. The AFE properties of the films are monitored using measurements of the polarization versus the electric field.

DS 31.9 Wed 15:00 P1A

Low-temperature characterization of ultra-strongly driven nanomembrane resonators — •Mengqi Fu, Fan Yang, and Elke Scheer — University of Konstanz, Konstanz, Germany

Ultra-strong nonlinear vibrations of nanoresonators with very high amplitude at room temperature recently have attracted broad interest[1,2]. However, the mechanism behind some of the observations (e.g. squeezing) cannot be derived from the existing theoretical models for strong nonlinearities and including thermal fluctuations.

To reduce the effects of thermal fluctuations of the environment and to elucidate other possible origins of these ultra-strong nonlinear effects, we developed a low-temperature (down to 4K) measurement system to detect flexural vibrations by using on-chip nanoelectrodes and the electromagnetic induction effect in a magnetic field. We characterize this novel detection scheme by studying the flexural vibrations of nanomembrane resonators from the linear to the ultra-strong nonlinear regime at variable temperature. The accuracy of the amplitude detection is 1 nm or better with high stability at all temperatures (4 K to 300 K). In addition, because the deflection signal is converted into high-frequency voltage signals rather than to the commonly used optical interference signal, the inductive scheme presented here is not subject to fundamental limitations imposed by the optical wavelength and is thus well-suited for measurements of the ultra-strong nonlinear regime with high deflection amplitudes.

References [1] F. Yang et al., Phys. Rev. Lett. 122, 154301 (2019). [2] J.S. Huber et al., [arXiv:1903.07601v2].

DS 32: Poster: Optical Analysis of Thin Films

Time: Wednesday 15:00–18:00 Location: P1A

DS 32.1 Wed 15:00 P1A

Revealing The Chemical Structures Of Silicon Nanoribbons On Ag(110) Via DFT And Raman Spectroscopy — •Alexander Ehm[1], Dmytro Solonenko[1], Jorge I. Cerda[2], Dietrich R. T. Zahn[1], and Patrick Vogt[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Instituto de Ciencia de Materiales de Madrid, ICMM-CSIC, Cantoblanco, 28049 Madrid, Spain

Silicon nanoribbons grown on Ag(110) exhibit a pentagonal Si structure along the missing row arrangement of the Ag surface [1]. Depending on the deposition temperature, nanoribbons can form a single- or a double-strand structure, which differs by the distance between the neighbouring chains. Even though double-strand nanoribbons have no bonds between the strands, the properties of the two single ribbons are influenced by their close proximity. In order to elucidate this interaction, we performed a combined study of single- and double-strand Si nanoribbons by Raman spectroscopy and density functional theory (DFT). The results show that nanoribbons exhibit a vibrational fingerprint distinct from 3D bulk Si or 2D silicene [2]. The vibrational signature is not only related to the pentagonal building block of nanoribbons, but also to their electronic properties, which are altered, when two Si nanoribbons are located in close proximity. This leads to a prominent Raman band around 380 cm^{-1}, a marker for the formation of double strand ribbons. The possible mechanisms and the origin of this band are discussed.

DS 32.2 Wed 15:00 P1A

Ultrafast pump-probe microscopy on MoSe2 — •Konrad Birkmeier[1,2], Lucas Lange[1], Edoardo Amarotti[1], and Achim Hartschuh[1] — [1]Department of Chemistry and CeNS, LMU Munich, Germany — [2]Toptica Photonics AG, Graefelfing, Germany

We investigate single and few layer MoSe2 by ultrafast pump-probe spectroscopy and microscopy giving insight to the decay dynamics in the 2D material. The excitation of different excitonic states by the pump pulse causes changes in the transient reflectivity and can be probed and spectrally resolved by broadband whitelight pulses rangig from the visible to the near infrared. By the subsequent use of ultra short, wavelength tunable probe pulses the decay dynamics of the excited states can be investigated further with a high signal to noise ratio. In combination with the high spatial resolution of confocal microscopy the carrier dynamics at boundaries, wrinkels and other inhomogeneities will be discussed.

DS 32.3 Wed 15:00 P1A

Transient Scattering Microscopy and Non-Linear Raman response of Single-Layer Graphene — •Lucas Lange, Veit Giegold, Richard Ciesielski, and Achim Hartschuh — Department of Chemistry and CeNS, LMU Munich, Germany

We investigate the ultrafast response of graphene using transient scattering and non-linear Raman microscopy. In general, high electronic temperatures reached for pulsed excitation cause a partial Pauli-blocking of optical transitions. This leads to reduced transient absorption and hence enhanced reflection. Importantly, the transient reflectivity signal detected at different time delay and energy detuning between pump and probe pulse features pronounced spatial inhomogenities in as prepared single-layer graphene. We discuss the decay dynamics of this transient response based on complementary Raman spectra. In addition, the hot electronic temperatures reached upon pulsed excitation are found to cause a partial Pauli-blocking of interfering quantum pathways contributing to resonant Raman scattering in graphene. As a consequence, the signal of the two dominant Raman bands G and 2D together with their ratio strongly depend on the laser intensity and result in a super-linear and sub-linear increase of the G band and 2D band intensity, respectively.

DS 32.4 Wed 15:00 P1A

Evaluation of thicknesses of polymer films on steel surfaces with spectroscopic ellipsometry — •Friedrich Bürger, Maria Sonnenberg, Lienhard Wegewitz, and Wolfgang Maus-Friedrichs — Clausthaler Zentrum für Materialtechnik, Technische Universität Clausthal, Leibnizstraße 9, 38678 Clausthal-Zellerfeld, Germany

In the production of polymeric foils, on the used steel surfaces a polymer residue builds up, that needs to be cleaned off after a certain film thickness. For this process it is important to have an idea of the films thickness remaining on these surfaces in situ. Here we evaluate if spectroscopic ellipsometry could be adapted for this purpose. Various thin polycarbonate (PC) films were therefore prepared by spin-coating. To change the film thickness in a different manner the samples were here treated with a dielectric barrier discharge (DBD) plasma. Afterwards measurements with an ellipsometer and a confocal laser scanning microscope (CLSM) were performed. This was repeated several times with different PC film thicknesses and plasma treatment times. Additionally, X-ray photoelectron spectroscopy was performed on different samples to detect possible change in composition of the films and the steel surfaces due to plasma treatment. As the thickness of the film measured by the CLSM decreased with increasing plasma treatment time, the measurements with the ellipsometer reflected this change. This indicates that spectroscopic ellipsometry could be adapted to evaluate the thickness of PC films in situ on steel surfaces when other methods are unavailable.

DS 32.5 Wed 15:00 P1A

Effect of lattice strain on the surface structure of epitaxial manganite thin films — •Leonard Schüler, Jonas Wawra, Sebastian Merten, and Vasily Moshnyaga — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Our recent study of the surface-enhanced Raman spectroscopy (SERS)

revealed that $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) thin films grown in a stress-free state on MgO(200) substrates possess an electron-enriched surface, that manifests itself by the appearance of strong Jahn-Teller stretching and antistretching modes in SERS spectra [1]. Here we were focusing on the effect of epitaxy strain on the surface structure of LSMO films, grown on $LaAlO_3$, $SrTiO_3$ and sapphire substrates by a metalorganic aerosol deposition (MAD) technique. Raman intensity of the substrate background has been reduced by optimizing the confocal setup of the spectrometer. The surface structure was then determined by comparing the conventional Raman spectra of films with their respective SERS spectra, obtained by coating the films with Au nanoparticles using the same MAD. Furthermore, the influence of the MAD surface modification on the SERS spectra has been investigated. Financial support of the DFG via SFB1073 is acknowledged.
[1] S. Merten et al. Phys. Rev. Mater. 3, 060401(R) (2019)

DS 32.6 Wed 15:00 P1A

IN-SITU INVESTIGATION OF ELECTROCHROMIC RADIATION PROCESSES IN TUNGSTEN TRIOXIDE THIN FILMS BY OPTICAL SPECTROSCOPY — •Alexander Strack[1], Simon Burkhardt[1,2] und Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Center for Materials Research(LaMa), Heinrich-Buff-Ring 16, 35392 Giessen

Smart-Windows with thin films of tungsten trioxide in the fenestration of buildings help to regulate heat transfer though windows and thus to reduce energy consumption for climatization.This approach is coast efficient and may contribute significantly to CO2 reduction in the atomsphere. For the best performance of the smart window it is essential to understand what happens in the tungsten film and how to optimize the coloration process. Different spectroscopic techniques are employed to investigate the electrochromic coloring process in thin tungsten films. Ramanspectroscopy reveals the differant crystalline phases of WO3 which occur during coloration. Simultaneous measuring the absorption and the current allows one to correlate the degree of coloration with the incorporated charge and with the crystalline phase of the material.

DS 32.7 Wed 15:00 P1A

Real-time pump-probe microscopy of single-shot laser thin film ablation — •Till Wachweger — Universität Bayreuth

The interaction of single ultrashort laser pulses with materials allows for tailored phase changes and precise microprocessing. Despite existing ultrafast instrumentations, insights into fast irreversible phenomena in inhomogeneous materials and at individual positions are severely limited due to the lack of real-time acquisition. We present an interferometric real-time pump-probe microscopy setup which is used to study the lift-off of a metallic thin film layer. A sub-200fs laser pulse induces the ablation, and the lift-off progress is monitored via high repetitive interferometry based on the time-stretch Dispersive Fourier Transformation.

DS 32.8 Wed 15:00 P1A

Hyperspectral and Time-Resolved IR Laser Polarimetry — •Christoph Kratz, Andreas Furchner, and Karsten Hinrichs — Leibniz-Institut für Analytische Wissenschaften -ISAS- e.V., Berlin, Germany

Beyond classical FT-IR and synchrotron IR spectroscopy, the analysis of composition, structure and heterogeneity of complex surfaces and thin films is significantly advanced by a new generation of IR polarimeters [1]. We developed a novel laser-based IR technique enabling time and spatially resolved 5D analytics by combining a tunable QC laser with a single-shot ellipsometer [2,3]. Specifications are 0.5 cm^{-1} spectral resolution, <125 μm spatial resolution, 20 μs temporal resolution for single wavelength and 100 ms for spectral investigations [2,3]. Large area mapping (50 x 50 mm^2) and time-resolved studies under ambient conditions [2], as well as coupling with humid or liquid flow cells for in-situ IR spectroscopy (e.g. IR nL microfluidics [4]) are possible. Presented examples are chemical and structural heterogeneity investigations of organic thin films, and the solid-liquid phase transition of a myristic acid film. Funding: EFRE 1.8/13, in cooperation with Sentech Instruments GmbH.

[1] K. Hinrichs et al, JVST B 37, 060801 (2019).
[2] A. Furchner et al., Optics Letters 44.19: 4893-4896 (2019).
[3] A. Furchner et al., Optics Letters 44.17: 4387-4390 (2019).
[4] C. Kratz et al., ACS Sensors, 3:299-303 (2018).

DS 32.9 Wed 15:00 P1A

Controlling the phase-change of $Ge_2Sb_2Te_5$ via ion beam doping — •Robin Schock, Martin Hafermann, Konstantin Ruffert, and Carsten Ronning — Institut of Solid State Pyhsics, Friedrich Schiller University Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The phase-change material $Ge_2Sb_2Te_5$ (GST) builds the basis for reconfigurable optical devices like rewritable data storage or switchable metasurfaces, because of its drastic differences in the electrical and optical properties accompanying the phase-change. In such devices switching between crystalline and amorphous states can be triggered by either electrical, thermal or optical external stimuli that exceeds a specific energy threshold. Although there is already a wide field of applications, a major flaw is the inability to tune the phase-change threshold for various applications. Doping of GST can be utilized to change the crystallization kinetics and enables the manipulation of the energy threshold. As doping during the growth process of GST films is limited, we used ion beam implantation for non-equilibrium doping, which enables us additional control of the lateral doping distribution. Thus, we implanted various ion species and doping concentrations into GST thin films and directly observed the phase-change via differential reflection measurements during heating of our samples. We show that ion beam doping is a powerful tool to tailor the phase-change temperature of GST over a broad temperature range.

DS 33: Poster: Thin Films: Applications, Transport and Phase Change Materials

Time: Wednesday 15:00–18:00 Location: P1A

DS 33.1 Wed 15:00 P1A

Towards a large-scale quantum simulator at room temperature — Philipp J. Vetter[1], Thomas Unden[1], Nikolas Tomek[1], Tamara Sumarac[2], Elana K. Urbach[2], Timo Weggler[1], •Maximilian G. Hirsch[1], Hideyuki Watanabe[3], Kohei M. Itoh[4], Boris Naydenov[5], Mikhail D. Lukin[2], Martin B. Plenio[6], and Fedor Jelezko[1] — [1]Institute for Quantum Optics and Center for Integrated Quantum Science and Technology, Universität Ulm — [2]Department of Physics, Harvard University — [3]Correlated Electronics Group, Electronics and Photonics Research Institute, National Institute of Advanced Industrial Science and Technology, Tsukuba — [4]Department of Applied Physics and Physico-Informatics, Faculty of Science and Technology, Keio University — [5]Helmholtz-Zentrum Berlin für Materialien und Energie — [6]Institute for Theoretical Physics and Center for Integrated Quantum Science and Technology, Universität Ulm

Quantum simulators enable the study of strongly-correlated many-body systems that may exhibit exotic phases, such as spin liquids and supersolids. We present our progress of creating a large-scale quantum simulator at room-temperature, which is based on the nitrogen vacancy center in diamond, coupled to surrounding nuclear spins. We demonstrate the fabrication of a 1 nm thin 13C layer in diamond which is polarized and coherently controlled by the NV center. 2D-Materials which offer a clearly identifiable symmetry and thickness are transferred onto the diamond surface. The nuclear spins within the transferred flake are sensed via the NV center aiming for full polarization.

DS 33.2 Wed 15:00 P1A

MoS2 as universal charge selective layer in Sb2S3 based TF solar cells — •Leonid Shupletsov[1,2], Pascal Büttner[1], Yuanyuan Cao[1], and Julien Bachmann[1,3] — [1]FAU, IZNF, Cauerstraße 3, 91058 Erlangen, Germany — [2]FHI, Faradayweg 4-6, 14195 Berlin, Germany — [3]Institute of Chemistry, Saint Petersburg State University, Universitetskii pr. 26, 198504 St. Petersburg, Russia

To comply with the rising demand in green energy, new durable photovoltaic devices, which use earth abundant, non-toxic and affordable materials, are required. Antimony (III) sulphide (Sb2S3), with a direct band gap of 1.7 eV and very high absorption coefficient, is a promising absorption material candidate for novel thin film (TF) photovoltaics.

Better charge selective materials must be found to achieve economically viable efficiencies, and avoid organic compounds. We demonstrate the proof of principle for the utilization of bulk MoS2 as a universal selective carrier material in Sb2S3 based TF solar cells, capable of replacing the usually organic hole transport (HTL) and the metal oxide electron transport layers (ETL). Cyclovoltammetric deposition of uniform amorphous MoS2 thin films from aqueous solution on ITO with tens of nanometres thickness was optimized and compared to atomic layer deposition (ALD). Thermal treatment was employed to convert the as grown layers into a crystalline phase. The layer properties vary depending on the deposition method which allowed to build devices with MoS2 as ETL, HTL or both. High current extraction was achieved with MoS2 replacing both charge selective layers. This study shows the great tunability and application potential of bulk MoS2.

DS 33.3 Wed 15:00 P1A

Lithographical Fabrication of Single Crystal OFET Arrays by Area Selective Growth and Solvent Vapor Annealing — •Zhifang Wang[1,2], Hong Wang[1], Wenchong Wang[1], and Lifeng Chi[2] — [1]Physikalisches Institut and Center for Nanotechnology (CeNTech), Universität Münster, 48149 Münster, Germany. — [2]Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Institute of Functional Nano & Soft Materials (FUNSOM), Joint International Research Laboratory of Carbon-Based Functional Materials and Devices, Soochow University, 199 Ren'ai Road, Suzhou, 215123, Jiangsu, P.R. China

OFET arrays based on miniaturized organic single crystals play an important role in reading-out circuit, which is crucial for high peformance and high level integration organic electronics. Here, we achieved high uniformity and high density single crystal OFET arrays by using a lithography compatible strategy that combines area selective growth and subsequent solvent vapor annealing process. The organic semiconductor molecule triethylsilylethynyl anthradithiophene (TES-ADT) can first selectively grow on prepatterned drain-source electrodes, then further convert into discrete single crystals by solvent vapor annealing. The results show that the crystals very uniform in size, with two orders of improvement in carrier mobility in comparison to that of amorphous/polycrystalline film. With the method, crosstalk between devices can be completely surpressed. OFET and basic logic gate arrays with reading-out electrodes are further demonstrated.

DS 33.4 Wed 15:00 P1A

Transport properties in thin films of the chiral RhSi compound — •Hua Lv, Anastasios Markou, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Unconventional chiral fermions attract a lot of attention due to their unusual quantum phenomena and unique electrical properties, such as quantized photogalvanic optical response. Recent studies demonstrated the large surface Fermi arc [1] and quantized photocurrent in bulk RhSi crystal [2].

In this work, we systematically study the magneto transport properties of magnetron sputtered RhSi films with different thickness. We find the surface scattering plays an important role in the thinner films and Kohler's rule dominates the longitudinal magnetoresistance.

References:

[1] Daniel S. Sanchez et al, Nature 567, 500-505 (2019).

[2] Dylan Rees et al, arXiv: 1902.03230v2.

DS 33.5 Wed 15:00 P1A

Magnetoconductance of Bi quantum films in parallel magnetic fields — •Doaa Abdelbarey[1], Christoph Tegenkamp[1,2], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Institut für Physik, TU Chemnitz

Bismuth has attracted a lot of interest because of its unique electronic properties such as low carrier concentrations and high carrier mobilities, In particular, strong Rashba splitting of the edge states appears in quantum films generated by epitaxial growth. Thus high-quality thin films open new pathways to tailor the electronic properties further. Magneto-conductance of films grown epitaxially on Si(111) with a thickness of 10 to 100 bilayers (BL) was measured at T= 9 K in parallel magnetic fields up to 4T. For B-fields in plane and parallel to the current direction only WAL is observed irrespective of thickness. However, if the B-fields are in plane, but perpendicular to the current, a crossover from weak anti-localization (WAL) to weak localization (WL) and back is seen for films up to 70 BL. For thicker films only WAL is observed. The observed coherent part of conductance in parallel B-fields perpendicular to current is characterized by an intriguing change from strong to weak coupling between edge states as a function of layer thickness and their hybridization with the quantized bulk states.

DS 33.6 Wed 15:00 P1A

In-operando studies on thiophene based organic field-effect transistors — •Manuel Johnson[1], Tim Hawly[1], Baolin Zhao[2], Marcus Halik[2], and Rainer Fink[1] — [1]Lehrstuhl für Physikalische Chemie II, FAU Erlangen-Nürnberg, Germany — [2]Lehrstuhl für Werkstoffwissenschaften II, FAU Erlangen-Nürnberg, Germany

Organic field effect transistors have drawn growing interest for novel electronic applications like backplanes for flexible displays or low-cost circuits for sensor applications. Main reason for this has been their increased performance due to the development of materials with improved charge carriers mobility and environmental stability [1]. Nevertheless, there are still open questions regarding charge carrier transport and its mechanism. To address this issue we performed Raman and Kelvin probe force microscopy studies to get an insight into our devices, based on pentacene and different thiophene derivatives while operating the devices. We observe a permanent change in the surface potential after the first device stress (i.e. functional operation) and a reversible potential increase during device operation. Furthermore, we found that the permanent potential change is homogenous across the device while the reversible effect is strongly correlated to the local microstructure. We interpret these findings as different effects of charge trapping, whereby the permanent charge trapping takes place inside the dielectric layer while the reversible charge trapping happens inside the organic semiconductor film and at the organic-dielectric interface. This research is funded by the DFG within GRK1896.

[1] D. Natali, et al., Adv. Mater. 2012, 24, 1357

DS 33.7 Wed 15:00 P1A

Investigation of Superconductivity in the Phase Change Material $In_3Sb_1Te_2$ — •Lisa Metzner[1], Elisabeth-Annemarie Gerhorst[1], Patrick Juraschitz[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 rapidly and reversibly between an amorphous and a crystalline state which show a big contrast in optical and electrical properties. It has been shown, that these chalcogenide-based materials can be classified by a unique bonding mechanism, called metavalent bonding, which can account for many of the special properties of these materials. When these materials are put on a map, besides their suitability for memory applications, many topological insulators, good thermoelectrics or superconductors can be identified, since strong electron-phonon interactions play a prominent role in these metavalent materials.

The aim of this work is to investigate the superconductivity in the phase change material $In_3Sb_1Te_2$. Therefore, thin film samples for both structural characterization and electrical transport measurements are deposited by sputter deposition. Furthermore, tunnel contacts are produced to analyse the superconducting energy gap alongside the critical temperatures and fields for films of various thicknesses.

DS 33.8 Wed 15:00 P1A

Electrical and Thermal Transport Properties of Ion-Beam Sputtered Epitaxial Manganite Perovskite Films — •Tim Sievert, Gottfried Schnabel, Birte Kressdorf, Jörg Hoffmann, and Christian Jooss — Institut für Materialphysik, Georg-August-Universität Göttingen

Perovskite oxides are a promising class of materials for microelectronics and energy harvesting. Strongly correlated manganite thin films reveal interesting transport properties which can be drastically altered by phase transitions. Due to their dependence on strain, off-stoichiometry and point defects, they are influenced by ion beam sputtering conditions. Thus, it is crucial to understand the impact of fabrication on the resulting material and fundamental processes within the material.

In this contribution we examine the interrelation between fabrication parameters, growth and film properties like strain, composition, electric and thermal transport of manganite perovskites, such as $La_{1-x}Sr_xMnO_3$, $Pr_{1-x}Ca_xMnO_3$ on $SrTiO_3(100)$ substrates. The temperature dependence of thermal, electrical and optical conductivity as well as magnetization between 5 K to 400 K are correlated with the microstructure and phase transitions in order to improve the understanding of the impact of defects on the phase diagram and transport phenomena. For the study of photo-electric characteristics, steps into the growth of optically transparent conducting contacts are pursued based on sputtering of indium tin oxide films.

DS 34: Annual General Meeting of the Thin Films Division

Time: Wednesday 18:15–19:15 Location: CHE 91

Duration 1 hour

DS 35: 2D Materials and their Heterostructures II (joint session DS/O/HL)

Time: Thursday 9:30–10:45 Location: CHE 89

DS 35.1 Thu 9:30 CHE 89

Longitudinal Nonlinear Spin Sensitive Response in two-dimensional Materials — •Dominik Kreil, Mario Graml, and Helga M. Böhm — Institute of Theoretical Physics, Johannes Kepler University Linz, Altenbergerstr. 69, A-4040 Linz, Austria

Future spin- and valleytronic devices will demand a deeper understanding of electronic systems. [1] With increasing intenstitys of state of the art terahertz lasers linear approximations become more imprecise. Nonlinear plasmonic effects arising from coherent oscillations of free charge carriers in metals or highly doped semiconductors serve to enhance optical processes. The underlying dynamics of electrons (or holes) was successfully treated semi-classically [2] in three-dimensional (3D) nanostructures; quantum expressions for up to the third order of the longitudinal nonlinear polarizabilities of the 3D, 2D and 1D homogeneous electron gases as well as graphene are also known. We here present a general discussion of higher order response functions resulting from time-dependent perturbation theory. Using the random phase approximation as in Ref. [3] we also derive a closed formula for longitudinal nonlinear spin sensitive response functions in arbitrary order. It holds for all the above listed systems and for imbalanced spin- or valley-polarizations. An application to the 2D spin-polarized electron gas with parabolic dispersion and in graphene [4,5] is presented.

References: [1] Vitale et al., Small 14, 1801483 (2018). [2] Krasavinet al., Laser & Photonics Reviews 12, 1700082 (2018). [3] Mikhailov, Phys. Rev. B. 93, 085403 (2016). [4] D. Kreil et al., Phys. Rev. B. 92, 085403 (2015). [5] D. Kreil et al., Lithuanian J. Phys. 59, 35 (2019).

DS 35.2 Thu 9:45 CHE 89

Predicting Exfoliability of MAX Phases into MXenes Using Ab-initio Thermodynamics — •Ali Muhammad Malik, Delwin Perera, Jochen Rohrer, and Karsten Albe — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

In recent years, research on 2D MAX-derived MXenes has expanded significantly due to their potential application in energy storage systems, electromagnetic interface shielding, electrocatalysis and gas detection. Almost 40 MAX phases have been predicted to be exfoliable based on force constant calculations and exfoliation energies. However, in experiment only 21 have so far been chemically exfoliated. In this work, we present a descriptor that combines calculated reaction energies and surface stabilities under experimentally relevant conditions. In agreement with experiments, we show that this descriptor is indeed capable of predicting the exfoliability of MXenes from Ti-based MAX phases in HF, whereas Cr-based MAX phases are predicted to decompose into Cr_3C_2 (carbide). We suggest that this descriptor is capable to guide experimental synthesis efforts in particular with respect to the choice of etchant and concentration.

DS 35.3 Thu 10:00 CHE 89

Characterization and Stability of Janus TiXY (X/Y= S, Se, and Te) Monolayers — Aybey Mogulkoc[1], Yesim Mogulkoc[1], Seymur Jahangirov[2], and •Engin Durgun[2] — [1]Department of Physics, Ankara University, 06100, Ankara, Turkey — [2]UNAM and Institute of Materials Science and Nanotechnology, Bilkent University, 06800, Ankara, Turkey

The addition of third element to binary 2D structures can lead to superior properties, hence extensive analyses on the characterization of such systems are required to reveal their full potential. In this study, we examine the structural, mechanical, electronic, thermal, and optical properties of TiXY (X/Y= S, Se, and Te) monolayers by using first-principles techniques. The stability of 1T and 2H-phases are revealed by phonon spectrum analysis and molecular dynamics simulations. Following the investigation of the mechanical response, electronic structures are examined together with partial density of states analysis. While monolayers of 1T-TiXY are found to be semimetals, monolayers of 2H-TiXY are semiconductors with indirect band gap. The optical spectrum is obtained by calculating the imaginary dielectric function and is correlated with the electronic structure. The variation of heat capacity with temperature is investigated and low/high temperature response is shown. Finally, possible structural distortions are also taken into account and charge density wave transition in 1T-TiSeS due to Peierls instability is demonstrated. Our results not only reveal the stable Janus monolayers of TiXY but they also point out these systems as promising candidates for nanoscale applications.

DS 35.4 Thu 10:15 CHE 89

Semiconducting defect-free polymorph of borophene: Peierls distortion in two dimensions — Semran Ipek[2], Aybey Mogulkoc[1], •Seymur Cahangirov[2], and Engin Durgun[2] — [1]Department of Physics, Ankara University, 06100, Ankara, Turkey — [2]UNAM and Institute of Materials Science and Nanotechnology, Bilkent University, 06800, Ankara, Turkey

In contrast to the well-defined lattices of various two-dimensional (2D) systems, the atomic structure of borophene is sensitive to growth conditions and type of the substrate which results in rich polymorphism. By employing ab initio methods, we reveal a thermodynamically stable borophene polymorph without vacancies which is a semiconductor unlike the other known boron sheets, in the form of an asymmetric centered-washboard structure. Our results indicate that asymmetric distortion is induced due to Peierls instability which transforms a symmetric metallic system into a semiconductor. We also show that applying uniaxial or biaxial strain gradually lowers the obtained band gap and the symmetric configuration is restored following the closure of the band gap. Furthermore, while the Poisson's ratio is calculated to be high and positive in the semiconducting regime, it switches to negative once the metallicity is retrieved. The realization of semiconducting borophene polymorphs without defects and tunability of its electronic and mechanical response can extend the usage of boron sheets in a variety of nanoelectronic applications

DS 35.5 Thu 10:30 CHE 89

First-principles study of hydrogenation on bilayer GaN — •Anh Khoa Augustin Lu[1], Tetsuya Morishita[1,2], Tomoe Yayama[3], and Takeshi Nakanishi[1,2] — [1]MathAM-OIL, AIST, Sendai, Japan — [2]CD-FMat, AIST, Tsukuba, Japan — [3]Department of Applied Physics, Kogakuin University, Tokyo, Japan

In the last decade, a large number of two-dimensional materials has been discovered. In recent years, two-dimensional III-V materials have arisen with the experimental demonstration of two-dimensional GaN. Here, we focus on the case of bilayer GaN. While the atomic structure of pristine bilayer GaN is relatively well understood, the impact that hydrogenation remains unclear since unlike transition metal dichalcogenides, pristine GaN has dangling bonds. In that respect, the present work focuses on the atomic structure, stability and electronic properties of bilayer GaN passivated by hydrogen atoms, with a large range of hydrogen coverage. First-principles calculations based on the density functional theory were performed to identify the structures with the lowest energy. While previous studies have focused on structures oriented along the c-plane, our results reveal that depending on the hydrogen concentration, the plane orientation of the most stable structure (c-, m-, or a-plane) is different. In particular, at high hydrogen concentration, structures oriented along the m- and a-planes have the lowest energy. Their stability is confirmed by first-principles molecular dynamics simulations performed at finite (room) temperature. By modulating the hydrogen concentration, one can therefore tailor the atomic structure and properties of bilayer GaN.

DS 36: Thin Oxides and Oxide Layers I (joint session DS/HL/O)

Time: Thursday 9:30–10:45 Location: CHE 91

DS 36.1 Thu 9:30 CHE 91

Atomically sharp epitaxial interface between Ba_2SiO_4 and Si(001)

— •Julian Koch and Herbert Pfnür — Leibniz Universität Hannover, Institut für Festkörperphysik

Epitaxial growth of Ba_2SiO_4 on Si(001) is a challenge, since neither crystal symmetry nor lattice constants match in a simple manner, but as we show, it has the potential to become the first high quality crystalline high-k gate dielectric. We combined X-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED) and aberration-corrected scanning transmission electron microscopy (STEM) in order to optimize the epitaxial growth by molecular beam epitaxy. The films were grown by a co-deposition method that requires no diffusion of Si from the substrate. While 400 °C turned out to be sufficient to form chemically homogeneous films, crystalline films required an annealing step to $670-690\,^\circ$C with the break-up of interfacial Si-O bonds as crucial step. STEM confirms that the interface is atomically sharp and that a single layer of the silicate is changed to a (2×3) structure at the interface from the (2×1.5) bulk structure. Electrical measurements on MOS-diodes with this material show small hysteresis in CV-curves, low interface trap densities ($< 6 \times 10^{10}$ cm^2eV^{-1}) and low leakage currents.

DS 36.2 Thu 9:45 CHE 91

Nano-scale spectroscopic analysis of $LaAlO_3/SrTiO_3$ interfaces using scattering-type Scanning Near-field Optical Microscopy

— •Yigong Luan[1], Julian Barnett[1], Marc Rose[2], Felix Gunkel[2], Martin Lewin[1], and Thomas Taubner[1] — [1]Institute of Physics (IA) RWTH Aachen — [2]PGI-3, Forschungszentrum Jülich

In the group of functional oxide materials, the interface of bulk insulators $LaAlO_3$ and $SrTiO_3$ (LAO/STO) attracts attention due to its highly confined and conductive two-dimensional electron gas (2DEGs), which could be interesting for high-electron-mobility transistors. 2DEGs at oxide interfaces result from electronic reconstruction, which is highly dependent on the local structure [1]. The extraction of their electronic properties is difficult for far-field spectroscopy and conventional nano-resolved microscopy (e.g. STM), as the conducting layer is highly confined and buried below an insulating layer (LAO). We overcome these limitations by using scattering-type Scanning Near-field Optical Microscopy for a quantitative extraction of electron properties from "phonon-enhanced spectroscopy", as the presence of free charge carriers leads to significant changes to the phonon resonance due to plasmon-phonon coupling [2]. We use an improved model (Finite Dipole Model) combining with Transfer Matrix Method to interpret the experimental results, investigating the influence of both LAO layer and 2DEGs on the STO phonon near-field resonance in detail, which allows us to extract the local electronic properties.

[1] A. Ohtomo et al., Nature 427, 423 (2004)
[2] M. Lewin et al., Adv. Funct. Mater, 28. 1802834 (2018)

DS 36.3 Thu 10:00 CHE 91

Optoelectrical properties of VO_2 ultra-thin films

— •Maximilian Obst[1], Laura Rodríguez[2], Gustau Catalan[2,3], Susanne C. Kehr[1], and Lukas M. Eng[1,4] — [1]Institute of Applied Physics, Technische Universität Dresden, Germany — [2]Institut Catalá de Nanociéncia i Nanotecnologia and The Barcelona Institute of Nanoscience and Technology, Campus UAB, Barcelona, Catalonia — [3]ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Catalonia — [4]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, Technische Universität Dresden, Germany

Vanadium dioxide (VO_2) is a material that is in the central research focus due to its metal-to-insulator phase transition (MIT) at room temperature. Experimentally, this temperature-regime is easily accessible, and hence allows profound MIT-studies while dreaming of interesting applications, such as phase-change memories. Although thicker VO_2 films are intensively investigated, the properties and physical behavior of ultrathin VO_2 layers are far from being understood.

In this work, an epitaxial VO_2-film of 10 nm grown on a rutile(001) single-crystal is explored, applying a broad set of electrical and optical methods. While Raman-spectroscopy revealed no structural phase transition of the film, electrical transport measurements as well as spectrally-resolved (UV to mid-IR) reflectivity measurements clearly show the MIT at ~300 K. In conclusion, the structural and electrical phase transition seems to be completely disentangled in these ultrathin films. However, thin VO_2-films might easily oxidize to V_2O_5, as was indicated by measuring the vanadium $2p_{3/2}$-peak using XPS.

DS 36.4 Thu 10:15 CHE 91

Towards quasi two-dimensional β-Ga2O3

— •Constance Schmidt, Mahfujur Rahaman, and Dietrich R. T. Zahn — Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

β-Ga2O3 is a transparent oxide semiconductor with outstanding properties due to its wide bandgap (Eg = 4.9 eV). It is already intensively studied in its bulk and thin film form. Studies on ultrathin films or even quasi-2D films are less common. Nevertheless, for nano electronics quasi-2D β-Ga2O3 can be beneficial as semiconductor or insulator, depending on layer thickness and doping [1]. β-Ga2O3 is not a van-der-Waals material, which makes conventional exfoliation challenging. Attempts show that layer thicknesses below 60 nm are not yet possible by exfoliating β-Ga2O3 [2]. To overcome this difficulty, we use a van-der-Waals material (GaSe), exfoliate thin flakes on Si with 300 nm SiO2, HOPG and Mica substrates, and oxidize these flakes by thermal annealing ((600 - 1000)°C, 30 min, in air) to obtain quasi 2D β-Ga2O3. In this work, we show the preparation of Se free quasi-2D β-Ga2O3 by annealing using temperatures higher than 700°C. The thin flakes obtained have thicknesses in the range of (0.5 - 50) nm as measured with atomic force microscopy. Energy dispersive X-ray spectra reveal the chemical composition of the 2D flakes and most importantly the absence of Se. Raman spectroscopy (excitation: 325 nm) verifies the β-Ga2O3 phase.

[1] J. Su, et al., J. Phys. Chem. C 122 43 24592-24599 (2018) [2] Y. Kwon, et al., APPLIED PHYSICS LETTERS 110 131901 (2017)

DS 36.5 Thu 10:30 CHE 91

Thermal phase transformations through iron oxides/ oxide substrates interfaces

— •Mai Hussein Hamed[1,2], David N. Mueller[1], Tomáš Duchoň[1], Ronja Hinz[1], Claus M. Schneider[1,3], and Martina Müller[1,4] — [1]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich GmbH, Germany — [2]Faculty of Science, Helwan University, Cairo, Egypt — [3]Fakultät für Physik, Duisburg-Essen Universität , Germany — [4]Experimentelle Physik I, Technische Universität Dortmund, Germany

Oxide heterostructures possess a wide range of electrical and magnetic properties arising, in particular, vie interactions across their interfaces. Therefore, our primary goal is understanding, controlling and tuning the interface properties. In this study, using hard X-ray photoelectron spectroscopy (HAXPES), we demonstrate phase transformations from Fe_3O_4 to either γ-Fe_2O_3 or FeO through active redox reactions across three relevant interfaces, i.e. (1) the outside atmosphere/Fe_xO_y film interface, (2) the interface between phase-transformed Fe_xO_y/Fe_xO_y intralayers and (3) the Fe_xO_y/oxide substrate interface. We find that the "active" oxide substrates ($SrTiO_3$ or YSZ) play an important role as an additional oxygen supplier or scavenger. This leads to a clear alteration of the standard temperature-pressure phase diagram of iron oxides. Accordingly, we calculate the effective oxygen pressure through the interfaces and adjust the phase diagram. Our findings allow us not only to control the interfaces but more importantly, to tune their physical functionalities by a controlled thermal phase design, giving access to far from equilibrium phases.

DS 37: Focus Session: Functional Metal Oxides for Novel Applications and Devices II (joint session HL/DS)

Metal oxides exhibit a myriad of fascinating physical properties that enable a large variety of potential applications such as sensors and detectors, solar energy harvesting, transparent and potentially bendable electronics, power electronics, high-electron-mobility transisitors, memristors, topological quantum computation and so on. These functionalities typically require homo- or heteroepitaxial layers of high crystallinity with bendable amorphous semiconducting oxides as an exception. This session sets a focus on growth of bulk and thin films, experimental and theoretical investigation of their physical properties as well as fabrication and characterization of demonstrator devices.

Organizers: Oliver Bierwagen (Paul-Drude-Institut für Festkörperelektronik, Berlin), Holger Eisele (TU Berlin), Jutta Schwarzkopf (Leibniz-Institut für Kristallzüchtung, Berlin) and Holger von Wenckstern (Universität Leipzig).

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

Invited Talk DS 37.1 Thu 9:30 POT 81

Basics of Gas Sensing with Semiconducting Metal Oxides — •Nicolae Barsan — University of Tuebingen, Tuebingen, Germany

This contribution will present the basic knowledge needed to understand gas sensing with semiconducting metal oxides. It will explain how the interaction with atmospheric gases changes both surface charge and free charge carriers concentration and will descrice that in terms of reception and transduction functions. The body of essential data needed for the understanding of sensing for the case of two representative oxides, namely SnO2 and WO3 will be presented together with the description of the most relevant operando investigation techniques, namely Kelvin probe work function changes measurements and Diffuse Reflectance Infrared Fourier Transform Spectroscopy.The example of CO detection in the presence of humidity will be in the focus. It will be shown how this knowledge can be formalized with the help of the quasi-chemical reactions. Furthermore it will be explained how the charging of the surface changes the properties of the oxide and how this can be quantified with the help of the Poisson and electro-neutrality equations for both n and p-type materials.

DS 37.2 Thu 10:00 POT 81

Optical and photocatalytic properties of gallium-zinc-oxynitrides thin films grown by molecular beam epitaxy — •Elise Sirotti, Max Kraut, Florian Pantle, and Martin Stutzmann — Walter Schottky Institut and Physics Department, Technische Universität München, Am Coulomwall 4, 85748 Garching, Germany

GaN and ZnO are two well-studied materials with favorable energy positions of their band edges with respect to the redox levels of many electro-chemical reactions. However, their large band gap limits the use for simultaneous efficient solar light absorption and photocatalytic activity. By forming an alloy of both materials, the band gap can be reduced by more than 1 eV, while the energetic position of the conduction band stays almost constant. We present the growth of GZNO thin films by means of plasma-assisted MBE on c-plane sapphire. The quality and composition of the quaternary compound have been optimized by varying the temperature, metal fluxes and nitrogen-to-oxygen ratio during deposition. We performed photo-thermal deflection spectroscopy, valence band XPS and EDX measurements to investigate the influence of the composition on the electronic properties. As a result, the influence of the different components on the energetic positions of the conduction band and valence band has been clarified. With electrochemical measurements, we gain insights into the photo-catalytic activity and stability of the thin films. The high flexibility gained by MBE growth allows us to acquire additional knowledge about the fundamental principles of the band gap narrowing process.

DS 37.3 Thu 10:15 POT 81

Surface Stability of β-Ga$_2$O$_3$ at Realistic Temperature and Pressure Conditions from First Principles — •Konstantin Lion[1,2], Sergey V. Levchenko[3,2], Matthias Scheffler[2,1], and Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin, Berlin, DE — [2]Fritz-Haber-Institut der MPG, Berlin, DE — [3]Skolkovo Institute of Science and Technology, Moscow, RU

The surface properties of a material play a vital role in epitaxial growth and electrical contacts. Depending on the miscut direction on off-oriented (100) β-Ga$_2$O$_3$ substrates, homoepitaxially grown layers show distinct surface morphologies, i.e., the formation of $(\bar{2}01)$ facets [1]. In a first-principles approach, it is important to account for the experimental growth conditions, since they can influence surface stability and thus surface faceting. In this work, we study the stability of all symmetrically inequivalent low-index surfaces of β-Ga$_2$O$_3$ at realistic conditions using *ab initio* atomistic thermodynamics. In the calculation of the phase diagrams of all surfaces, we include vibrational contributions to the surface free energy. We find that $(\bar{2}01)$ faceting on (100) substrates is thermodynamically favored at $T = 825\,^\circ\mathrm{C}$ and an oxygen partial pressure of 1 mbar, the conditions during homoepitaxial growth. This shows that thermal equilibrium has been reached during growth. Also, we find that the (001) surface is stabilized at higher oxygen chemical potentials, which explains its role as a cleavage plane at ambient conditions.

[1] R. Schewski *et al.*, APL Materials **7**, 022515 (2019)

DS 37.4 Thu 10:30 POT 81

Investigations of β-Ga$_2$O$_3$(100) cleavage surfaces by scanning tunneling microscopy and spectroscopy — •Celina Seraphin Schulze[1], Jonathan Hofmann[1], Christian Bruckmann[1], Martin Franz[1], Zbigniew Galazka[2], Wjatscheslav Martyanov[1], and Holger Eisele[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung (IKZ), Berlin, Germany

We present surface investigations of three differently doped β-Ga$_2$O$_3$ crystals by scanning tunneling microscopy and spectroscopy. One sample is unintentionally doped, while both others are doped by Si and Sn. All the bulk β-Ga$_2$O$_3$ single crystals were grown from the melt by the Czochralski method [1,2] and cleaved *in situ* under a base pressure below 1×10^{-8} Pa for experimental investigation. On the flat β-Ga$_2$O$_3$(100) cleavage surfaces of each sample dark contrasts occur that can be partially assigned to unintentional background doping by Si. By low energy electron diffraction measurements on the β-Ga$_2$O$_3$(100) surfaces we observed an unreconstructed surface with a 1×1 diffraction pattern. Scanning tunneling spectra show intrinsic electronic states within the band gap, induced most likely by oxygen vacancies. This project was supported by the Leibniz Association, Leibniz Science Campus GraFOx, project C2-3.

[1] Z. Galazka *et al.*, ECS J. Solid State Sci. Technol. 6, Q3007 (2017)

[2] Z. Galazka *et al.*, J. Crystal Growth 529, 125297 (2020)

DS 37.5 Thu 10:45 POT 81

Growth and characterization of Si delta-doped β-Ga$_2$O$_3$ layers by MOVPE — •Saud Bin Anooz, Raimund Grüneberg, Robert Schewski, Martin Albrecht, Andreas Fiedler, Klaus Irmscher, Zbigniew Galazka, Günter Wagner, and Andreas Popp — Leibniz-Institut für Kristallzüchtung (IKZ), Max-Born-Str. 2, 12489 Berlin, Germany

Si delta-doped β-Ga$_2$O$_3$ layers have been grown on (100) and (010) β-Ga$_2$O$_3$ substrates by MOVPE. AFM images of the grown layer on (010) oriented substrate show 2D island growth, while for layers grown on (100) with 6o miscut angle substrate step flow growth mode has been found resulting in a lower surface roughness for the (100) surface compared to (010). The amount of Si incorporated into the grown layers as well as the shape of the interface were studied by secondary ion mass spectrometry (SIMS). The SIMS depth profile for the Si delta-doped layer grown on a (010) substrate shows a gradual transition from the high Si doped to the unintentionally doped regime. However, the Si depth profile of the layer grown on (100) 6° off substrate shows sharp interfaces between the high and low doped regions, a clear advantage with regard to later devices. This could be explained by the surface morphology of the grown layers on (010) and (100) substrates.

30 min. break

Invited Talk DS 37.6 Thu 11:30 POT 81

Ultra-thin oxides on InGaN nanowires: Passivation layers for nanostructured photoelectrodes and optical analysis of chemical processes — Paula Neuderth[2], Mariona Coll[3], Jörg Schörmann[2], Christian Reitz[6], Jordi Arbiol[4], Roland Marschall[5], and •Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Institute of Experimental Physics I Justus Liebig University Giessen Germany — [3]Institut de Ciencia de Materials de Barcelona ICMAB-CSIC, Spain — [4]ICREA Pg. Lluís Companys 23 08010 Barcelona, Spain — [5]Physical Chemistry III, University of Bayreuth, Germany — [6]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology, Germany

We demonstrate an experimental strategy for systematically assessing the influence of surface passivation layers on the photocatalytic properties of InGaN nanowire (NW) photoanodes by combining photocurrent analysis, photoluminescence spectroscopy and high resolution transmission electron microscopy. We apply this approach to separate the influence of different mechanisms recombination and transport processes of photogenerated carriers and to compare the effect of TiO2, CeO2 and Al2O3 coatings deposited by atomic layer deposition. Due to efficient charge transfer from the InGaN NW core a stable TiO2-covered photoanode with visible light excitation is realized. As a second application we demonstrate that due to the sensitivity of the InGaN NW photoluminescence to surface adsorbed oxygen the optical analysis of oxygen diffusion in ultrathin ceria coatings deposited by atomic layer deposition is possible.

DS 37.7 Thu 12:00 POT 81

Growth Window, Solubility Limit and Material Properties of κ-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ PLD thin films — •A. Hassa[1], C. Wouters[2], M. Kneiss[1], P. Storm[1], H. von Wenckstern[1], D. Splith[1], C. Sturm[1], M. Albrecht[2], and M. Grundmann[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstraße 5, 04103 Leipzig, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, D-12489 Berlin, Germany

The orthorhombic polymorph of Ga_2O_3, namely κ, is of increasing interest because of its predicted large polarization of 23 μC/cm^2 [1] rendering it well suited for possible usage e.g. in HEMT's. The high bandgap of about 5 eV [2] can be enlarged by alloying with Al_2O_3 enabling such heterostructure-based devices. We present κ-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ thin films grown on (00.1)Al_2O_3 by tin-assisted pulsed laser deposition (PLD) [2]. For some thin films a homogeneous target with a defined composition and for an 2 inch in diameter thin film a two-fold PLD target consisting of Ga_2O_3/Al_2O_3 semicircular segments were utilized to grow a sample with laterally continuous composition spread [3]. Al content, growth rates and the occurrence of single phase κ-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ depends systematically on growth conditions. Further, we present the dependence of structural and optical properties on alloy composition. The maximum observed Al incorporation in the κ-phase was $x = 0.46$ with a bandgap of 5.85 eV.
[1] M. B. Maccioni *et al.*, Appl. Phys. Express 9, 04102 (2016).
[2] M. Kneiß *et al.*, APL Materials 7, 022516 (2019).
[3] H. von Wenckstern *et al.*, CrystEngComm 15, 10020 (2013).

DS 37.8 Thu 12:15 POT 81

Epitaxy of κ-(Al,Ga)$_2$O$_3$ heterostructures and superlattices by VCCS-PLD — •Philipp Storm[1], Max Kneiss[1], Thorsten Schultz[2], Daniel Splith[1], Holger von Wenckstern[1], Norbert Koch[2], Michael Lorenz[1], and Marius Grundmann[1] — [1]Universität Leipzig, Felix-Bloch Institut für Festkörperphysik — [2]Humboldt Universität zu Berlin, Institut für Physik

Ga_2O_3 is a wide band gap semiconductor with pronounced polymorphism. The thermodynamically stable and therefore most often investigated polymorph is the monoclinic β-phase. However, the metastable, orthorhombic κ-phase gained significant interest due to its high predicted spontaneous polarization of 23 μC/cm^2 [1]. Exploiting the polarization differences at κ-$Ga_2O_3/CaCO_3$ [2] or κ-Ga_2O_3/κ-(Al,Ga)$_2$O$_3$ heterointerfaces could allow for the formation of 2DEGs with high carrier densities, crucial for QWIP or HEMT devices. Nevertheless, only little is known about κ-(Al,Ga)$_2$O$_3$ heterostructures [3]. In this work, VCCS-PLD (vertical continuous composition spread pulsed laser deposition) [4] was utilized for the growth of κ-(Al,Ga)$_2$O$_3$ heterostructures and superlattices that were investigated regarding structural, morphological and optical properties to evaluate their potential for device applications.
[1] M. B. Maccioni *et al.* : Appl. Phys. Express 9, 041102 (2016)
[2] S. B. Cho *et al.* : Appl. Phys. Lett. 112, 162101 (2016)
[3] P. Storm *et al.* : APL Mater. 7, 111110 (2019)
[3] M. Kneiß *et al.* : ACS Comb. Sci. 20, 643 (2018)

DS 37.9 Thu 12:30 POT 81

Tin-assisted growth of κ-(Al$_x$Ga$_{1-x}$)$_2$O$_3$/(In$_x$Ga$_{1-x}$)$_2$O$_3$ superlattice heterostructures by pulsed laser deposition — •Max Kneiss, Philipp Storm, Anna Hassa, Daniel Splith, Chris Sturm, Holger von Wenckstern, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik

The orthorhombic κ-phase of Ga_2O_3 possesses a similarly high bandgap of 5 eV as the thermodynamically stable β-phase, but further is expected to exhibit a high spontaneous electrical polarization of 23 μC/cm^2 [1]. Polarization differences at interfaces of κ-phase heterostructures can be utilized for polarization doping to localize a 2DEG that typically features large carrier densities as well as high mobility. We present the coherent growth of κ-(Al$_x$Ga$_{1-x}$)$_2$O$_3$/(In$_x$Ga$_{1-x}$)$_2$O$_3$ quantum-well (QW) superlattices on c-sapphire substrates by pulsed laser deposition. Tin containing targets were necessary for the stabilization of the orthorhombic phase [2]. We found narrow superlattice oscillations up to the ninth order and up to $x \approx 0.5$ in XRD 2θ-ω scans as well as in reciprocal space maps for up to 15 layer pair superlattices confirming excellent crystal quality and abrupt interfaces. The evolution of superlattice oscillations as well as the optical properties will be evaluated in dependence on the QW and barrier width as well as on the composition of the QW and barrier layers. AFM measurements confirm smooth surface morphology for all samples. [1] Maccioni *et al.*, Appl. Phys. Expr. **9**, 041102 (2016) [2] Kneiß *et al.*, APL Materials **7**, 022516 (2019)

DS 37.10 Thu 12:45 POT 81

Band offsets at κ-([Al,In]$_x$Ga$_{1-x}$)$_2$O$_3$/MgO interfaces — •Thorsten Schultz[1,2], Max Kneiss[3], Philipp Storm[3], Daniel Splith[3], Holger von Wenckstern[3], Marius Grundmann[3], and Norbert Koch[1,2] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Berlin, Germany — [2]Helmholtz-Zentrum für Energie und Materialien GmbH, Berlin, Germany — [3]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Leipzig, Germany

Conduction and valence band offsets are amongst the most crucial material parameters for semiconductor heterostructure device design. Due to its expected high spontaneous electrical polarization and the possibility of polarization doping at heterointerfaces, the metastable orthorhombic κ-phase of Ga_2O_3 and its indium and aluminum alloy systems are an interesting material class. We report on valence and conduction band offsets of κ-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ and κ-(In$_x$Ga$_{1-x}$)$_2$O$_3$ thin films to MgO as reference dielectric by X-ray photoelectron spectroscopy. The determined band alignments reveal the formation of a type I heterojunction to MgO for all compositions with conduction band offsets of at least 1.4 eV, providing excellent electron confinement. We further found that the conduction band offsets in the alloy system are mainly determined by the evolution of the bandgaps. Therefore, tunable conduction band offsets of up to 1.1 eV within the alloy system allow for subniveau transition energies in corresponding quantum wells from the IR to the visible regime, which are promising for application in, e.g., quantum-well infrared photodetectors.

DS 38: 2D Materials and their Heterostructures III (joint session DS/HL)

Time: Thursday 11:00–12:30 Location: CHE 89

DS 38.1 Thu 11:00 CHE 89

Controllable growth of few-layer graphene —

•Victor Aristov[1,2], Alexander Chaika[2,3], Olga Molodtsova[1,4], Sergey Babenkov[1,5], Dmitrii Potorochin[1,4,6], Andrea Locatelli[7], Tevfik Mentes[7], Alessandro Sala[7], and Dmitry Marchenko[8] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]Institute of Solid State Physics of the Russian Academy of Sciences, Chernogolovka, Moscow District 142432, Russian Federation — [3]CRANN, School of Physics, Trinity College Dublin, Dublin 2, Ireland — [4]ITMO University, 197101 Saint Petersburg, Russian Federation — [5]Institut fuer Physik, Johannes Gutenberg-Universita*t, D-55099 Mainz, Germany — [6]Institute of Experimental Physics, TU Bergakademie Freiberg, D-09599 Freiberg, Germany — [7]Elettra Sincrotrone Trieste, I-34149 Basovizza, Trieste, Italy — [8]Helmholtz-Zentrum Berlin fuer Materialien und Energie, D-12489 Berlin, Germany

Utilizing vicinal SiC/Si(001) wafers one can synthesize self-aligned graphene nanoribbons that exhibit energy transport gap on the order of 1 eV, large positive in-plane magnetoresistance, and the potential to work as a spin filter, opening opportunities for electronic and spintronic applications. This work demonstrates the capabilities to control the lattice and boundary orientations and the layer thickness in-situ, during the few-layer graphene synthesis in an ultra-high vacuum [1]. Supported by the RFBR (Grant Nos. 17-02-01139, 17-02-01291). [1] V.Yu.Aristov et al., ACS Nano 13, 526 (2019)

DS 38.2 Thu 11:15 CHE 89

Proximity-induced spin Hall effect in graphene/WSe$_2$ van der Waals heterostructures with tunable, highly efficient spin-to-charge conversion —

•Franz Herling[1,2], C.K. Safeer[1], Josep Ingla-Aynés[1], Nerea Ontoso[1], Luis E. Hueso[1,3], and Fèlix Casanova[1,3] — [1]CIC nanoGUNE, 20018 Donostia-San Sebastian, Basque Country, Spain — [2]QuESTech, Horizon 2020 ITN, Marie Sklodowska-Curie Action (No 766025) — [3]IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Basque Country, Spain

The proximity effect in two-dimensional materials opens ways to achieve important functions for future spintronic devices. In van der Waals heterostructures, transition metal dichalcogenides (TMD) can be used to enhance the spin-orbit coupling of graphene leading to highly efficient spin-to-charge conversion (SCC) by spin Hall effect (SHE) that is predicted to be controllable by a gate voltage. Here, we report for the first time the observation of the SHE in graphene proximitized with WSe$_2$. By Hanle precession measurements, we quantify the spin transport and SCC parameters from 10 K up to room temperature. Exceptional for graphene/TMD devices, the sole mechanism is the SHE for all measurements and no Rashba-Edelstein effect is observable. Importantly, we are able to amplify and turn off the SCC by applying a back-gate voltage, demonstrating the long-awaited milestone of an electrically-tunable SHE. The amplified SCC shows a high efficiency, measured with an unprecedented SCC length of up to 41 nm (with a lower limit of 20 nm).

DS 38.3 Thu 11:30 CHE 89

Thermal conductivity and thermal diffusivity of suspended few-layer h-BN using modified 3ω method —

•Sofia Blanter[1], Nicola Paradiso[1], Denis Kochan[2], Kenji Watanabe[3], Takashi Taniguchi[3], and Christoph Strunk[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

We present measurements of thermal conductivity and thermal diffusivity for few-layer suspended hexagonal boron nitride between 25 and 300 K. The measurements are performed on 5-13 nm thick and suspended over a length of 2-10 μm h-BN flakes using a modified version of the 3 omega method.

We generate a temperature gradient by an AC current through a metal heater. Then we measure the temperature difference and the phase shift of the AC temperature response between the heater and a thermometer a small distance away. This allows us to assess the thermal diffusivity of the flake separately from that of the substrate.

Varying the distance between the heater and thermometer, we observe that the phase shift becomes temperature independent for short distances.

DS 38.4 Thu 11:45 CHE 89

Dimensional crossover due to broken symmetry and enhanced thermoelectric performance in graphene antidot lattices —

•Mustafa Neşet Çinar and Hâldun Sevinçli — Deparment of Materials Science and Engineering, Izmir Institute of Technology, 35430 Urla Izmir Turkey

Graphene antidot lattices (GALs) are monolayers with periodically placed holes in otherwise pristine graphene. We investigate the electronic properties of symmetric and symmetric GAL structures having hexagonal holes, and show that anisotropic GALs can display a dimensional crossover such that quasi-one-dimensional (Q1D) electronic structures can be realized in two-dimensional systems around the charge neutrality point. We investigate the transport and thermoelectric properties of these Q1D GALs by using non-equilibrium Green function (NEGF) method. Dimensional crossover manifests itself as transmission plateaus, a characteristic feature of Q1D systems, and enhancement of thermoelectric efficiency, where thermoelectric figure of merit, zT, can be as high as 0.9 at room temperature. We further study the transport properties in the presence of Anderson disorder and and that mean-free-paths of Q1D electrons of anisotropic configuration are much longer than those of isotropic one at the same energies.

DS 38.5 Thu 12:00 CHE 89

Electronic structure of thin topological insulator films —

•Thomas Naimer, Klaus Zollner, and Jaroslav Fabian — Universität Regensburg, Deutschland

We investigate the electronic structure of thin slabs of the 3D topological insulators Bi2Se3 and Bi2Te3 by means of density functional theory. We present an extensive study of the effects of perpendicular electric fields on the topological surface states. Additionally we examine exchange proximity effects in Cr2Ge2Te6-Bi2Te3 heterostructures. We acknowledge the support of the EU Graphene Flagship program.

DS 38.6 Thu 12:15 CHE 89

Interacting two-electron states in electrostatically confined bilayer graphene quantum dots —

•Angelika Knothe and Vladimir Fal'ko — National Graphene Institute, University of Manchester, Manchester M13 9PL, United Kingdom

Successfully utilizing the properties of two-dimensional materials in quantum nanostructure devices could lead to unprecedented electronics applications. We study the possible states of two interacting electrons in a quantum dot electrostatically confined in gapped bilayer graphene. The properties of the material's electronic structure, such as the three minivalleys around each valley, and the corresponding orbital magnetic moment, translate into the features of the dot states. In the weakly gapped case, the single-particle level scheme is that of an almost quadratic band, featuring a singly-degenerate ground state and angular momentum duplet degeneracies. For a sufficiently strong gap, threefold degenerate "minivalley triplets" emerge. For two electrons in the dot, the long-range part of the screened Coulomb interaction defines the orbital configuration of the interacting two-particle state. Short-range contributions breaking the symmetries on the lattice scale determine the ordering in spin and valley space. We identify the set of orbital, spin, and valley levels of the interacting two-particle states.

DS 39: Thin Oxides and Oxide Layers II (joint session DS/HL)

Time: Thursday 11:00–12:15 Location: CHE 91

DS 39.1 Thu 11:00 CHE 91

Structural, Optical and Electrical Properties of Indium Tungsten Oxide upon High Temperature Annealing — •Dorothee Menzel and Lars Korte — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekulestrasse 5, 12489 Berlin, Germany

High work function metal oxides, such as tungsten oxide (WOx) have recently been investigated as charge selective p-contacts for silicon heterojunction solar cells: They provide a higher optical transparency, and due to their high work function (WF) it is expected that they can improve the cell's fill factor due to a more efficient carrier separation. However, WOx suffers from a rather poor conductivity. Indium oxide (InOx), on the other hand, has a moderate WF but a much higher conductivity. We vary the ratio of In-to-W oxide by thermal co-evaporation, spanning the full range from pure WOx to pure InOx and search for a tradeoff of high WF and high conductivity. Using in-situ (X-ray and UV) PES and surface photovoltage measurements, we found a pronounced decrease of the WF from 6.3eV for pure WOx down to 4.5eV for 40% of InOx-content in the InWOx mixture. This was accompanied by a decrease of the band bending in the c-Si substrate by 200meV [1]. Further studies focused on the material properties, such as optical, electrical and structural properties of indium tungsten oxide thin films on glass. We will discuss the changes in these properties with changing In-to-W ratio and upon high temperature annealing up to 700°C.

[1] D. Menzel et al., Appl. Phys. Lett., 112, 1-13, 2018.

DS 39.2 Thu 11:15 CHE 91

In-situ observation of sub-unit-cell nonlinear polarization in superlattices of layered oxides — •Johanna Nordlander[1], Marco Campanini[2], Marta D. Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]ETH, Zurich, Switzerland — [2]EMPA, Dübendorf, Switzerland

When approaching the 2D-limit of a material, finite size, edge or confinement effects often lead to phenomena that differ from the bulk behavior and promote novel functionalities. In materials with a layered structure, the individual sub-unit-cell layers that form their fundamental building blocks may exhibit a different symmetry, and hence different properties, than those of the parent material. For example, strong nonlinear optical properties may arise from broken inversion symmetry in fractional unit-cells of an otherwise centrosymmetric layered oxide. Here we use in-situ optical second harmonic generation (ISHG) during thin-film deposition to access these unique symmetry properties of sub-unit-cell layers in ultrathin, naturally layered hexagonal manganites. A strong nonlinear polarization directly originating from the inversion-symmetry breaking of individual half-unit-cell layers leads to a striking modulation of ISHG intensity connected to the periodic cancellation and reappearance of a non-centrosymmetric thin-film structure as each half-unit-cell layer is added during thin-film synthesis. We thus reveal the unexpectedly strong optical response of these sub-unit-cell blocks that perfectly cancel in the bulk limit. We furthermore make use of this characteristic dynamic ISHG signature to create oxide superlattices through sub-unit-cell symmetry control.

DS 39.3 Thu 11:30 CHE 91

Ellipsometric study of defect induced magnetism in spinel ferrite thin films — •Vitaly Zviagin[1], Chris Sturm[1], Pablo Esquinazi[1], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1,2] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik — [2]Now at: Technische Universität Ilmenau, Institut für Physik

We present the magnetic properties of normal spinel $ZnFe_2O_4$ (ZFO) thin films in dependence on fabrication and annealing temperature as well as atmosphere. The increase in the net magnetic response with decreasing substrate temperature correlates with the increase in cation disorder, evident by an increase in O^{2-}2p-Fe^{3+}_{Td}3d electronic transition amplitude in the dielectric function (DF) spectra.[1] Absorption in the low energy range (∼0.9 eV) is related to an electronic transition between d orbitals of Fe^{2+} and Fe^{3+} cations and shows a strong dependence on fabrication and annealing atmosphere. Comparing the cation distribution in film bulk (optical transitions in the DF) to near-surface region (X-ray absorption), it is found that an inhomogeneous cation distribution leads to a weaker magnetic response in films of inverse configuration, whereas defects in normal spinel are likely to be found at the film surface. The presented results show that it is possible to engineer and to probe the defect distribution in the magnetic spinel ferrite film structure and to tailor their magnetic properties on demand.

[1] V. Zviagin *et al.*, Appl. Phys. Lett. **108**, 13 (2016)

DS 39.4 Thu 11:45 CHE 91

Fast sweep and voltage pulse studies on HfO_2/TiO_2- bilayer resistive switching memories — •Nils Quiring[1], Felix Cüppers[1], Alexander Hardtdegen[1], Susanne Hoffmann-Eifert[1], and Rainer Waser[1,2] — [1]PGI-7, Forschungszentrum Jülich GmbH, Germany — [2]IWE-2, RWTH Aachen University, Germany

Redox-based resistive random access memories (ReRAM) are promising contenders for future information technology applications. Compared to the respective monolayers, bilayer oxide stacks of HfO_2/TiO_2 revealed enhanced switching stability [1]. Yet, the origin of this stability is not fully understood. The inherent variability of properties such as the resistance states, switching voltages and times need further investigation.

In this study, bilayer oxide stacks of HfO_2/TiO_2 sandwiched between a Pt and a Ti electrode are electrically characterized by voltage sweep and pulse measurements. The switching behavior at different voltages, durations and signal waveform geometries with a current limitation is examined. Cells during switching are characterized with respect to cycle to cycle and device to device variability.

[1] A. Hardtdegen et al., " Improved Switching Stability and the Effect of an Internal Series Resistor in HfO_2/TiO_2 Bilayer ReRAM Cells " *IEEE TED*, vol. 65, 8, 2018, pp. 3229-3236.

DS 39.5 Thu 12:00 CHE 91

TiO_x formation during ALD metal oxide growth on Ti for resistive switches — •Ivonne Bente, Stephan Aussen, and Susanne Hoffmann-Eifert — Peter Grünberg Institut, Forschungszentrum Jülich GmbH

We studied the formation of TiO_x at the interface of Ti metal and a metal oxide film, which is grown onto the Ti layer by atomic layer deposition (ALD). For the metal oxide we investigated stoichiometric oxide films (MO) including Al_2O_3, TiO_2 and HfO_2 layers. The 25 nm thick dense Ti films are deposited on thermal oxidized Si wafers in an off-axis sputter tool with a base pressure $< 10^{-10}$ mbar. The Ti films with hexagonal crystal structure exhibit a low surface roughness. The films were transferred under ultra-high vacuum into an ALD plasma system. 2 to 3 nm thick oxide layers are deposited at 250°C using O_2-plasma as the oxygen source and standard metalo-organic precursors for the metal sources. The resulting stacks are investigated by x-ray photoelectron spectroscopy showing different Ti oxidation states (0 to 4^+) and a clear TiO_x thickness dependence on the ALD process. The switching behavior of the resulting stacks is investigated. In addition, complementary resistive switching experiments are performed on equivalent stacks, i.e. $Pt/MO/TiO_x/Ti$. The correlation between the XPS results and the resistive switching characteristics (pristine leakage current, electroforming voltage, etc.) is discussed.

DS 40: Thin Film Properties: Structure, Morphology and Composition I

Time: Thursday 15:00–16:30 Location: CHE 89

DS 40.1 Thu 15:00 CHE 89

Novel Type of Bent-Lattice Nanostructure in Crystallizing Amorphous Films: from Transrotational Crystals to Amorphous Models — •Vladimir Kolosov — Ural Federal University, Ekaterinburg, Russia

Unusual transrotational thin crystals with curvilinear lattice [1] have been discovered by transmission electron microscopy (TEM) for crystal growth in thin (10-100 nm) amorphous films for growing number of different substances. The formation of unexpected transrotational nanostructures can be traced in situ in TEM column. Transrotation (unit cell translation is complicated by small rotation realized round an axis lying in the film plane) can result in strong regular lattice orientation gradients (up to 300 degrees per 1 micron) of different geometries: cylindrical, ellipsoidal, toroidal, saddle, etc. Complex skyrmion-like lattice orientation texture is observed in some spherulite crystals. The transrotation phenomenon is the basis for novel lattice-rotation/strain nanoengineering. Transrotational micro crystals have been eventually recognized in some vital thin film materials, i.e. PCMs for memory [2-3]. New nanocrystalline models of amorphous state are proposed: fine-grained structures with lattice curvature. Going to 3D clusters of positive/negative curvature and dynamics we propose the hypothesis of "dilatons" and "contractons" pulsating or/and circulating in amorphous/glassy solids. [1] V.Yu. Kolosov and A.R.Tholen, Acta Mat., 48 (2000) 1829. [2] B.J. Kooi and J.T.M. De Hosson, JAP, 95 (2004), 4714. [3] E. Rimini et al, JAP, 105 (2009), 123502.

DS 40.2 Thu 15:15 CHE 89

Evaluation of atomically-resolved high-resolution TEM images of Di-and Tri- Re molecules @ SWNT with convolutional neural networks — •Christopher Leist, Kecheng Cao, and Ute Kaiser — Central Facility of Electron Microscopy Materials Science, Ulm University, 89081 Ulm, Germany

Single-walled carbon nanotubes (SWNT) containing transition metal Di- and Tri- Re molecules are investigated using atomic resolution transmission electron microscopy (TEM).The images are taken at 80kV with the Cc/Cs-corrected SALVE instrument operated at 80kV, where the nanotube can be stable and sub-Angstrom resolution can be achieved. Detailed analysis of the Re atom distances is not only time consuming, also many interesting image features are close to the scale of the pixel error, and the manual evaluations are prone to user bias. Here we use deep learning routines which have the potential of both speeding up the evaluation process considerable as well as reducing the accompanied bias. The neural networks are trained on simulated TEM images. Here we present our progress in training the neural network and thereby automating the image investigation.

DS 40.3 Thu 15:30 CHE 89

Helium Ion Microscope (HIM) Imaging and Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) depth profiling of sample cross sections — •Nico Klingner, René Heller, and Gregor Hlawacek — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstr. 400, 01328 Dresden, Germany

The HIM is well known for its high-resolution imaging and nanofabrication performance. We have recently developed and presented a time-of-flight secondary ion mass spectrometer that can be retrofitted to existing microscopes [1,2].

Depth profiling in SIMS in general is usually done by sputtering into deeper layers and plotting the signal intensity over time. The actual milling depth can only be estimated and the common approach is to measure the crater depth with atomic force microscopy every time a compositional change is observed.

Direct imaging and chemical analysis of a cross-section with high spatial resolution can avoid this challenge. The cross sections will be prepared ex-situ by milling, grinding and low energy argon ion polishing.

[1] Klingner, N.; Heller, R.; Hlawacek, G.; von Borany, J.; Notte, J. A.; Huang, J. and Facsko, S.; Ultramicroscopy 162(2016), 91-97

[2] Klingner, N.; Heller, R.; Hlawacek, G.; Facsko, S. and von Borany, J.; Ultramicroscopy 198(2019), 10-17

DS 40.4 Thu 15:45 CHE 89

Impurity-Enhanced Solid-State Amorphization and Its Influence on Thin Film Formation — •Koen van Stiphout — Instituut voor Kern- en Stralingsfysica, KU Leuven, 3001 Leuven, Belgium — 2nd Institute of Physics, Georg-August-University Göttingen, 37077 Göttingen, Germany

The growth of amorphous compound thin films at the interface between a metal film and a semiconductor substrate upon annealing, has been studied extensively in the past. However, little is known about the influence of impurities of such a *solid-state amorphization (SSA)* reaction. Using *in situ* techniques, including synchrotron X-ray diffraction (XRD) and Rutherford backscattering spectrometry (RBS), we show that when small amounts of nitrogen impurities (< 2 at.%) are implanted under the right conditions, the amorphous, intermixed layer during the Ni-Si reaction can reach thicknesses of almost 70 nm before crystallizing, an order-of-magnitude thicker than in the unimplanted system[1]. The delayed crystallization of the amorphous layer has profound effects on the reaction path of the system, as the early stages of phase formation become an interplay of long-range diffusion and kinetic nucleation barriers. Furthermore, we show that the increased stability of the amorphous phase is not just a particularity of the solid-phase reaction, but a general property of the Ni-Si system. At the heart of this *impurity-enhanced* SSA reaction lies the strong asymmetry in atomic mobility of the elements, which is increased due to the addition of an immobile, insoluble impurity element.

[1] K. van Stiphout *et al.* 2019, J. Phys. D: Appl. Phys. **52**, 145301

DS 40.5 Thu 16:00 CHE 89

Band Engineering in Photonic Crystals with multi-order Square Lattice — •Jiaxu Chen, Fanzhou Lv, Yudie Huang, Zhihang Wang, Shiyao Jia, Yi Wang, and Wenxin wang — Harbin Engineering University, Harbin, China

2D Photonic crystals (PCs) can be artificially arranged as periodic arrays to arise interesting optical characteristics, because of their intrinsic photonic band structures that are obviously determined by the lattice parameters. Therefore, the idea of band engineering can be realized by nanofabrication and provides an effective way to control the optical performance. However, most studies focus on band engineering by embedding elements at high symmetry points (Γ, X, M) of Brillouin zone in reciprocal-space, systemic studies along the path (Δ, Σ, Z) between symmetry points are still lacking. Here, 2D PCs with square lattice are engineered into muti-order lattices by carefully embed with other periodic elements at specific positions that correspond embedding lattice sites at non-high-symmetry points of Brillouin zone. This work proves non-high-symmetry point embedding is also an approach for photonic band engineering in photonic crystals as well as high-symmetry point and it is an effective way to modulate the photonic performances. As a result, the engineered photonic bands of PCs exhibit Dirac-like conical dispersions and flat band structure.

DS 40.6 Thu 16:15 CHE 89

Band Engineering in Photonic Crystals with multi-order Square Lattice — •Chen jiaxu — Harbin Engineering University, Harbin, China

2D Photonic crystals (PCs) can be artificially arranged as periodic arrays to arise interesting optical characteristics, because of their intrinsic photonic band structures that are obviously determined by the lattice parameters. Therefore, the idea of band engineering can be realized by nanofabrication and provides an effective way to control the optical performance. However, most studies focus on band engineering by embedding elements at high symmetry points (Γ, X, M) of Brillouin zone in reciprocal-space, systemic studies along the path (Δ, Σ, Z) between symmetry points are still lacking. Here, 2D PCs with square lattice are engineered into muti-order lattices by carefully embed with other periodic elements at specific positions that correspond embedding lattice sites at non-high-symmetry points of Brillouin zone. This work proves non-high-symmetry point embedding is also an approach for photonic band engineering in photonic crystals as well as high-symmetry point and it is an effective way to modulate the photonic performances. As a result, the engineered photonic bands of PCs exhibit Dirac-like conical dispersions and flat band structure.

DS 41: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions V (joint session O/HL/DS/CPP)

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

Invited Talk DS 41.1 Thu 15:00 GER 38

Huge quantum effects on the 250 K superconducting lanthanum hydride — •Ion Errea — University of the Basque Country, Donostia/San Sebastián, Spain

The discovery of superconductivity at 200 K in the hydrogen sulfide system at large pressures was a clear demonstration that hydrogen-rich materials can be high-temperature superconductors. The recent synthesis of LaH10 with a superconducting critical temperature (Tc) of 250 K place these materials at the verge of reaching the long-dreamed room-temperature superconductivity. Here we show that quantum atomic fluctuations stabilize in the superconducting pressure range a high-symmetry Fm-3m crystal structure consistent with experiments, which has a colossal electron-phonon coupling of 3.5. Even if ab initio classical calculations predict this structure to distort below 230 GPa yielding a complex energy landscape, the inclusion of quantum effects evidences the Fm-3m as the true ground state. The agreement between the calculated and experimental Tc values further supports this phase as responsible for the 250 K superconductivity. The relevance of quantum fluctuations questions many of the crystal structure predictions made for hydrides within a classical approach that at the moment guide the experimental quest for room-temperature superconductivity. Furthermore, quantum effects are revealed to be crucial to stabilize solids with extraordinary electron-phonon coupling, which may otherwise be destabilized by the large electron-phonon interaction, reducing the pressures needed for their synthesis.

DS 41.2 Thu 15:30 GER 38

Self-Interaction Corrected SCAN for Solids: All-Electron Implementation with Numeric Atom-Centered Basis Functions — •Sheng Bi[1], Igor Ying Zhang[2], Christian Carbogno[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Fudan University, Shanghai, China

For all semi-local density-functional approximations (DFAs), electronic self-interaction errors lead to an erroneous description of charge-transfer processes, a systematic underestimation of band gaps in semiconductors, and incorrect total energies [1]. These errors can be alleviated via localized-orbital scaling corrections [2] or via self-interaction corrections (SIC) [3]. In this work, we have implemented a reciprocal-space formulation of self-consistent SIC in the all-electron, numeric atomic-orbitals code *FHI-aims*, which is applicable for all semi-local DFAs, including the promising meta-GGA "strongly constrained and appropriately normed" (SCAN) functional [4]. We validate our implementation by inspecting charge transfer, cohesive energies, and band gaps for a test set of molecules and solids, showing that SIC considerably improves SCAN calculations and yields results on par with standard *GW* calculations at a fraction of the computational cost. This allows us to use SCAN-SIC for studying the adsorption of organic molecules on the H-Si(111) surface.

[1] A. J. Cohen *et al.*, *Chem. Rev.* **112**, 289 (2011).
[2] N. Q. Su *et al.*, *Proc. Natl. Acad. Sci.* **115**, 9678 (2018).
[3] Z. Yan *et al.*, *Phys. Rev. A* **95**, 052505 (2017).
[4] J. Sun *et al.*, *Phys. Rev. Lett.* **115**, 036402 (2015).

DS 41.3 Thu 15:45 GER 38

Understanding the lattice dynamics of 3D hexagonal boron nitride (h-BN): beyond the LDA approach — •Luigi Cigarini, Michal Novotný, and František Karlický — Department of Physics, Faculty of Science, University of Ostrava, Czech Republic

It is fundamental to achieve a clear depiction of the lattice dynamics of 3D h-BN in order to understand the experimental outcomes. Five different stacking conformations are possible for 3D h-BN and at least two or three of them are systematically present in samples in variable amounts [1-2], resulting as a source of irreproducibility for experiments, such as the infrared optical response [3-4].

The lattice dynamics of h-BN is particularly tough to describe, stated the different nature of the forces participating in it: covalent bonds and Van der Waals interactions. The LDA approach seemed to be the most effective compromise, at the DFT level [1,5-6].

In this work we explain the surprisingly good performance of LDA. We also show that it is possible to achieve better results, in comparison with experimental IR spectra, by using, instead, the GGA approach to DFT and treating separately the two parts of the dynamical matrix. Besides, we found that IR spectroscopy is able to give some information about stacking composition. [1]. Liu, L. et al., Phys. Rev. B, 68(10), 104102 (2003). [2]. Constantinescu, G. et al., Phys. Rev. Lett., 111(3), 036104 (2013). [3]. Çamurlu, H.E. et al., Ceram. Int., 42(5), 6312-6318 (2016). [4]. Mukheem, A. et al., Nanomaterials, 9(4), 645 (2019). [5]. Cuscó, R. et al., Phys. Rev. B, 97(15), 155435 (2018). [6]. Serrano, J. et al., Phys. rev. lett., 98(9), 095503 (2007).

DS 41.4 Thu 16:00 GER 38

Error Estimation of Energy-per-Atom of Semiconductor Compounds Using Statistical Learning — •Daniel T. Speckhard[1,2], Sven Lubeck[2], Christian Carbogno[1], Luca Ghiringhelli[1], Claudia Draxl[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

Material databases such as NOMAD give researchers the ability to work with millions of material simulation results [1]. However, it is typically unclear to which extent calculations performed with different numerical settings and computer codes can be trusted and related to each other. This project presents statistical learning strategies to model errors in energies for two all-electron DFT codes, *FHI-aims* and `exciting`, for different basis-set sizes and **k**-point densities. Specifically, we use mutual information scores to select features that are able to capture the energy-per-atom errors. With respect to several metrics, random forest regression on the selected features shows the most promising results. This work lays the foundation for estimating errors in DFT data in NOMAD and helps to save computing resources by *a priori* predicting the DFT simulation settings required to achieve a desired level of precision. This also enables us to estimate the basis-set and **k**-point converged results of not fully converged calculations.

[1] C. Draxl and M. Scheffler, *J. Phys. Mat.*, **2** 036001 (2019). https://nomad-coe.eu

DS 41.5 Thu 16:15 GER 38

Force balance approach for advanced approximations in density functional theories — •Mary Leena Tchenkoue[1], Markus Penz[1], Iris Theophilou[1], Michael Ruggenthaler[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, New York NY 10010, USA

We propose a systematic and constructive way to determine the exchange-correlation potentials of density-functional theories including vector potentials. The approach does not rely on energy or action functionals. Instead it is based on equations of motion of current quantities (force balance equations) and is feasible both in the ground-state and the time-dependent setting. This avoids, besides differentiability and causality issues, the optimized-effective-potential procedure of orbital-dependent functionals. We provide straightforward exchange-type approximations for different density functional theories that for a homogeneous system and no external vector potential reduce to the exchange-only local-density and Slater Xα approximations.

DS 41.6 Thu 16:30 GER 38

Combining embedded mean field theory with linear-scaling density functional theory — •Joseph Prentice[1,2], Robert Charlton[2], Arash Mostofi[2], and Peter Haynes[2] — [1]St Edmund Hall and Department of Materials, University of Oxford, Oxford, UK — [2]Department of Materials, Department of Physics and the Thomas Young Centre, Imperial College London, London, UK

We demonstrate the capability of embedded mean field theory (EMFT) within the linear-scaling density-functional theory code ONETEP, which enables DFT-in-DFT quantum embedding calculations on systems containing thousands of atoms at a fraction of the cost of a full calculation. We perform simulations on a wide range of systems from molecules to complex nanostructures to demonstrate the performance of our implementation with respect to accuracy and efficiency. This work paves the way for the application of this class of quantum embedding method to large-scale systems that are beyond the reach of existing implementations.

DS 41.7 Thu 16:45 GER 38

Topological semimetallic phase in PbO_2 promoted by temperature — •Bo Peng[1], Ivona Bravić[1], Judith L. MacManus-Driscoll[2], and Bartomeu Monserrat[1] — [1]Cavendish Laboratory, University of Cambridge, United Kingdom — [2]Department of Materials Science and Metallurgy, University of Cambridge, United Kingdom

Materials exhibiting topological order host exotic phenomena that could form the basis for novel developments in areas ranging from low-power electronics to quantum computers. The past decade has witnessed multiple experimental realization and thousands of predictions of topological materials. However, it has been determined that increasing temperature destroys topological order, restricting many topological materials to very low temperatures and thus hampering practical applications. Here, we propose the first material realization of temperature promoted topological order. We show that a semiconducting oxide that has been widely used in lead-acid batteries, β-PbO_2, hosts a topological semimetallic phase driven by both thermal expansion and electron-phonon coupling upon increasing temperature. We identify the interplay between the quasi-two-dimensional nature of the charge distribution of the valence band with the three-dimensional nature of the charge distribution of the conduction band as the microscopic mechanism driving this unconventional temperature dependence. Thus, we propose a general principle to search for and design novel topological materials whose topological order is stabilized by increasing temperature. This provides a clear roadmap for taking topological materials from the laboratory to technological devices.

DS 41.8 Thu 17:00 GER 38

How Electric Fields Affect Intermolecular van der Waals Interactions — •Mohammad Reza Karimpour, Dmitry Fedorov, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

van der Waals (vdW) dispersion interactions between atoms or molecules originate from electromagnetic forces caused by the zero-point quantum-mechanical fluctuations of electronic charge densities. They are ubiquitous in nature and present in many areas of physics, chemistry, biology, and nanotechnology. Recently, it has been shown that the strength of vdW interactions can be controlled and tailored by external electric charges [1]. In addition, an external field strongly modifies the dispersion interaction between two hydrogen atoms and can change both its spatial dependence and its attractive or repulsive character [2]. To describe such important phenomena in large molecular systems, we employ the Many-Body Dispersion (MBD) method [3] based on the quantum Drude oscillator model. Since the conventional MBD method includes only dipole-dipole coupling, it does not capture the effects of external fields on vdW interactions. Therefore, we first extend the approach to dipole-quadrupole and quadrupole-quadrupole couplings. Then, the developed formalism is applied to calculate the MBD energy in the presence of an external electric field for low-dimensional systems including bilayer graphene.

[1] Kleshchonok and Tkatchenko, Nat. Commun. **9**, 3017 (2018)
[2] Fiscelli *et al.* arXiv:1909.03517 (2019)
[3] Tkatchenko *et al.* Phys. Rev. Lett. **108**, 236402 (2012)

DS 41.9 Thu 17:15 GER 38

Electronic structure of β-SiAlON: effect of Al/O doping and of finite temperature — •Saleem Ayaz Khan[1], Ondrej Šipr[2], Jiří Vackář[2], Robin Niklaus[3], Wolfgang Schnick[3], and Jan Minár[1] — [1]University of West Bohemia, Plzen, Czech Republic — [2]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [3]LMU Munich, Germany

Electronic structure of a series of ordered and disordered β-Si_{6-z}Al_{z}O_{z}N_{8-z} systems is investigated by means of ab initio calculations, using the FLAPW method as implemented in the wien2k code and Green function KKR method as implemented in the SPR-KKR code. Finite temperature effects are included within the alloy analogy model. We found that the trends with the Al/O doping are similar for ordered and disordered structures. The electronic band gap decreases with increasing z by about 1 eV when going from z=0 to z=2. The optical gap decreases analogously as the electronic band gap. The changes in the density of states (DOS) at Si and N atoms introduced by doping β-Si_{3}N_{4} with Al and O are comparable to the DOS at Al and O atoms themselves. The bottom of the conduction band in β-Si_{6-z}Al_{z}O_{z}N_{8-z} is formed by extended states residing on all atomic types. Increasing the temperature leads to a shift of the bottom of the conduction band to lower energies. The amount of this shift increases with increasing doping z.

DS 42: Focus Session: Functional Metal Oxides for Novel Applications and Devices III (joint session HL/DS)

electronics, power electronics, high-electron-mobility transisitors, memristors, topological quantum computation and so on. These functionalities typically require homo- or heteroepitaxial layers of high crystallinity with bendable amorphous semiconducting oxides as an exception. This session sets a focus on growth of bulk and thin films, experimental and theoretical investigation of their physical properties as well as fabrication and characterization of demonstrator devices.

Organizers: Oliver Bierwagen (Paul-Drude-Institut für Festkörperelektronik, Berlin), Holger Eisele (TU Berlin), Jutta Schwarzkopf (Leibniz-Institut für Kristallzüchtung, Berlin) and Holger von Wenckstern (Universität Leipzig).

Time: Thursday 15:00–16:30 Location: POT 81

DS 42.1 Thu 15:00 POT 81

Ab-initio investigation of first-order Raman scattering in gallium oxide — •Rouven Koch, Pasquale Pavone, Dmitrii Nabok, and Claudia Draxl — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Germany

In this work, we investigate the Raman tensors and first-order spectra of the β and α phase of Ga_2O_3 by means of first-principles calculations using the *ab-initio* methodology implemented in the software package `exciting` [1]. We start from the determination of the equilibrium crystal structure of both polymorphs. Then, we explore the lattice dynamics of the two phases, paying special attention to the characterization of the phonons at the Γ point. The peculiar properties of the polar phonon modes of the β phase are addressed, including the LO-TO splitting and reflectivity spectra. Then, we compute the frequency-dependent dielectric tensors within the random-phase approximation. The lattice-dynamical properties and the dielectric tensors are used for the calculation of the Raman spectra in different polarizations. The obtained polarized Raman spectra for α- and β-Ga_2O_3 are compared to available data in the literature [2]. Our results highlight the fact that excitonic effects do not play a significant role on off-resonance Raman spectra. The overall good agreement with the experiments indicates the accuracy of the approximations used in this calculation.

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

[2] C. Kranert *et al.*, Scientific Reports **6** (2016) 35964.

DS 42.2 Thu 15:15 POT 81

Raman-Spectroscopy of corundum-like α-Ga_2O_3 grown by HVPE — •Jona Grümbel[1], Pingfan Ning[1,3], Jürgen Bläsing[1], Dae-Woo Jeon[2], Martin Feneberg[1], and Rüdiger Goldhahn[1] — [1]Otto-von-Guericke-Universität Magdeburg — [2]Korean Institute of ceramic Engineering and Technology, Seoul, South Korea — [3]School of Electronics and Information Engineering, Tiangong University, China

Ga_2O_3 is a high-bandgap semiconductor, whose stable β-phase is already applicable to semiconductor power devices like FETs and Schottky-Diodes. The metastable, corundum-like α-phase is less discussed, but allows bandgap-engineering by alloying with α-Al_2O_3 (sapphire) or α-In_2O_3.

Here, we investigate the lattice vibrations in the context of crystal quality. Therefore, three different samples grown by three different variations of HVPE (halide vapor phase epitaxy) are investigated. For the characterization of phonon modes, Raman Spectroscopy is employed.

All seven Raman-active phonon modes are identified in different Raman setup configurations. We investigate the correlation of phonon energies and lattice parameters as determined by x-ray diffraction. A small but detectable influence of phonon deformation potentials is found. Moreover, we find a very pronounced influence of crystal quality - as witnessed by ω-scan relative amplitudes - on certain Raman-active phonon modes which might be used as marker for ample quality.

DS 42.3 Thu 15:30 POT 81

Raman spectroscopy as a tool to determine the Néel temperature of NiO thin films in correlation with their structural characteristics — •Johannes Feldl, Melanie Budde, Carsten Tschammer, Oliver Bierwagen, and Manfred Ramsteiner — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5–7, 10117 Berlin, Germany

NiO is one of the most common natural antiferromagnetic (AF) oxides and a transparent p-type semiconductor making this material interesting for both, applications in the fields of spintronics and transparent-oxide electronics. One of the crucial magnetic parameters of AF materials is the Néel temperature (T_N). For thin epitaxial films of NiO, T_N will depend on the growth conditions and their resulting structural properties and is therefore expected to deviate from the value of 523 K for bulk NiO. Here, we utilize Raman spectroscopy to study the magnetic and structural properties of NiO thin films. The films are grown on MgO(100) substrates by plasma-assisted molecular beam epitaxy at different substrate temperatures. For the assessment of the structural properties, Raman scattering by optical phonons is analysed. Regarding the experimental determination of T_N, we demonstrate a reliable approach by analyzing the temperature dependence of the two-magnon (2M) peak in the Raman spectra. The obtained T_N values are below 480 K and are found to be correlated with the in-plane strain and the degree of lattice disorder in the NiO films.

DS 42.4 Thu 15:45 POT 81

Phonons and free-carrier contributions of spinel $ZnGa_2O_4$ by spectroscopic ellipsometry — •Alwin Wüthrich[1], Martin Feneberg[1], Zbigniew Galazka[2], and Rüdiger Goldhahn[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Leibniz Institute for Crystal Growth, Berlin, Germany

Ga based spinels with the general formula of $MeGa_2O_4$, where Me is a divalent metal, such as $MgGa_2O_4$ or $ZnGa_2O_4$ offer an ultra wide band gap and good electrical conductivity. These transparent semiconducting oxides (TSOs) have been receiving greater interest in the last years due to an outstanding importance in a wide range of scientific disciplines, such as photoelectronics, sensing systems or optical applications. Here, bulk $ZnGa_2O_4$ single crystals were grown directly from the melt by the vertical gradient freeze (VGF) method. This study presents a characterisation of these bulk crystals by spectroscopic ellipsometry, from which the complex dielectric function (DF) was deduced. Free-carrier concentrations (n) up to 10^{19} cm^{-3} were investigated in the infrared spectral range, where the phonons and plasmons were determined. The former agrees well to prior theoretical and experimental studies while from the latter the dependence of the effective electron mass on n is achieved, indicating a non-parabolicity of the conductive band.

DS 42.5 Thu 16:00 POT 81

Electric and Thermoelectric Properties of $ZnGa_2O_4$ Bulk Crystals — •Johannes Boy[1], Martin Handwerg[1], Rüdiger Mitdank[1], Zbigniew Galazka[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, Max-Born-Strasse 2, 12489 Berlin, Germany

In the past years, intense research has been done in the field of oxide semiconductor materials, which are promising candidates for the design of novel high power devices, optoelectronics and sensing systems due to their wide bandgap. $ZnGa_2O_4$ is a transparent material of blue coloration, with a high bandgap E_g=4.6 eV at room temperature [1]. The majority charge carrier type is n-type. Electron mobilities up to 100 cm^2/Vs with charge carrier concentrations in the order of 10^{18} - 10^{19} cm^{-3} have been reported [1]. In this work, we manufactured microlabs on the chip [2] to investigate the temperature dependence of the Seebeck coefficient S, Hall charge carrier density n and mobility μ between $T = 10$ K and $T = 320$ K. At high bath temperatures $T > 230K$, the scattering is determined by electron-phonon-interaction. At low bath temperatures (between 10 and 150 K) we observe a temperature-independent maximum, which can be explained by electrons interacting with ionized impurities. The room temperature Seebeck coefficient is $S_{(300K)} = (-120\pm3)$ μV/K and decreases with decreasing bath temperature.[1] Z. Galazka, *et al.*; APL Materials **7**, 022512 (2019).

[2] J. Boy, *et al.*; APL Materials **7**, 022526 (2019).

DS 42.6 Thu 16:15 POT 81

Low-frequency noise characterization of MOCVD-grown β-Gallium Oxide — •Christian Golz[1], Günter Wagner[2], Saud Bin Anooz[2], Zbigniew Galazka[2], Andreas Popp[2], Fariba Hatami[1], and W. Ted Masselink[1] — [1]Department of Physics, Humboldt-Universität zu Berlin, Newton-Str. 15, D-12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin, Germany

Low-frequency noise spectroscopy was used to characterize defects and trap states in β-Ga_2O_3 epilayers. These high-quality Si-doped layers were homoepitaxially grown by metal-organic chemical vapour deposition (MOCVD)[1] on insulating Mg-doped β-Ga_2O_3 substrates prepared from bulk crystals obtained by the Czochralski method [2].

For noise measurements, lithographically defined Greek cross mesa structures were etched using hot H_3PO_4. Ohmic Ti/Au contacts were processed by e-beam evaporation. Generation-recombination noise, thermal noise, and 1/f noise are well resolved. Measured Hooge parameter values between 10^{-5} and 10^{-3} indicate a high structural quality of the epilayer. Generation-recombination noise was analyzed between 80 K and 400 K, finding up to three deep trap levels. Each of these deep traps is characterized in terms of their density, thermal activation energy, capture cross section prefactor, and binding energy.

[1] R. Schewski et al., APL Mater. 7, 022515 (2019); [2] Z. Galazka et al., ECS J. Solid State Sci. Technol. 6, Q3007 (2017)

DS 43: Thin Film Properties: Structure, Morphology and Composition II

Time: Thursday 16:45–18:15 Location: CHE 89

DS 43.1 Thu 16:45 CHE 89

Growth and electronic structure of hexagonal BN on a curved Rh(111) crystal — •Khadiza Ali[1], Laura Fernandez[1], Anna Makarova[2], Igor Piš[3], Federica Bondino[3], Enrique Ortega[1], and Fredrick Schiller[1] — [1]Centro de Física de Materiales (CSIC-UPV/EHU), 20018, San Sebastian, Spain — [2]Institut für Festkörperphysik, TU Dresden, D-01069 Dresden, Germany — [3]Elettra Sincrotrone Trieste, Strada Statale 14 Km 163.5, I-34149 Trieste, Italy

Understanding the growth of a hexagonal boron nitride (h-BN) monolayer has gained interest in the scientific community owing to its many-sided impact in the field of two-dimensional materials. We have investigated the growth and electronic structure of h-BN on vicinal rhodium surfaces in a systematic manner, using a crystal curved around the (111) face. While at the flat Rh(111) h-BN forms the *nanomesh* structure due to the lattice mismatch and strong chemical interaction to the substrate, h-BN on Rh vicinal surfaces leads to substrate faceting with well-ordered step arrays, that is, in a slightly different way as on vicinal Ni . Using STM we observe nanoribbons with hole and wire regions at the (111) facets that are separated by multiple steps. The electronic structure (using XAS, XPS and ARPES) reveals that the interaction of h-BN and the substrate gets stronger for densely stepped Rh substrates, contrary to nickel . For large vicinal angles α >10°, the (111) facets are too short for establishing the nanomesh and a stable side facet emerges tilted by approx. α=23° with respect to the Rh(111). ARPES measurements finds characteristic h-BN bands for this stable nanofacet.

DS 43.2 Thu 17:00 CHE 89

Broad Absorptance Behavior of High Entropy Oxide (MgCoNiCuZn)O — •Maria Barrera, Emeline Michele, Lars Wening, and Matthias Wuttig — IA Instutute of Physics RWTH Aachen University, Aachen, Germany

Near-equimolar High Entropy Oxides (HEO), which are stabilized due to the entropy-driven formation of simple-phases, provide an interesting combination of properties including colossal dielectric constants. (MgCoNiCuZn)O high entropy oxide films have been deposited onto silicon and glass via reactive magnetron sputtering using a MgCoNiCuZn target. Thin films show an unusually broad absorptance (1-R-T) ranging from the ultraviolet to the near-infrared regime. The origin of this unconventional absorption is related to the crystallographic structure, grain size, and composition for films deposited at different oxygen partial pressures.

DS 43.3 Thu 17:15 CHE 89

Investigation of thin boron layers on silicon (PureB) by means of x-ray photoelectron spectroscopy (XPS) — •Annika Stefanie Burkowitz[1], Marie Schmitz[1], Lukas Kesper[1], Ulf Berges[1], Stefan Dreiner[2], Daniel Weier[2], Lis Karen Nanver[3], and Carsten Westphal[1] — [1]DELTA/Experimentelle Physik I, TU Dortmund, Maria-Goeppert-Mayer-Straße 2, 44221 Dortmund, Germany — [2]Fraunhofer Institute for Microelectronic Circuits and Systems, Finkenstr. 61, 47057 Duisburg, Germany — [3]University of Twente, Drienerlolaan 5, 7522 NB Enschede, The Netherlands

We present an investigation of thin pure boron layers (PureB) on silicon. The name PureB was introduced in order to distinguish pure boron layers that lie on top of the substrate from boron doped into the substrate.

PureB systems yield excellent results regarding detection of ultraviolet light and low-energy electrons. The required extremly shallow pn-junctions can be fabricated by growing a few nanometers thick boron layer to ultra-pure silicon substrate wafers. Detectors using the PureB technology show a sensitivity close to the theoretical limit and a good robustness as well as an exceptionally low leakage current.

These outstanding properties are associated with the boron-silicon interface. Therefore, the aim of this research is to analyze the interface between the silicon substrate and the boron adsorbate by means of x-ray photelectron spectroscopy (XPS). XPS studies reveal information about chemical bonding types present in the boron layer and about the composition of the surface.

DS 43.4 Thu 17:30 CHE 89

Important factors influencing the electrical properties of polycrystalline AZO thin films — •Petr Novák[1], Tomáš Kozák[2], Petra Šotová[1], Lucie Prušáková[1], and Rostislav Medlín[1] — [1]New Technologies - Research Centre, University of West Bohemia, Plzeň, Czech Republic — [2]Department of Physics and NTIS - European Centre of Excellence, University of West Bohemia, Plzeň, Czech Republic

The aluminium-doped zinc oxide (AZO) may have similar electrical and optical properties to more expensive Indium-tin oxide (ITO), which is mostly used material for transparent conductive electrodes. Nevertheless, it is difficult to obtain comparable conductivity at deposition temperatures below 100°C. The fundamental benefit of ITO films is good conductivity also in the nanocrystalline or amorphous phase. On the contrary, well crystalline structure is required to obtain suitable properties of AZO. The present work deals with investigation of the relation between electrical properties of AZO and the film structure observed by electron microscopy. The structural defects formed under different conditions such as grain boundary or basal edge dislocations were observed by SEM and TEM. In particular, the investigation focuses on the grain boundary scattering, which reduces the mobility of the free carriers. The work is also devoted to the influence of oxygen conditions on the carrier concertation, which corresponds to the presence of various intrinsic defects at oxygen poor and oxygen rich conditions.

DS 43.5 Thu 17:45 CHE 89

Low-temperature growth of Ga_2O_3 thin films by PEALD — •Ali Mahmoodinezhad[1], Christoph Janowitz[1], Franziska Naumann[2], Paul Plate[2], Hassan Gargouri[2], Karsten Henkel[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, K.-Zuse-Str. 1, 03046 Cottbus, Germany — [2]SENTECH Instruments GmbH, Schwarzschildstraße 2, 12489 Berlin, Germany

Thin films of gallium oxide (Ga_2O_3) were deposited on silicon (100) through plasma-assisted atomic layer deposition with alternating supply of trimethylgallium and oxygen plasma at low substrate temperatures of 80 to 200 °C. The optical and electrical properties as well as the chemical composition of the Ga_2O_3 films were investigated by spectroscopic ellipsometry (SE), capacitance-voltage (C-V) measurements, and X-ray photoelectron spectroscopy (XPS) documenting the high quality of the films. A constant growth rate of ~ 0.66 Å per cycle accompanied by a low inhomogeneity of $\leq 2\%$ was determined from the SE data for all temperatures. We found a temperature-independent refractive index (1.86±0.01 at 632.8 nm) whereas the optical bandgap decreased with increasing temperature (from 4.68 to 4.57 eV). XPS analysis revealed an almost ideal Ga:O ratio of 2:3 for all temperatures, with the lowest carbon contamination ($\sim 10\%$) for deposition at 150 °C. Furthermore, from the C-V data a permittivity of 9.7±0.2 (at 10 kHz) as well as fixed and mobile oxide charge densities in the order of 1 to 4×10^{12} cm^{-2} were deduced.

DS 43.6 Thu 18:00 CHE 89

Transitions between growth modes in lattice KMC simulations — •Eelco Empting, Miriam Klopotek, and Martin Oettel — Insitut für angewandte Physik, University of Tübingen, Germany

We study heteroepitaxial growth on the lattice using Kinetic Monte Carlo (KMC) with nearest-neighbor interactions between particles and contact particle-substrate interactions as well as Ehrlich-Schwöbel (ES) barriers. Two different models are implemented: (i) a solid-on-solid (SOS) model and (ii) a model in which particles are allowed to desorb from the film and diffuse in the gas phase (colloidal growth model, CGM).

Typical experimental growth modes (layer-by-layer, island and 3D growth) are recovered and we identify several dynamical transitions between these.

In the extreme case of an infinite ES barrier, the CGM model results in a behavior which significantly differs from that of the SOS model due to the possible desorption to and resorption from the gas phase.

DS 44: Magnetic Coupling and Anisotropy in Thin Films (joint session MA/DS)

Time: Friday 9:30–13:00 Location: HSZ 04

DS 44.1 Fri 9:30 HSZ 04

Imaging of ultrafast spin dynamics using high-harmonic radiation — •Sergey Zayko[1], Ofer Kfir[1], Michael Heigl[2], Michael Lohmann[1], Jakob Hagen[1], Murat Sivis[1], Manfred Albrecht[2], and Claus Ropers[1] — [1]IV Physical Institute, University of Göttingen — [2]Experimental physics IV, University of Augsburg

The demand for next-generation information processing methodologies increases the interest in spintronic devices, as they may offer energy-efficient operation at THz frequencies [1,2]. Such developments require means for tracking of magnetic dynamics with nanoscale resolution and a temporal precision well below a picosecond, as highlighted in a first experimental effort [3]. Here we utilize MCD (magnetic circular dichroism) imaging with high-harmonic radiation [4] for the mapping of spin-texture dynamics. Our experiment captures magnetic movies with a combined 40 nm spatial- and 40 femtosecond temporal resolutions, and images with resolution better than 20 nm. We use these capabilities to follow the ultrafast responses of magnetic domains in materials with perpendicular magnetic anisotropy, such as local ultrafast demagnetization and non-local dynamics near domain walls. We believe that our approach will yield deeper insights into the corresponding physics of the ultrafast magnetism and become an indispensable tool for applied research.

[1] A. Fert, V. Cros, and J. Sampaio, Nat Nano 8, 152 (2013). [2] Nature Nanotech 10, 185 (2015). [3] C. von Korff Schmising et al., Phys. Rev. Lett. 112, 217203 (2014). [4] O. Kfir, S. Zayko et al.,

Science Advances 3, eaao4641 (2017).

DS 44.2 Fri 9:45 HSZ 04

Complex spin textures and domain-wall pinning in Sm-Co magnets — Leonardo Pierobon[1], András Kovács[2], Robin E. Schäublin[1], Stephan S. A. Gerstl[1], Urs Wyss[3], •Jan Caron[2], Rafal E. Dunin-Borkowski[2], Jörg F. Löffler[1], and Michalis Charilaou[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland — [2]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, FZ Julich, Germany — [3]Arnold Magnetic Technologies, Switzerland

Sm-Co alloys are the best-performing permanent magnets at high temperatures due to their cellular microstructure, which consists of a Sm2Co17 matrix and SmCo5 cells intersected by Zr-rich platelets. Although extensive research has been done to understand the connection between the magnet's microstructure and its magnetic properties, theory and experiments have still not converged. To tackle this issue, we use Lorentz transmission electron microscopy, off-axis electron holography and micromagnetic simulations. We find that the magnetization reversal starts by domain-wall nucleation at the interfaces between Zr-rich platelets and the Sm2Co17 matrix. Despite strong pinning at the SmCo5 cells, curling instabilities form where all three phases meet, further propagating the reversal. Unexpectedly, we also find topologically non-trivial structures with 2π winding that significantly affect the reversal. Based on this, we propose a modification of microstructure to increase the coercivity and remanence.

DS 44.3 Fri 10:00 HSZ 04

Titanium d-ferromagnetism with perpendicular anisotropy in defective anatase — •Markus Stiller[1], Alpha T. N'Diaye[2], Hendrik Ohldag[2], José Barzola Quiquia[1], Pablo D. Esquinazi[1], Thomas Amelal[3], Carsten Bundesmann[3], Daniel Spemann[3], Martin Trautmann[4], Angelika Chassé[4], Hichem Ben Hamed[4], Waheed A. Adeagbo[4], and Wolfram Hergert[4] — [1]Felix-Bloch-Institute for Solid-state Physics, University of Leipzig, Germany — [2]ALS, Lawrence Berkeley National Laboratory, USA — [3]Leibniz Institute of Surface Engineering, Germany — [4]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany

Undoped TiO2 anatase thin films were grown on LAO and STO substrates. Ferromagnetism was generated at the surface of anatase films by low-energy ion irradiation. Ar+-ion irradiation resulted in a thin (10nm) ferromagnetic surface layer. Field hysteresis as well as zero-field cooled and field cooled curves reveal that, after irradiation the samples show ferromagnetism at room temperature with an out-of-plane easy axis and low remanence. Magnetic force microscopy reveals that this low remanence is due to oppositely aligned magnetic domains. XMCD measurements at room temperature show that the band at the titanium L-edges is spin polarized, not at the O K-edge. Together with DFT calculations, the results indicate that Ti vacancy-interstitial pairs are responsible for the magnetic order. These results open up interesting possibilities for future applications, e.g. single domain patterns of μm size can be easily prepared. Further, they contradict the theory of paramagnetism due to vacuum fluctuations proposed by Coey.

DS 44.4 Fri 10:15 HSZ 04

Magnetic anisotropy of disordered FeRh thin films probed by X-band ferromagnetic resonance — •Jonas Wiemeler[1], Anna Semisalova[1], Benjamin Zingsem[1], Nicolas Josten[1], Ralf Meckenstock[1], Rantej Bali[3], Kay Potzger[3], Jürgen Lindner[3], Jürgen Fassbender[3], Thomas Thomson[2], and Michael Farle[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]The University of Manchester, UK — [3]Institute of Ion Beam Physics and Materials Research, HZDR, Germany

The ion irradiation induced disorder in FeRh thin films changes certain magnetic properties, such as phase transition temperature from AF to FM states and saturation magnetisation. Furthermore, the free energy density changes correspondingly to the magnetocrystalline anisotropy variation in irradiated films. Here, ferromagnetic resonance (FMR) experiments were carried out to analyse the magnetic anisotropy of 25 keV Ne^+-irradiated 40 nm thick $Fe_{50}Rh_{50}$ films. A total of 6 films, irradiated with an ion fluence of $1 \cdot 10^{13} - 4 \cdot 10^{14}\ \frac{\text{Ions}}{\text{cm}^2}$, were characterised with FMR at 100 - 400 K and compared with a non-irradiated film.

The anisotropy of Ne-irradiated FeRh thin film changes from cubic for a low ion fluence to a mixture of cubic and in-plane uniaxial anisotropy, the latter contribution turns out to be dominating for higher fluence. The sign of the perpendicular magnetic anisotropy constant $K_U = K_{2\perp}$ was found to reverse while Ne^+ fluence is increasing. Supported by DFG SE2853/1-1, BA5656/1-1.

DS 44.5 Fri 10:30 HSZ 04

Ferromagnetic writing on B2 $Fe_{49}Rh_{51}$ thin films using ultra-short laser pulses — •Alexander Schmeink[1,2], Benedikt Eggert[3], Jonathan Ehrler[1], Mohamad-Assaad Mawass[4], René Hübner[1], Kay Potzger[1], Jürgen Lindner[1], Jürgen Fassbender[1,2], Florian Kronast[4], Heiko Wende[3], and Rantej Bali[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Fakultät für Physik, Technische Universität Dresden, Germany — [3]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Germany — [4]Helmholtz-Zentrum Berlin, Germany

Laser manipulation of magnetic properties has potential applications in data storage. The equiatomic B2 FeRh alloy is well-known to show a metamagnetic isostructural antiferromagnetic (AFM) to ferromagnetic (FM) transition at ≈370 K. In contrast to the temperature-driven transition an AFM B2 → FM B2 transition can be induced via a decrease of short-range atomic order, which can be realised in alloy thin films using ion beams as well as laser pulses.[1]

Here we irradiate B2 $Fe_{49}Rh_{51}$ thin films of ≤ 30 nm thicknesses with ~ 100 fs laser pulses and observe the induced magnetic and structural changes. Depending on the laser fluence transitions of AFM to FM B2 $Fe_{49}Rh_{51}$ and with further disordering to the paramagnetic A1 structure are observed. The deposited energy influences the resolidifcation of the alloy, thereby determining the structure.

This work is funded by the DFG (BA 5656/1-1 and WE 2623/14-1).

[1] J. Ehrler et al. *ACS Applied Materials & Interfaces* **2018** 10 (17), 15232-15239

DS 44.6 Fri 10:45 HSZ 04

Magnetic structure and coupling phenomena of DyCo alloys — •Dieter Lott[1], Kai Chen[2], André Philippi-Kobs[3], and Valeria Lauter[4] — [1]Institute of Material Research, Helmholz-Zentrum Geesthacht, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, 12489 Berlin, Germany — [3]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, Germany — [4]Neutron Scattering Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

In the last years, alloys of rare-earth elements and 3d transition metals (RE-TM) became again in the focus of attention due there rich variety of magnetic effects owed to the different anisotropies of both material classes. Despite of their amorphous composition, this material class exhibits complex magnetic ordering resulting into non-collinear spin structures and the occurrence of magnetic chirality effects. Lately, different exchange bias phenomena were discovered in DyCo single films and in heterostructures [1,2]. In a very recent study, the occurrence of skyrmions in a single DyCo film could be observed. The analysis of the magnetic microstructure is one of the important keys for understand the underlying mechanism behind these intriguing phenomena. In this work, we report recent results on DyCo/NiFe thin films investigated via polarized neutron reflectometry. The analysis of the magnetic and chemical depth profiles at different magnetic fields and temperature allows one to gain insights into the coupling mechanism in these heterostructures.

15 min. break.

DS 44.7 Fri 11:15 HSZ 04

Crystallographic and magnetic structure in Co thin films investigated by NMR — •Patrizia Fritsch[1], Juriaan Lucassen[2], Casper F. Schippers[2], Marcel A. Verheijen[2,3], Erik J. Geluk[4], Beatrice Barcones[4], Rembert A. Duine[2,5], Henk J. M. Swagten[2], Bert Koopmans[2], Reinoud Lavrijsen[2], and Sabine Wurmehl[1,6] — [1]IFW Dresden, Germany — [2]Department of Applied Physics, TU Eindhoven, the Netherlands — [3]Eurofins Materials Science, Eindhoven, the Netherlands — [4]NanoLab@TU/e, TU Eindhoven, the Netherlands — [5]Institute for Theoretical Physics, Utrecht University, the Netherlands — [6]Institute of Solid State and Materials Physics, TU Dresden, Germany

Co thin films sandwiched between Pt and Ir (Pt (4 nm) / Co (t) / Ir (3 nm)) with t = 5 - 25 nm were grown. These films showed an increase in the out of plane (oop) magnetic anisotropy constant K above a critical thickness t_{cr}. The increase in the anisotropy K is linked to the formation of hcp Co on top of fcc Co due to lattice relaxation with increasing thickness t. We measured two films with Co thicknesses t

$= 10$ nm $> t_{cr} > t = 25$ nm by means of ^{59}Co zero-field nuclear magnetic resonance spectroscopy (ZF NMR) exploiting the internal field of the ferromagnetic material. ZF NMR is sensitive to changes in the local crystallographic and magnetic environment. In this contribution we will explain the overall increase of the anisotropy K due to magnetocrystalline (intrinsic) and magnetoelastic (extrinsic) effects on the basis of the ^{59}Co ZF NMR data.

DS 44.8 Fri 11:30 HSZ 04

Magneto-optical signal dependence on Co-layer thickness asymmetry in Co/Pt/Co-films — •Ramon Weber[1], Carmen Martín Valderrama[1,2], Lorenzo Fallarino[1], and Andreas Berger[1] — [1]CIC nanoGUNE, E-20018 Donostia-San Sebastian, Spain — [2]Faculty of Science, University of Valladolid, E-47011 Valladolid, Spain

Ever since the first observation of interlayer exchange coupling, magnetic multilayers have been a research subject of tremendeous importance, leading to many surprising phenomena. In a recent study, Tomita *et al.* [1] observed a most significant enhancement of the magneto-optical response in Fe/Pt multilayers that followed an inverse Fibonacci thickness stacking in comparison to periodically modulated reference samples. This effect could not be explained by classical electromagnetic theory assuming local material dependent dielectric properties, but might be related to quantum mechanical interferences associated with non-periodic stacking of nm-scale magnetic films and their resulting quantum well states. To test this explanation, we fabricated a series of Co/Pt/Co bilayer structures with pre-defined and variable thickness asymmetry of the Co layers, while keeping the total Co thickness constant. The optical and magneto-optical properties of these films were measured using Generalized Magneto-optical Ellipsometry, both as a function of the Co-layer thickness asymmetry and the Pt interlayer thickness.
[1] S. Tomita, T. Suwa, P. Riego, A. Berger, H. Nobuyoshi, and H. Yanagi, Phys. Rev. Appl. 11, 064010 (2019).

DS 44.9 Fri 11:45 HSZ 04

Interlayer exchange coupling in Fe/MgO[001] multilayers — •Tobias Warnatz[1], Fridrik Magnus[2], Sarah Sanz[1], Hasan Ali[3], Klaus Leifer[3], and Björgvin Hjörvarsson[1] — [1]Department of Physics and Astronomy, Uppsala University, Sweden — [2]Science Institute, University of Iceland, Reykjavik, Iceland — [3]Department of Engineering Sciences, Uppsala University, Sweden

Fe/MgO/Fe tunnel junctions are well known for their magnetoresistance, but their interlayer exchange coupling (IEC) [1] is less explored. Recently, we reported a sequential magnetic switching in interlayer exchange coupled Fe/MgO[001] superlattices [2]. The presented results were consistent with a beyond nearest neighbor IEC. Here, we report the first systematic investigation on the range of IEC in epitaxial Fe/MgO[001] multilayers. For that, samples with various Fe/MgO bilayer repetitions (N) were grown on single crystalline MgO(001) substrates. Hystereses curves with discrete magnetization steps were obtained, consistent with our previous results [2]. Taking only nearest-neighbor interactions into account, a reduction of the IEC by a factor of (1-1/N) should be observed [3] (the missing neighbor of the outermost layers becomes less important for many N). Our results deviate drastically from this prediction and verify a strong contribution from beyond nearest neighbor interactions. The results are essential for the understanding of the IEC in tunnel junctions and could even serve as a base for the development of three-dimensional data structures.

[1] Phys. Rev. Lett. 89, 106602 (2002) [2] Phys. Rev. B 97, 74424 (2018) [3] Appl. Phys. Lett. 58, pp. 1473-1475 (1991)

DS 44.10 Fri 12:00 HSZ 04

Probing the origin of ferromagnetic stability in LSMO/SRO — •Anna Zakharova — Swiss Light Source, Paul Scherrer Institut

The technological application of optimally doped mangnite is hindered due to the existence of a magnetic dead layer. However, when in contact with $SrRuO_3$ $La_{0.7}Sr_{0.3}MnO_3$ remains magnetic down to 1-2 u.c. Therefore in this work we investigate the origin of the ferromagnetic stability of LSMO in LSMO/SRO bilayers by using resonant x-ray spectroscopy varying thickness of LSMO and SRO deposited on $SrTiO_3$. Magnetic switching of LSMO in proximity with 20 u.c. SRO was observed even below critical thickness of LSMO. Moreover, 4 u.c. of LSMO shows remanence above SRO T_c. The XLD data evidences a preferential $d3z^2 - r^2$ occupation of Mn in LSMO/SRO interface in agreement with theoretical predictions. In addition, different Mn valence is observed for ultra-thin LSMO/SRO in comparison to LSMO//STO. These results combined can explain why the ferromagnetism is stabilized at LSMO/SRO interface.

DS 44.11 Fri 12:15 HSZ 04

Influence of structure and cation distribution on magnetic anisotropy and damping in Zn/Al doped nickel ferrites — •Julia Lumetzberger, Martin Buchner, Santa Pile, Verena Ney, and Andreas Ney — Johannes Kepler University Linz, Institute for Semiconductor and Solid State Physics, Linz, Austria

In spintronics one aims to obtain pure spin currents as an additional degree of freedom. To ensure a pure spin component ferromagnetic insulators are the material of choice. Promising results are obtained by cubic NiZnAl ferrite thin films grown on spinel MgAl$_2$O$_4$[1].In this contribution we use reactive magnetron sputtering as a preparation method to optimise the magnetic properties. All samples are analysed with X-ray diffractometry for their crystallographic properties. Furthermore, the angular and frequency dependence of the resonance position is measured by ferromagnetic resonance (FMR) and fitted to quantify the anisotropy fields as well as magnetic damping. Additionally, transmission electron microscopy is performed to investigate the interface on an atomic scale and the chemical composition by means of ion beam analysis. In a last step x-ray magnetic circular dichroism (XMCD) and XMCD (H) at the L$_{3,2}$ edge of Ni and Fe are performed to complement the integral SQUID magnetometry measurements and evidence their magnetic contributions to the hysteresis separately. A comparison between similarly strained materials revealed the importance of site occupancy as a major tuning factor for magnetic anisotropy and damping [2]. [1] S. Emori et. al., Adv. Mater. (2017), 29, 1701130 [2] J. Lumetzberger, arXiv:1908.08257 (2019)

DS 44.12 Fri 12:30 HSZ 04

Artificial bulk metamaterials based on graded epitaxial Co-alloy films — •Lorenzo Fallarino, Mikel Quintana, Ramon Weber, and Andreas Berger — CIC nanoGUNE, 20018 Donostia-San Sebastian, Basque Country, Spain

A very promising alternative to traditional magnetic information storage is based upon encoding information via non-collinear magnetic textures. They occur in certain materials with structure inversion asymmetry, a property that in conjunction with spin-orbit coupling leads to the Dzyaloshinskii-Moriya interaction (DMI). At interfaces between magnetic layers and heavy metals the DMI can be strong enough to promote non-collinear spin textures as ground states [1]. However, any real multilayer is prone to growth induced imperfections at each interface that can strongly affect the energetic landscape. Likewise, interfaces are the only portions that can be influenced in such multilayers, inherently limiting the total active contributions to a small fraction of an entire structure. Along these lines, we have devised an innovative approach by means of artificial bulk metamaterials Co$_{1-x}$A$_x$ (with A = Ru, Pt, Cr) exhibiting pre-defined graded composition structures, allowing for an expansion of DMI generating interfaces into the entirety of the material, thus enabling all-interface-bulk metamaterial. [1] A. Fert, N. Reyren, and V. Cros, Nat. Rev. Mat. 2, 17031 (2017).

DS 44.13 Fri 12:45 HSZ 04

Growth, structure, and magnetic properties of artificially layered NiMn in contact to ferromagnetic Co on Cu$_3$Au(001) — •Tauqir Shinwari[1], Ismet Gelen[1], Melek Villanueva[2], Yasser A. Shokr[1,3], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Division of Permanent Magnets and Applications, IMDEA Nanoscience, 28049, Madrid, Spain — [3]Faculty of Science, Department of Physics, Helwan University, 17119 Cairo, Egypt

A series of experiments is carried out to identify the fundamental mechanisms leading to the exchange-bias effect in ultrathin epitaxial layered ferromagnetic/antiferromagnetic (FM/AFM) samples on Cu$_3$Au(001). The studied samples are single-crystalline antiferromagnetic artificially layered [Ni/Mn] films covered by ferromagnetic Co layers, deposited under ultrahigh-vacuum conditions. The approach is to study the structural and magnetic properties of artificially ordered layers of Ni and Mn in contact to Co by using low-energy electron diffraction (LEED) and magneto-optical Kerr effect, respectively, and comparing with disordered Ni$_x$Mn$_{1-x}$ alloy films with the same Ni/Mn ratio and the same film thickness. We found from LEED I(V) curves that the perpendicular interatomic lattice distance is decreased in the artificially layered [Ni/Mn] samples in comparison to the disordered Ni$_x$Mn$_{1-x}$ alloy films. This change in the structure causes higher coercivity, exchange bias, and stronger exchange coupling in artificially layered [Ni/Mn] samples compared to disordered Ni$_x$Mn$_{1-x}$ alloy films.

DS 45: Thin Film Properties: Structure, Morphology and Composition III

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

DS 45.1 Fri 9:30 CHE 89

L1$_0$-ordered ferrimagnetic Fe$_{100-x}$Cr$_x$Pt(001) thin films. — •Nataliia Schmidt[1], Ritwik Mondal[2], Andreas Donges[2], Laszlo Szunyogh[3], Ulrich Nowak[2], and Manfred Albrecht[1] — [1]Institute of Physics, University of Augsburg, Germany — [2]Department of Physics, University of Konstanz, Germany — [3]Department of Theoretical Physics, Budapest University of Technology and Economics, Hungary

Tuning the properties of hard magnetic L1$_0$ FePt thin films is of high interest from a fundamental as well as technological point of view[1]. In this regard, 10 nm thick (Fe$_{100-x}$Cr$_x$)$_{50}$Pt$_{50}$ films (where $x = 0-100$ at.%) were prepared by epitaxial growth on MgO(100) substrates at 800°C. All samples reveal pronounced L1$_0$ chemical ordering. Strong perpendicular magnetic anisotropy (PMA) at 300 K persists up to 20 at.% Cr on Fe sites in L1$_0$ lattice. With addition of 45 at.% Cr, PMA gets strongly reduced. The coercive field in out-of-plane direction decreases from 42.94 kOe to 10.82 kOe with addition of 20 at.% Cr, which is attributed to a strong modification of the film morphology changing from island-like to a more continuous film. Depending on the Cr concentration, magnetic moments of Fe and Cr experience strong frustration due to antiferromagnetic coupling of Fe-Cr and Cr-Cr, but ferromagnetic interaction between Fe-Fe. For direct comparison with our experiments ground state as well as thermal properties were calculated within the framework of atomistic spin model simulations where the model parameters rest on first principles calculations.

[1] N. Y. Schmidt et al., Phys. Rev. B **100**, 064428 (2019).

DS 45.2 Fri 9:45 CHE 89

From colloidal Cu2ZnSnS4 (CZTS) nanocrystals to highly conductive p-type thin films — •Oleksandr Selyshchev[1], Alexandra Raevskaya[1], Volodymyr Dzhagan[2,3], Serhiy Kondratenko[3], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Institute of Semiconductor Physics, Nat. Acad. Sci. of Ukraine, 03028 Kyiv, Ukraine — [3]Department of Physics, Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine

CZTS is object of intensive research due to its perspectives in light harvesting applications. The benefits of the material are the direct tunable bandgap (1.5-2.0 eV), the high absorption coefficient, and the earth abundance and low toxicity of the constituents. In the focus of our research are aqueous colloidal CZTS nanocrystals (NCs) prepared in a green way. Details on the synthesis and spectral characteristics can be found in ref. [1]. Here we report on 50-100 nm thin CZTS films prepared by spin coating of a CZTS NC ink (a concentrated coloidal solution of CZTS NCs) on glass substrates. The conductivity of the films reaches 250 S/cm (300 K). The p-type conductivity is evident from the non-zero density of states at the Fermi edge in the X-ray photoemission spectra (XPS). The kesterite crystal structure of the material was confirmed by Raman spectroscopy. Composition and chemical states of the elements on the surface were examined by XPS. The optical absorption/reflection were studied in the visible, near-, and middle-infrared ranges. [1] Stroyuk et al., Sci Rep,(2018)8,13677, DOI:10.1038/s41598-018-32004-1.

DS 45.3 Fri 10:00 CHE 89

Metal phosphide deposited by atomic layer deposition for efficient electrochemical water splitting — •Haojie Zhang[1], Stefan L. Schweizer[1], and Ralf B. Wehrspohn[1,2] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, Heinrich-Damerow-Straße 4, 06120 Halle (Saale), Germany. — [2]Fraunhofer Institute for Microstructure of Materials and Systems, Walter-Hülse-Straße 1, Halle (Saale), Germany.

Transitional metal phosphide (TMP) has attracted great research interests due to its tunable crystal phases and excellent catalytic activity for electrochemical water splitting. However, TMP prepared by atomic layer deposition (ALD) has not be reported to date. Therefore, we herein report an improved ALD process to produce well-crystalline TMP ultrathin films. Our optimized ALD recipe demonstrated a controllably layer-by-layer deposition behavior. Furthermore, the deposited TMP exhibited a better hydrogen evolution reaction performance than that prepared by the traditional post-phosphorization method. Our strategy shows a huge application potential in various electrochemical areas.

DS 45.4 Fri 10:15 CHE 89

Investigation of early stage kinetics of SBS glasses in aqueous solutions using a slow positron beam — •Eric Hirschmann[1,3], Maik Butterling[1], Oskar Liedke[1], Ahmed Gamal Attallah[1], Andreas Wagner[1], Dirk Enke[2], and Reinhard Krause-Rehberg[3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Universität Leipzig, Leipzig, Germany — [3]Martin-Luther-Universität Halle-Wittenberg, Halle(Saale), Germany

Thin porous layers at the surface of sodium borosilicate glass(200-2000 nm) were generated via a combination of phase separation and selective leaching. It is possible to control the range of pore size by modifying the heat treatment and the layer thickness by varying the leaching process. The kinetic reaction of the leeching process in SBS is currently described by Sirenek et al. Unfortunately, all approximations base on experiments with high acid concentrations and long leeching periods. Furthermore, due to the thickness and roughness of the thin porous layer it becomes hard to analyse the layer with standard methods like SEM or liquid nitrogen adsorption. In thin porous layers the amount of material becomes so small that most conventional techniques fail caused by a leak of accessibility. Also, an imaging procedure like SEM is difficult due to the isolating properties of glass. Therefore, we used the mono energetic positron source (MePS) at HZDR in Dresden to characterize the layer thickness and pore size simultaneously. As a result we could calculate the layer thickness for different samples using Makhovian profiles and additionally the pore size as well as the pore size distribution based on the extended Tao-Eldrup model.

DS 45.5 Fri 10:30 CHE 89

Si nanopillar deformation by heavy polyatomic ion impacts — •Lothar Bischoff[1], Wolfgang Pilz[1], Hans-Jürgen Engelmann[1], Xiaomo Xu[1], Wolfhard Möller[1], Karl-Heinz Heinig[1], Sadegh Ghaderzadeh[1], Gregor Hlawacek[1], Ahmed Gharbi[2], and Raluca Tiron[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden — [2]CEA-Leti, Grenoble, France

Si nanopillars for the fabrication of vertical nanowire gate-all-around Single Electron Transistors [1], have been irradiated with Si^{++}, Pb^{+}, Pb^{++}, Au^{+}, Au^{++}, Au$_2^{+}$, and Au$_3^{+}$ ions accelerated by 30 kV. A FIB of mass separated ions, extracted from a Liquid Metal Alloy Ion Source [2], has been scanned over regular arrays of Si nanopillars of different diameters and pillar distances. The irradiations have been performed at RT and 400°C. Different morphological changes of the pillars like thinning, height reduction, tilting etc. have been observed which can be attributed to ion erosion (sputtering), impact-induced viscous flow or even transient nanosecond-scale melting [3]. The pillars were imaged by AFM, SEM, TEM and HIM. 3D Monte Carlo simulations [4] of ion and recoil trajectories based on the Binary Collision Approximation and Molecular Dynamics calculations have been carried out in order to discriminate the dominating processes.

[1] EU project Ions4SET, Horizon 2020 grant No. 688072 [2] L. Bischoff, et al., Appl. Phys. Rev. 3 (2016) 021101 [3] C. Anders, K.-H. Heinig, H. Urbassek, Phys. Rev. B87 (2013) 245434 [4] W. Möller, NIM B322 (2014) 23

DS 45.6 Fri 10:45 CHE 89

Magneto-dielectric Effect in Relaxor Dipolar Glassy Tb$_2$CoMnO$_6$ Film — •Rajesh Mandal[1,2], Mohit Chandra[3], Vladimir Roddatis[4], Malvika Tripathi[3], Ram Janay Choudhary[3], and Vasily Moshnyaga[1] — [1]Department of Physics, Indian Institute of Science Education and Research, Pune 411008, India — [2]Erstes Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]UGC-DAE Consortium for Scientific Research, Indore Centre, University Campus, Khandwa Road, Indore 452017, India — [4]Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Relaxor ferroelectrics are recognized as a family of disordered or partially ordered materials that are classified as a special class of dipolar glass with the formation of weakly interacting polarized nano domains (PNR) bellow a certain temperature. Here we report the observation of magneto-dielectrically coupled ferroelectric relaxation at quite high temperature (200K) in Tb_2CoMnO_6/STO(100) double perovskite thin film. Partially B site disordered film has been grown by means of a metal-organic aerosol deposition (MAD) technique. This material is reported as ferromagnetic insulator with TC around 90K. Here we observe an enhanced transition temperature of 110K due to in plane strain. The deviation from the Curie-Weiss law far above TC indicates the development of short range spin correlation which is getting coupled with the electric dipoles present in the system.

DS 46: Thin Film Properties: Structure, Morphology and Composition IV

Time: Friday 11:15–12:45 Location: CHE 89

DS 46.1 Fri 11:15 CHE 89

Noble metal nanoparticles in organic matrix — •Olga Molodtsova[1,2], Irina Aristova[3], Sergey Babenkov[4], Igor Khodos[5], Dmitrii Potorochin[1,2,6], Serguei Molodtsov[2,6,7], and Victor Aristov[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]ITMO University, 197101 Saint Petersburg, Russia — [3]Institute of Solid State Physics of Russian Academy of Sciences, 142432 Chernogolovka, Russia — [4]Institut für Physik, Johannes Gutenberg-Universität, D-55099 Mainz, Germany — [5]Institute of Microelectronics Technology and High-Purity Materials of Russian Academy of Sciences, 142432 Chernogolovka, Russia — [6]Institut fuer Experimentelle Physik, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [7]Europian XFELGmbH,22869 Schenefeld, Germany

The structure and morphology of nanocomposites created by silver NPs which are self-organize in a thin organic film CuPcFx, x=0; 4, depending on the amount of deposited metal, were studied in UHV using HR-TEM and HR-PES measurements. Metallic atoms deposited on the surface of an organic substrate diffuse into the substrate, forming NPs with a narrow size distribution. With HR-TEM the distance between the atomic planes of individual silver nanoparticles was determined and the steady gathering of individual nanoparticles into agglomerates and then into nanocrystals with inter-crystallite boundaries was observed. PES revealed a generally weak interaction between silver NPs and the organic matrix. However, a strong band bending in the organic film at small coatings with metal atoms was observed.

DS 46.2 Fri 11:30 CHE 89

Morphological and electrical characterization of mixed valence coordination polymers containing rhodium paddle wheels — •Daniel Steinbach, René Schmidt, and Florian Mertens — Institut für Physikalische Chemie, TU Bergakademie Freiberg

To overcome one of the disadvantages of most MOFs being isolators, conjugated coordination polymers are investigated regarding their electrical conductivity. Therefore paddle-wheel structures with a documented metal-metal bond, here rhodium derivates, were linked via conjugated organic molecules like pyrazine. Coordination polymers of this type were first synthesized as bulk materials, characterized using XRD, BET and XPS and then deposited as coatings on gold surfaces. Subsequently the topography of the deposited layers was measured. Different morphologies mainly determined by AFM were obtained by using spin coating and dip coating. Depending on the composition of the coordination polymer well distributed crystals or network like structures were found. The surface layers were further investigated by XPS and XRD. Direct current measurments were carried out on these systems by conductive AFM. The conductivity of our coordination polymers could be altered by oxidizing or reducing some metal atoms of the paddle-wheel structure, either via chemical or electrochemical oxidation, resulting in mixed valences. The dependency of the conductivity of the coordination polymer on the degree of oxidation was determined.

DS 46.3 Fri 11:45 CHE 89

Suitability of the solid electrolyte LiPSON with respect to solid electrolyte interphase formation in battery systems — •Fabian Michel[1,2], Martin Becker[1,2], Florian Kuhl[1,2], Jürgen Janek[2,3], and Angelika Polity[1,2] — [1]Institue of Experimental Physics I, JLU Giessen, 35392 Giessen — [2]Center for Material Research (ZfM/LaMa), JLU Giessen, 35392 Giessen — [3]Institute of Physical Chemistry, JLU Giessen, 35392 Giessen

Solid electrolytes play in upcoming role an future battery cell concepts. Therefore, the physical and electrochemical properties of the lithium-based solid electrolyte LiPSON are investigated with regard to an use in energy storage systems. An additional XPS in-situ experiment is performed to gain knowledge about the so-called solid-electrolyte-interphase (SEI) between metallic lithium and the electrolyte used. Similar investigations were carried out on the LiPSON-based material system LiPON. There a positive effect of the SEI was shown so the comparison and the possible substitution of LiPON by LiPSON is of importance for future cell concepts.

DS 46.4 Fri 12:00 CHE 89

Solution-based thin films of bridged triarylamines: Unravelling the self-assembly — •Tim Hawly[1], Fabian Streller[1], Manuel Johnson[1], Sandra Míguez-Lago[1], Milan Kivala[2], and Rainer Fink[1] — [1]Department Chemie und Pharmazie, Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Centre of Advanced Materials, Universität Heidelberg, Germany

Columnar (1D) triarylamine thin films from a dip-coating approach have been discussed in literature as potential candidates for functional n-type semiconducting layers and regarding both their solution processability and crystal structure. Herein, we report on the growth behavior and realization of upstanding 2D-extended films of a series of bridged triarylamines via a solution-based processing method.

Film preparation is inspected at different length scales by optical microscopy (OM) and atomic force microscopy (AFM). Long-range order, crystallinity and layer thickness appeared to decisively depend on the nature of the peripheral substituents attached to the polycyclic aromatic backbone with flat core structures being preferred over non-planar ones. Electron diffraction (SAED) confirmed the crystalline structure of the obtained ultrathin films. Additionally, first steps to clarify the molecular orientation within prepared structures were taken via angle-resolved near edge x-ray absorption fine structure (NEXAFS) spectroscopy. Our work presents a fine tool ensemble for unambiguous design and structure elucidation of high-quality, 2D heterotriangulene systems aiming at potential application fields such as layered organic electronics. This research is funded by the DFG within GRK1896.

DS 46.5 Fri 12:15 CHE 89

Investigation of the interaction of an organic electron donor with graphene — •Joris de la Rie[1], Qiankun Wang[1], Kathrin Müller[1], Wenbo Lu[1], Mihaela Enache[1], Milan Kivala[2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Institute for Organic Chemistry, University of Heidelberg, Germany

Among others, graphene is widely known for its excellent electronic properties making it an extremely appealing candidate for usage in future (nano)electronic devices. Such applications often require modification of graphene's electronic properties to ensure compatibility with other device components. Deposition of a molecular layer has been shown to controllably modify graphene's work function as well as charge carrier type and concentration.

Here, we report on the self-assembly of the organic donor molecule 2,3,6,7,10,11-hexakis-alkoxytriphenylene (HAT) on graphene on Ir(111). Previous study of this molecule on Ag(111) identified it as a suitable candidate for use in organic electronics[1]. Employing scanning tunnelling microscopy and low energy electron diffraction, we found that these molecules assembled in a hexagonal network at up to monolayer coverages. We used X-ray and ultraviolet photoelectron spectroscopy to investigate the intermolecular and molecule-graphene interactions as well as to monitor changes of the electronic properties of graphene.

[1] Müller et al., Small 2019, 15, 1901741

DS 46.6 Fri 12:30 CHE 89

Dewetting assisted MWCNT ring formation — •Surita Basu[1], Prabir Patra[2], and Jayati Sarkar[1] — [1]Department of Chemical Engineering, Indian Institute of Technology Delhi, India — [2]Department of Biomedical Engineering, University of Bridgeport 126 Park Avenue, Bridgeport,CT 06604

The fabrication of finite arrangement with nanoscale materials is key to current technology and self-assembly and self-organization are considered efficient and cost-effective and so a preferred process for building ordered structure of nanoparticles. Carbon nanotubes are very interesting material for their properties and molecular structures. Carbon nanotubes can assemble in different morphologies depending on its physical synthesis method. The different morphologies of CNT are coiled CNTs, CNT junctions, and toroidal CNTs. Thin polymer film $<$ 100 nm also undergoes self-organization resulting in the formation of arrays of droplets. These spontaneously formed ordered patterns or structures on the surface has a wide range of technological applications. The retraction of fluid from the surface that it was supposed to cover leads to the phenomenon of dewetting causing the arrangement of droplets which act as a template for the self-assembly of the carbon nanotubes. The self-organized patterns on the thin PS film along with Marangoni flow are the driving force behind the circular ring formation of the carbon nanotubes without any external physical method.

DS 47: Overview Talk: Wiesendanger (joint session O/CPP/DS)

Time: Friday 14:00–14:45 Location: HSZ 02

Topical Talk DS 47.1 Fri 14:00 HSZ 02

Surface Science Aspects of Topological States of Matter — •Roland Wiesendanger — Universität Hamburg

Topological states of matter have raised great excitement in solid state physics in the past years, e.g. in the fields of topological insulators, topological spin textures (magnetic skyrmions), and topological superconductors hosting Majorana states. Surface and interface science plays a crucial role for all these fields, as has been demonstrated, e.g., by the discovery of ultimately small-scale skyrmions stabilized by interfacial Dzyaloshinskii-Moriya interactions [1,2] or the direct real-space observation of the emergence of Majorana states in atomic-scale magnet-superconductor hybrid systems [3,4]. In particular, the preparation of extremely clean surfaces of elemental s-wave superconductors, such as Re, Ta, La, and Nb has boosted recent studies of topological superconductivity in bottom-up constructed 1D and 2D hybrid systems, allowing for the atomic-scale design of Majorana states and a one-to-one comparison between results of theoretical toy models and experimental observations. Bringing together surface science concepts and advanced techniques for the fabrication of atomically well defined magnet-superconductor hybrid systems is a key ingredient for this exciting new research area which ultimately will allow for the realization of topological quantum computation schemes. [1] N. Romming et al., Science 341, 6146 (2013). [2] S. Heinze et al., Nature Physics 7, 713 (2011). [3] H. Kim et al., Science Advances 4, eaar5251 (2018). [4] A. Palacio-Morales et al., Science Advances 5, eaav6600 (2019).