Thin Films Division
Fachverband Dünne Schichten (DS)

Sprecher des Fachverbandes
Norbert Esser
Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V.
Research Department Interface Analytics
Schwarzschildstraße 8
12489 Berlin
norbert.esser@isas.de

Stellvertretender Sprecher
Jürgen Faßbender
Helmholtz-Zentrum Dresden-Rossendorf e.V.
Institute of Ion Beam Physics and Materials Research
PO Box 51 01 19
01314 Dresden
j.fassbender@hzdr.de

Overview of Invited Talks and Sessions

(Lecture rooms H8 and H11; Poster A)

Gaede Prize Talk

DS 21.2	Tue	14:00–14:30	H11	**Ultrafast dynamics of many-body effects in solids and at interfaces: Polarons, excitons and correlated electrons** — •Julia Stähler

Invited Talks

DS 4.1	Mon	9:30–10:00	H11	**Controlling and tailoring molecular thin film growth** — •Stefan Kowarik
DS 8.1	Mon	15:00–15:30	H8	**Materials characterization at the nanoscale by X-ray spectrometry** — •Burkhard Beckhoff
DS 15.1	Tue	9:30–10:00	H8	**Heterostructures with Targeted Nanoarchitecture and Tunable Properties** — •David Johnson
DS 28.1	Wed	9:30–10:00	H8	**Surface analytics with electron spectroscopy on coated steel sheets** — •David Stifter
DS 36.1	Wed	15:00–15:30	H11	**Single site-controlled InGaAs quantum dots grown on patterned GaAs nanoholes** — •S. Höfling, S. Maier, S. Unsleber, M. Kamp, C. Schneider
DS 36.2	Wed	15:30–16:00	H11	**Nanometer scale correlation of structural and optical properties of individual GaAs/AlGaAs nanorodsby Scanning Transmission Electron Microscope Cathodoluminescence** — •Frank Bertram, Marcus Müller, Peter Veit, Jürgen Christen
DS 36.3	Wed	16:00–16:30	H11	**Local Heteroepitaxy for Large-Scale Integration** — •Heinz Schmid, Mattias Borg, Davide Cutaia, Kirsten Moselund, Moritz Knoedler, Nicolas Bologna, Heike Riel
DS 36.4	Wed	16:45–17:15	H11	**Fabrication and study of metal contacts on germanium nanowires using electrical biasing in a transmission electron microscope** — •Martien den-Hertog, Khalil El-Hajroui, Clemens Zeiner, Alois Lugstein, Eric Robin, Miguel Lopez-Haro, Jean-Luc Rouviere
DS 36.5	Wed	17:15–17:45	H11	**Cubic GaN on pre-patterned 3C-SiC/Si (001) substrates** — •Donat Josef As, Ricarda Maria Kemper, Thomas Riedl, Jörg K.N. Lindner
DS 40.1	Thu	9:30–10:15	H11	**Oxide semiconductors: materials design and applications** — •Hideo Hosono
DS 40.2	Thu	10:15–10:45	H11	**Mixing In and Ga sesquioxides - and their polar phases** — •Vincenzo Fiorentini
DS 40.3	Thu	10:45–11:15	H11	**Exploring and tailoring conductance phenomena in oxide films: An STM study** — •Niklas Nilius
DS 40.4	Thu	11:30–12:00	H11	**Miscibility and phase separation in $(\mathrm{In}_x\mathrm{Ga}_{1-x})_2\mathrm{O}_3$** — •Martin Albrecht, Robert Schewski, Toni Markurt, Tobias Schulz, Michele Baldini, Günter Wagner, Holger von Wenckstern, Marius Grundmann, Hartwin Peelaers, Joel Varley, Chris Van de Walle

DS 47.1	Thu	15:00–15:30	H8	**Bright and dark excitons in transition metal dichalcogenide monolayers** — Cedric Robert, Gang Wang, Aslihan Suslu, Bin Chen, Sije Yang, Sarah Alamdari, Iann Gerber, Thierry Amand, Sef Tongay, Bernhard Urbaszek, •Xavier Marie
DS 47.2	Thu	15:30–16:00	H8	**Exciton fine structure in transition-metal dichalcogenides monolayers** — •Mikhail Glazov
DS 47.3	Thu	16:00–16:30	H8	**Photonics and polaritonics with van der Waals heterostructures** — •Alexander Tartakovskii
DS 47.4	Thu	16:30–17:00	H8	**van der Waals Epitaxy of 2D materials** — •Sefaattin Tongay
DS 56.1	Fri	9:30–10:00	H11	**Processes at the nanoscale: Recent progress in understandings on ReRAMs** — •Ilia Valov
DS 56.2	Fri	10:00–10:30	H11	**Tunnel junction based memristors as artificial synapses** — •Andy Thomas

Invited talks of the joint symposium SYHP

See SYHP for the full program of the symposium.

SYHP 1.1	Mon	9:30–10:00	H1	**Perovskite Semiconductors: Opportunities and Challenges for Photovoltaic Materials Design** — •David B. Mitzi
SYHP 1.2	Mon	10:00–10:30	H1	**Perovskite Solar Cells: A new Paradigm in Photovoltaics** — •Mohammad Nazeeruddin
SYHP 1.3	Mon	10:30–11:00	H1	**Charge-Carrier Diffusion and Radiative Efficiencies in Hybrid Metal Halide Perovskites** — •Laura Herz
SYHP 1.4	Mon	11:15–11:45	H1	**Photovoltage losses in perovskite solar cells** — •Kristofer Tvingsted
SYHP 1.5	Mon	11:45–12:15	H1	**Computational screening of perovskite solar energy materials** — •Karsten W. Jacobsen

Invited talks of the joint symposium SYTI

See SYTIfor the full program of the symposium.

SYTI 1.1	Wed	9:30–10:10	H1	**Topological insulators and topological superconductors** — •Shoucheng Zhang
SYTI 1.2	Wed	10:10–10:50	H1	**Three-dimensional topological insulators and superconductors** — •Yoichi Ando
SYTI 1.3	Wed	10:50–11:30	H1	**Interplay of magnetic and electronic states in pyrochlore iridates** — •Leon Balents
SYTI 1.4	Wed	11:40–12:20	H1	**Magnetic imaging of edge states** — •Kathryn Moler
SYTI 1.5	Wed	12:20–13:00	H1	**Sub-nm wide edge states at the dark side of a weak topological insulator** — •Markus Morgenstern

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Intrinsic Transport Coefficients and Momentum Space Berry Curvatures** — •Allan H MacDonald
SYES 1.2	Fri	10:00–10:30	H1	**Berry phase linked spin-orbit torques in Ferromagnetic and Antiferromagnetic systems** — •Jairo Sinova
SYES 1.3	Fri	10:30–11:00	H1	**Transport in Topological Insulators and Topological Superconductors: In Search of Majorana Fermions** — •Ewelina Hankiewicz
SYES 1.4	Fri	11:15–11:45	H1	**Engineering Topological Quantum States: From 1D to 2D.** — •Jelena Klinovaja
SYES 1.5	Fri	11:45–12:15	H1	**Skyrmions – Topological magnetization solitons for future spintronics** — •Stefan Blügel

Sessions

DS 1.1–1.3	Sun	16:00–18:30	H18	**Tutorial: Hybrid and Perovskite Photovoltaics** **(Joint session of CPP, DF, DS and HL, organized by CPP)**
DS 2.1–2.5	Mon	9:30–12:15	H1	**Fundamentals of Hybrid and Perovskite Photovoltaics** **(Joint symposium of CPP, DF, DS and HL, organized by CPP)**
DS 3.1–3.14	Mon	9:30–13:15	H8	**Phase Change / Resistive Switching**

DS 4.1–4.11	Mon	9:30–12:45	H11	**Organic Thin Films I**
DS 5.1–5.11	Mon	9:30–13:00	H16	**Two-dimensional Materials** **(Joint session of DS and HL, organized by HL)**
DS 6.1–6.10	Mon	9:30–12:30	H17	**Graphene: Theory** **(Joint session of DS, DY, HL, MA, O and TT organized by HL)**
DS 7.1–7.8	Mon	14:45–17:45	H17	**Graphene: Transport** **(Joint session of DS, DY, HL, MA, O and TT organized by HL)**
DS 8.1–8.5	Mon	15:00–16:30	H8	**Thin Film Characterisation: Structure Analysis and Composition I**
DS 9.1–9.7	Mon	15:00–16:45	H11	**Organic Thin Films II**
DS 10.1–10.10	Mon	15:00–17:45	H18	**Transport: Topological Insulators - 2D** **(Joint session of DS, HL, MA, O and TT, organized by TT)**
DS 11.1–11.9	Mon	15:00–17:30	H38	**Hybrid and Perovskite Photovoltaics I** **(Joint session of CPP, DS and HL, organized by CPP)**
DS 12.1–12.55	Mon	17:00–19:00	Poster A	**Postersession DS**
DS 13.1–13.4	Mon	17:45–18:45	H17	**Graphene: Fabrication** **(Joint session of DS, DY, HL, MA, O and TT organized by HL)**
DS 14	Mon	19:00–20:00	H8	**Annual Meeting of the Thin Films Division**
DS 15.1–15.9	Tue	9:30–12:15	H8	**Thermoelectric Materials**
DS 16.1–16.13	Tue	9:30–13:00	H11	**Layer Properties: Electrical, Optical, and Mechanical**
DS 17.1–17.10	Tue	10:30–13:00	H24	**2D Materials: Structure and Electronic Properties** **(Joint session of DS and O, organized by O)**
DS 18.1–18.10	Tue	10:30–13:15	S052	**1D Metal Wires on Semiconductors I** **(Joint session of DS and O, organized by O)**
DS 19.1–19.8	Tue	10:45–13:00	H37	**Hybrid and Perovskite Photovoltaics II** **(Joint session of CPP, DS and HL, organized by CPP)**
DS 20.1–20.2	Tue	12:30–13:00	H8	**Topological Insulators: Status Quo and Future Directions** **(Joint session of DS, O and TT, organized by DS)**
DS 21.1–21.4	Tue	13:30–15:30	H11	**Gaede Prize Symposium** **(Joint session of DS and O, organized by DS)**
DS 22.1–22.6	Tue	14:00–15:45	H18	**Transport: Topological Insulators - 3D** **(Joint session of DS, HL, MA, O and TT, organized by TT)**
DS 23.1–23.7	Tue	14:00–16:00	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport I** **(Joint session of DS and O, organized by O)**
DS 24.1–24.8	Tue	14:00–16:00	S052	**1D Metal Wires on Semiconductors II** **(Joint session of DS and O, organized by O)**
DS 25.1–25.6	Tue	14:00–15:30	H37	**Organic Electronics and Photovoltaics I** **(Joint session of CPP, DS, HL and O, organized by CPP)**
DS 26.1–26.1	Wed	8:30– 9:15	H1	**Plenary Talk XI**
DS 27.1–27.5	Wed	9:30–13:00	H1	**Symposium Topological Insulators: Status Quo and Future Directions** **(Joint symposium of DS, HL, MA, O and TT, organized by TT)**
DS 28.1–28.8	Wed	9:30–12:00	H8	**Thin Film Applications**
DS 29.1–29.8	Wed	9:30–11:45	H11	**Hybrid and Perovskite Photovoltaics III** **(Joint session of CPP, DS and HL, organized by DS)**
DS 30.1–30.13	Wed	9:30–13:15	H22	**Transport: Graphene** **(Joint session of DS, DY, HL, MA, O and TT, organized by TT)**
DS 31.1–31.10	Wed	10:30–13:00	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport II** **(Joint session of DS and O, organized by O)**
DS 32.1–32.10	Wed	10:30–13:00	S053	**2D Materials: Growth** **(Joint session of DS and O, organized by O)**
DS 33.1–33.3	Wed	12:00–12:45	H11	**Frontiers of Electronic Structure Theory** **(Joint session of DS and O, organized by DS)**
DS 34.1–34.2	Wed	12:15–12:45	H8	**Atomic Layer Deposition**

DS 35.1–35.12	Wed	15:00–18:15	H8	**Thin Film Characterisation: Structure Analysis and Composition II**
DS 36.1–36.8	Wed	15:00–18:30	H11	**Focussed Session: Semiconductor Heteroepitaxy on Nanopatterned Substrates** **(Joint session of DS and HL, organized by DS)**
DS 37.1–37.12	Wed	15:00–18:30	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport III** **(Joint session of DS and O, organized by O)**
DS 38.1–38.10	Wed	15:00–17:45	H32	**Topological Insulators** **(Joint session of DS, HL, MA, O and TT, organized by MA)**
DS 39.1–39.6	Thu	9:30–11:00	H8	**Resistive Effects I**
DS 40.1–40.9	Thu	9:30–13:15	H11	**Focussed Session: Oxide Semiconductors for Device and Energy Applications I** **(Joint session of DS and HL, organized by DS)**
DS 41.1–41.13	Thu	9:30–13:00	H23	**Transport: Molecular Electronics and Photonics I** **(Joint session of CPP, DS, HL, MA, O and TT, organized by TT)**
DS 42.1–42.11	Thu	9:30–12:45	H40	**Organic Electronics and Photovoltaics II** **(Joint session of CPP, DS, HL and O, organized by CPP)**
DS 43.1–43.9	Thu	10:30–13:15	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport IV** **(Joint session of DS and O, organized by O)**
DS 44.1–44.8	Thu	11:15–13:15	H8	**Physics and Application of Emergent 2D-semiconductors and their Heterostructures I** **(Joint session of DS and HL, organized by DS)**
DS 45.1–45.13	Thu	14:45–18:30	H2	**Hybrid and Perovskite Photovoltaics IV** **(Joint session of CPP, DF, DS and HL, organized by HL)**
DS 46.1–46.8	Thu	14:45–17:15	H10	**Topological Insulators I** **(Joint session of DS and HL, organized by HL)**
DS 47.1–47.4	Thu	15:00–17:00	H8	**Focussed Session: Physics and Application of Emergent 2D-semiconductors and their Heterostructures II** **(Joint session of DS and HL, organized by DS)**
DS 48.1–48.7	Thu	15:00–16:45	H11	**Oxide Semiconductors for Device and Energy Applications II** **(Joint session of DS and HL, organized by DS)**
DS 49.1–49.4	Thu	15:00–16:00	H23	**Transport: Molecular Electronics and Photonics II** **(Joint session of CPP, DS, HL, MA, O and TT, organized by TT)**
DS 50.1–50.13	Thu	15:00–18:15	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport V** **(Joint session of DS and O, organized by O)**
DS 51.1–51.7	Thu	16:15–18:30	H23	**Transport: Spintronics and Magnetotransport** **(Joint session of DS, HL, MA and TT, organized by TT)**
DS 52.1–52.5	Thu	17:00–18:15	H11	**Ion and Electron Beam Induced Processes**
DS 53.1–53.37	Thu	16:00–19:00	Poster A	**Postersession DS/HL**
DS 54.1–54.5	Fri	9:30–12:15	H1	**Symposium on Frontiers of Electronic Structure Theory: Focus on Topology and Transport** **(Joint symposium of DS, HL, MA, MM and O, organized by O)**
DS 55.1–55.10	Fri	9:30–12:15	H8	**Organic Thin Films III**
DS 56.1–56.6	Fri	9:30–11:45	H11	**Focussed Session: Resistive Effects II**
DS 57.1–57.8	Fri	9:30–12:00	H15	**Topological Insulators II** **(Joint session of DS and HL, organized by HL)**
DS 58.1–58.9	Fri	9:30–12:00	H40	**Organic Electronics and Photovoltaics III** **(Joint session of CPP, DS, HL and O, organized by CPP)**

Annual Meeting of the Thin Films Division

Monday 19:00–20:00 H8

- Annual Report

DS 1: Tutorial: Hybrid and Perovskite Photovoltaics (Joint session of CPP, DF, DS and HL, organized by CPP)

Organizers: Lukas Schmidt-Mende (Universität Konstanz), Vladimir Dyakonov (Universität Würzburg) and Christoph Lienau (Universität Oldenburg)

Tremendous progress has been achieved in the performance of hybrid solar cells, with efficiencies now exceeding 20 % for devices based on organometallic halide perovskites. Aim of this tutorial is to introduce this topic of perovskite solar cells to prepare for the following symposium (SYHP) and allow vivid scientific discussions. A description of current state-of-the-art device fabrication methods and solar cell architectures will be given and their role on the device performance explained. The device physics will be discussed and charge carrier generation and recombination mechanisms in perovskite films explained and compared to other material systems. Additionally the important role of electronic structure of the different layers in hybrid perovskite will be covered.

Time: Sunday 16:00–18:30 Location: H18

Tutorial DS 1.1 Sun 16:00 H18

Perovskite photovoltaics: Synthesis, structure and device architecture — •Pablo Docampo — LMU Munich, Germany

Recently, organic-inorganic hybrid perovskites have been proven to be excellent photovoltaic materials, exhibiting outstanding light absorption, high carrier mobility and facile solution processability. Besides the manufacturing low costs of perovskite thin-films, the power conversion efficiencies demonstrated for this class of materials is already at the same level as poly-crystalline silicon and other thin film photovoltaic technologies. The pursuit of efficiency in the field of metal halide perovskite solar cells has been achieved mainly through the improvement to perovskite deposition processing and optimization of the device architecture.

In this tutorial I will focus on three topics. Firstly, the evolution of the device architecture, starting from sensitized mesoscopic solar cells to planar heterojunction devices employing organic contacts. Secondly, the commonly employed perovskite deposition techniques with special emphasis on the morphological quality of the prepared perovskite films. Thirdly, the perovskite structure and its stability both towards moisture and other factors such as UV-light, temperature and atmosphere. I will link these different aspects with device performance characteristics and introduce recent developments in the field towards surmounting the challenges the technology is currently facing from a materials point of view.

Tutorial DS 1.2 Sun 16:50 H18

Charge Carrier Generation and Recombination in Organic and Perovskite Solar Cells — •Andreas Baumann — Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), Magdalene-Schoch-Str. 3, D-97074 Würzburg

The new star on the photovoltaic (PV) horizon, are the so called organometal halide perovskite solar cells. This new kind of thin-film PV technology has experienced a tremendous, yet not seen increase in power conversion efficiency (PCE) compared to other types of PV technologies. Up to now the solar cell efficiency on lab scale could be improved from 3.8% in 2008 to above 20% in 2015 being already competitive with commercially available PV technologies. Especially this boost in PCE values has attracted attention of many researchers from all different PV research fields. Thereby, perovskite PV is one of the most promising thin film PV technologies regarding low-cost manufacturing combined with high PCE. However, the working principle of these solar cells is yet not completely understood and is strongly discussed in literature. Phenomena, such as the often observed anomalous hysteresis in the current-voltage characteristics or the giant dielectric constant and its impact on charge carrier generation and recombination are highly debated topics with so far different given possible explanations.

In this tutorial, the processes of charge carrier generation and recombination in perovskite solar cells will be highlighted and compared to those in well studied organic solar cells. Thereby, the aim is to give an overview of the published data on these processes in order to present the current status of research.

Tutorial DS 1.3 Sun 17:40 H18

The electronic structure in hybrid perovskite layers and devices — •Selina Olthof — University of Cologne, Institute for Physical Chemistry, Luxemburger Straße 116, 50939 Köln, Germany

The performance of optoelectronic devices strongly depends on the appropriate energetic alignment of the participating transport levels which directly influence the charge transport through the different layers. In order to optimize these interfaces in a non-trial-and-error fashion, one needs to know the conduction band minimum and valence band maximum of the perovskites to be able to select ideal transport layers as well as contact materials. While commonly vacuum level alignment is assumed at the interface to the substrate, this is actually rarely found in devices. Interfacial states, interface dipoles, and band bending can (and do) significantly alter the energy level landscape.

In this tutorial I will discuss the electronic structure of perovskites and introduce common measurement techniques that can shed a light on their energetic properties as well as the interface alignment relevant for devices. Combining reports from literature with our own recent results on the versatile electronic nature of this material I will elucidate the interplay between electronic structure and overall device performance.

DS 2: Fundamentals of Hybrid and Perovskite Photovoltaics (Joint symposium of CPP, DF, DS and HL, organized by CPP)

Time: Monday 9:30–12:15 Location: H1

Invited Talk DS 2.1 Mon 9:30 H1

Perovskite Semiconductors: Opportunities and Challenges for Photovoltaic Materials Design — •David B. Mitzi — Duke University, Edmund T. Pratt Jr. School of Engineering, Durham, NC 27708-0300 USA

Organic-inorganic and related halide-based perovskites (e.g., those based on Pb halide frameworks) have attracted substantial recent interest for solar cell and other optoelectronic technologies, because of the large optical absorption coefficients, high carrier mobilities, long minority carrier lifetimes, and relatively benign defects and grain boundaries. Indeed, these materials have enabled an unprecedented rapid improvement in photovoltaic (PV) performance to levels above 20% power conversion efficiency. Despite the great promise, challenges for the current generation of PV materials include replacing lead with more environmentally benign metals, improving PV device stability (moisture, UV and air) and controlling hysteresis. This talk will explore beyond the current focus on three-dimensional (3-D) lead(II)-based perovskites, to highlight the outstanding structural, chemical and electronic flexibility of the perovskite family. Particular focus will be afforded to systems in which divalent lead is replaced with other metal cations exhibiting a lone pair of electrons, such as Sn, Bi and Sb, since these systems share some of the beneficial electronic structure characteristics of the Pb-based systems. Further discovery within the perovskite structural and chemical space may offer prospects to solve the current technological challenges for perovskite PV and yield important opportunities for energy materials design.

Invited Talk DS 2.2 Mon 10:00 H1

Perovskite Solar Cells: A new Paradigm in Photovoltaics — •Mohammad Nazeeruddin — EPFL, GMF, Sion Switzerland

Perovskite solar cells exhibited significant leapfrog in efficiency due to a broad absorption, high optical absorption coefficient, very low exciton binding energy, long carrier diffusion lengths, efficient charge collection, and very high open circuit potential similar to III-IV semiconductors. Unlike silicon solar cells, perovskite solar cells can be developed a variety of low-temperature solution process from inexpensive raw materials. By engineering compositional ratio of perovskite absorber, film formation using anti-solvent, and interface engineering of charge transport materials a remarkable power conversion efficiency of over 21% has been demonstrated, highlighting the unique photovoltaic properties of perovskite materials. In this talk, we present the current progress in perovskite solar cells, various deposition methods for perovskite absorbing layer, synthesis and characterization of novel hole transporting materials, and highlight crucial challenges and prospects

Invited Talk DS 2.3 Mon 10:30 H1

Charge-Carrier Diffusion and Radiative Efficiencies in Hybrid Metal Halide Perovskites — •Laura Herz — University of Oxford, Oxford, UK

Hybrid metal halide perovskites (stoichiometry AMX_3) have recently emerged as low-cost active materials in PV cells with power conversion efficiencies in excess of 20%. In addition, hybrid perovskites show prospects for applications in low-cost light-emitting diodes and lasers.

Here we discuss how parameters essential for photovoltaic operation, such as charge carrier recombination and diffusion lengths are altered with substitutions of the organic A cation (e.g. methylammonium versus formamidinium), the metal M cation (e.g. Pb^{2+} or Sn^{2+}) and the halide X anion (I versus Br). We analyze distinct charge-carrier recombination mechanisms, such as trap-mediated, bi-molecular (electron-hole) and Auger recombination, which show different dependences on composition and temperature.

We use these insights to predict charge-carrier diffusion lengths and radiative efficiencies in the limit of ultra-low trap-related recombination, which could potentially be reached through further advances in material processing. We find that for hybrid lead iodide perovskites with typical charge-carrier mobilities of $\sim 30\mathrm{cm}^2/(\mathrm{Vs})$, charge-carrier diffusion lengths under solar irradiation are unlikely to exceed $\sim 10\mu\mathrm{m}$ even if all trap-related recombination is eliminated. We further show that if high radiative efficiencies are to be obtained for intermediate charge-carrier densities ($n \sim 10^{14}\mathrm{cm}^{-3}$), trap-related recombination lifetimes have to exceed microseconds.

15 min. break.

Invited Talk DS 2.4 Mon 11:15 H1

Photovoltage losses in perovskite solar cells — •Kristofer Tvingsted — Experimental Physics VI, Julius Maximilians Universität, Würzburg, Germany

Perovskite PVs have reached significant power conversion efficiency in a very short time period. Apart from providing a rather high photocurrent, they also retain a comparatively high open circuit voltage (VOC). The VOC of most solar cells is however far from its potential upper limit due to charge carrier recombination of various types, whose origin must be accurately determined. Herein, I summarize what we have learned about these photovoltage losses by studying the radiative part of recombination in Perovskites. By accurate determination of the present solar cells radiative efficiency, that is their ability to emit light, we conclude how far the solar cells are from their own thermodynamic upper limit and further, how they relate to a reference OPV cell. We evaluate the carrier density dependence of the radiative efficiency and associate it to the ideality factor, which in itself represents a uniform figure of merit for the dominant type of recombination. We show that, as the perovskite steady state photoluminescence is strong at open circuit conditions, but substantially quenched only at short circuit, they perform in this respect just as an ideal solar cell should do, and also very different from most OPVs or DSSC cells studied so far. Substantially improving the radiative efficiency to increase the open circuit voltage is a promising route to put these new photovoltaic converters in efficiency parity with the best inorganic counterparts.

Invited Talk DS 2.5 Mon 11:45 H1

Computational screening of perovskite solar energy materials — •Karsten W. Jacobsen — CAMD, Dept. of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

In the talk I shall describe computational efforts to idenfity new materials for efficient light absorption with particular focus on materials in the perovskite structure and water splitting. The materials have to obey a number of criteria in order to work for light absorption and water splitting depending on the particular design of the device. We consider in particular stability, appropriate bandgap and bandstructure for visible light absorption, and an adequate line-up of band edges to the water redox potential. We also identify descriptors to determine defect-sensitivity of the materials.

We have considered several classes of materials with most emphasis on the cubic perovskite structure and derivatives like double perovskites and layered perovskites (Ruddlesden-Popper and Dion-Jacobson phases) with anions O, N, F, or S. Also a range of Sn and Pb based organic and inorganic perovskites have been considered with different combinations of the anions I, Br, and Cl. The possibilities of band gap tuning using atomic-level heterostructures or strain will also be touched upon.

I shall finally mention presently available open databases of relevance for energy materials including the Computational Materials Repository (https://cmr.fysik.dtu.dk) where the discussed data are made publicly available.

DS 3: Phase Change / Resistive Switching

Time: Monday 9:30–13:15 Location: H8

DS 3.1 Mon 9:30 H8

MemFlash: Memristive operation mode of floating gate transistors — •Henning Winterfeld[1], Nico Himmel[1], Martin Ziegler[1], Henning Hanssen[2], Detlef Friedrich[2], Wolfgang Benecke[2], and Hermann Kohlstedt[1] — [1]Nanoelektronik, Technische Fakultät, Christian-Albrechts Universität zu Kiel, Germany — [2]Fraunhofer-Institut für Siliziumtechnologie (ISIT), Itzehoe, Germany

Memristive devices have great potential for the use as key elements in neuromorphic circuits. However, the system integration which requires a wafer level fabrication technology has turned out to be difficult. Therefore, MemFlash cells, i.e. single floating gate transistors operating in a memristive operation mode, are an interesting alternative to state-of-the-art memristive devices. Here, a semi-industrial fabrication process is presented, which allows us to tailor the device properties by using different gate stacks. Fabricated devices vary in channel length and width with tunneling windows between 4 $\mu\mathrm{m}^2$ and 100 $\mu\mathrm{m}^2$. Furthermore, tunnel barrier thicknesses between 3 nm up to 7 nm were realized. First hysteresis measurements show on-off resistance values of about 260 kOhm and 680 kOhm, respectively. The electrical characteristics of these devices will be presented, while based on this data, possible advantages and disadvantages of the MemFlash device with respect to conventional memristive devices will be discussed.

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

DS 3.2 Mon 9:45 H8

Memristive Functionality of a SONOS Memory Transistor — •Nico Himmel[1], Hannes Mähne[2], Steffen Thiem[2], Henning Winterfeld[1], Martin Ziegler[1], and Hermann Kohlstedt[1] — [1]Nanoelektronik, Technische Fakultät der Christian-Albrechts Universität Kiel, Germany — [2]X-FAB Dresden GmbH Co. KG, Dresden, Germany

Charge trap transistors of silicon-oxide-nitride-oxide-polysilicon (SONOS) type can be operated as a memristive device. In the talk, a two terminal wiring scheme for single depletion SONOS cells with one additional resistor will be introduced. The all-electric operation principle and established silicon manufacturing process of SONOS devices at the Semiconductor Foundry XFAB promise reliable operation, low parameter spread and large integration density. Experimental current-voltage curves show a pinched hysteretic shape within ±10 V with a polarity dependent asymmetry and $R_{off}/R_{on} > 25$ at 0.5 V. In addition the circuit response to voltage pulses, which is relevant for neuromorphic applications, is discussed. The circuit design is an implementation of the MemFlash concept, as proposed for a memristive operation of floating gate transistors [1].

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

[1] M. Ziegler et al., APL **101**, 263504 (2012)

DS 3.3 Mon 10:00 H8

Memristive circuits for the emulation of neuronal dynamics — •Marina Ignatov, Martin Ziegler, Mirko Hansen, Adrian Petraru, and Hermann Kohlstedt — AG Nanoelektronik, Christian-Albrechts-Universität zu Kiel, Germany

We discuss the capabilities of memristive devices for the emulation of neural dynamics in electronic circuits. Therefore, a memristive spiking neuron model is presented [1] which has been experimentally implemented in a compact electronic circuit comprising memristive and memcapacitive devices. In more detail, the strongly correlated electron material vanadium dioxide (VO_2) and a chemical electromigration cell Ag/TiO_{2-x}/Al have been employed to emulate neural spike coding, including firing frequency adaptation. The latter was first observed by E. D. Adrian in 1926 and is nowadays believed to be the basis of neural computing. Furthermore, the advantages of memristive oscillator systems for neural computing will be discussed. In this context, we present results on an electronic circuit which belongs to the class of van der Pol oscillators, which are considered as model systems to mimic higher brain functionalities.

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

[1] M. Ignatov et al., Front. Neurosci. 9: 376 (2015)

DS 3.4 Mon 10:15 H8

Memristive Devices for Neuromorphic Systems — •Mirko Hansen[1], Martin Ziegler[1], Finn Zahari[1], Lukas Kolberg[1], Sven Dirkmann[2], Thomas Mussenbrock[2], and Hermann Kohlstedt[1] — [1]AG Nanoelektronik, Christian-Albrechts-Universität zu Kiel, Germany — [2]Lehrstuhl für Theoretische Elektrotechnik, Ruhr-Universität Bochum, Germany

The intensified development of memristive devices for memory applications led to several other possible fields of operation. Among them, their use for neuromorphic systems is one of the most promising applications. While several neuron-based learning concepts have been successfully demonstrated using single devices, the realization of neuromorphic systems using many memristive devices remains challenging.

We present TiO_x and Nb_xO_y-based memristive devices [1] with different device properties. The devices are fabricated on 4 inch wafers using a four mask lithography process with etching and deposition steps to yield a large number of high quality devices. A wafer-scale electronic characterization of these devices allows obtaining device parameters from a large number of devices. These parameters are employed for a network simulation which is able to recognize patterns [2]. Based on simulations, essential device requirements and device parameters for neuromorphic systems will be discussed.

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

[1] M. Hansen et al., Scientific Reports, vol. 5, p. 13753 (2015)

[2] F. Zahari et al., AIMS Materials Science 2: 203-216 (2015)

DS 3.5 Mon 10:30 H8

Critical ReRAM Stack Parameters Controlling Complementary versus Bipolar Resistive Switching — •Alexander Schönhals[1], Dirk J. Wouters[1], Astrid Marchewka[1], Thomas Breuer[2], Katharina Skaja[2], Stephan Menzel[2], and Rainer Waser[1,2] — [1]Institut für Werkstoffe der Elektrotechnik II, RWTH Aachen University, Aachen, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Jülich, Germany

Today's memory technologies in the semiconductor industry are approaching their scalability limits. As one of the leading candidates for the future non-volatile memory technology, redox based resistive switching memory (ReRAM) has attracted increased attention.

Resistance change in a valence change mechanism (VCM) based ReRAM cell can be achieved by applied voltage modulation and is accounted for a redistribution of the ionic species within the active layer. VCM-type Metal-Oxide ReRAM cell usually consists of a transition metal-oxide layer acting as an active switching layer and a metallic layer acting as a reservoir for oxygen scavenging. The thickness of the oxygen scavenging metal layer, forming the Ohmic contact in TaOx based ReRAM device, was found to be the critical experimental parameter controlling stable bipolar resistive switching versus the occurrence of single-cell complementary switching. Here it is argued that the physically controlling parameter is the effective work function difference between top and bottom electrode contact of the ReRAM cell. For a thin metal cap layer, oxidation increases the effective work function changing from Ohmic to a more blocking contact behavior.

DS 3.6 Mon 10:45 H8

Resistive switching in oxygen engineered TaO_x and Ta:HfO_x based RRAM devices grown by MBE — •Merin Jissy Joseph[1], S.U. Sharath[1], Stefan Vogel[1], Erwin Hildebrandt[1], Philipp Komissinskiy[1], Thomas Schroeder[2], and Lambert Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, Germany — [2]IHP, Frankfurt (Oder), Germany

With conventional flash based non-volatile memories (NVM) gradually approaching its limitations of scaling, resistive random access memory (RRAM) based on CMOS compatible metal oxides (HfO_x, TaO_x etc.) is among the widely investigated choices of next generation NVM. Techniques like oxygen engineering [1] and doping is of interest in reducing the forming voltage and improving the effective device yield in HfO_x based RRAM devices. Resistive switching characteristics were investigated in TaO_x and Ta:HfO_x thin films grown on titanium nitride (TiN) electrodes by reactive molecular beam epitaxy (MBE). TaO_x based devices show a strong dependence of the forming voltage on oxidation conditions. A comparison of amorphous and polycrystalline Ta:HfO_x based devices showed tunable and opposite forming voltage trends with changing composition and doping, highlighting the role of grain-boundaries. One important result is that Ta doping increases the stability of the resistive states, irrespective of crystallinity. Under fixed oxidation conditions, Ta doping in HfO_x was found to reduce the forming voltage while at the same time the resistance ratio is even increased to above ten thousand (10.000).

[1] S. U. Sharath *et al.*, Appl. Phys. Lett. **104**, 063502 (2014).

DS 3.7 Mon 11:00 H8

Time domain analysis of resistive switching in $SrTiO_3$ — •Karsten Fleck[1,2], Camilla La Torre[1,2], Nabeel Aslam[2,3], Susanne Hoffman-Eifert[2,3], Ulrich Böttger[1,2], Rainer Waser[1,2,3], and Stephan Menzel[2,3] — [1]Institut für Werkstoffe der Elektrotechnik II, RWTH Aachen, Aachen, Germany — [2]JARA Fundamentals of Future Information Technology, Jülich, Germany — [3]PGI 7, Forschungszentrum Jülich GmbH, Jülich, Germany

The bipolar resistive switching in metal oxides has gained much attention for the potential application in memory and logic devices. Resistive random access memories based this effect (ReRAM) combine several advantages. Beside their good scalability, high endurance and fast switching they are also very energy efficient. ReRAM cells basically consist of a metal-insulator-metal structure that can be switched between a low and a high resistive state. During an initial electroforming step an oxygen-vacancy enriched highly conductive filament evolves in the oxide. By application of appropriately polarized voltages the oxygen vacancy concentration at one of the metal-oxide interfaces can either be decreased or increased thereby either disableing or enableing electronic conduction. This work presents an analysis of the current during resistive switching in Pt/$SrTiO_3$/TiN nano-crossbars covering the timescale from 10 ns up to 10^5 s. The $SrTiO_3$ layer is deposited by ALD. A pulse scheme is used for cycling thereby monitoring the transient currents. The results are compared to an electro-thermal compact-model thereby illustrating the importance of a thermal runaway due to Joule heating for fast switching.

15 min. break.

DS 3.8 Mon 11:30 H8

Resistive switching in oxygen engineered Al_2O_3/HfO_x based RRAM devices grown by MBE — •Stefan Vogel[1], S. U. Sharath[1], Erwin Hildebrandt[1], Jonas Hunka[1], Christian Wenger[2], Thomas Schroeder[2], and Lambert Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, Germany — [2]IHP, Frankfurt (Oder), Germany

Recently, resistive random access memory (RRAM) has gained a lot of attention due to its promising properties: fast switching times, high endurance, and low power consumption. RRAM devices are non-volatile memories (NVM) based on switching between a low and high resistance state (LRS/HRS) by conducting filaments (CF) which are formed and disrupted by applying voltages of different polarities. RRAM devices usually have a simple metal-insulator-metal stack (MIM) structure. Insulating transition metal oxides like hafnium oxide (HfO_2) are promising for embedded RRAM due to its established CMOS compatibility.

In-situ stacks of TiN/HfO_x with oxygen deficient stoichiometry were deposited by molecular beam epitaxy (MBE) using radical sources with different gases (oxygen and nitrogen) [1]. Device stacks of $Pt/HfO_x/TiN$ with varying device areas were patterned using lithography. Since the forming process of the filament is crucial for good device endurance, the temperature of formation was varied to investigate its influence on the forming process and the endurance. The effect of Al_2O_3 interlayers acting as oxygen diffusion barriers on switching performance has also been investigated.
[1] S. U. Sharath *et al.*, Appl. Phys. Lett. **104**, 063502 (2014).

DS 3.9 Mon 11:45 H8

Non-volatile capacitive switching of BiFeO3-coated Si3N4 /Ge/Si structures — •Kefeng Li[1,2], Lars Rebohle[2], Nan Du[1], Tiangui You[1], Slawek Prucnal[2], Ilona Skorupa[1], Danilo Bürger[1], Thomas Schröder[3], Oliver G. Schmidt[1,4], and Heidemarie Schmidt[1] — [1]Faculty of Electrical and Information Engineering, TU Chemnitz — [2]Institute of Ion Beam Physics and Materials Research, HZDR — [3]Institut for Innovative Microelectronics, IHP Frankfurt/Oder — [4]Institute for Integrative Nanosciences, IFW Dresden

Multiferroic BiFeO3 (BFO) has a large remnant polarization [1]. Ca. 75 nm thick amorphous BFO layers have been grown by pulsed laser deposition at 25 °C on Si3N4/Ge/Si and afterwards recrystallized by applying a 20 ms long flash lamp annealing pulse in oxygen atmosphere [2]. Here we report on the non-volatile capacitive switching in Au/BFO/Si3N4/Ge/Si/Al structures between high capacitance state (HCS) and low capacitance state (LCS) which have a lower power consumption in comparison to the current-driven resistive switching between low resistance state and high resistance state in Au/BFO/Pt/Ti structures [3]. Whereas the HCS is rather stable for the BFO-coated and for the uncoated Si3N4/Ge/Si, the LCS is only stable for the BFO-coated Si3N4/Ge/Si. [1] S. Sakai, M.Takahashi, Materials, 3, 4950 (2010).[2] Subsecond Annealing of Advanced Materials, (Eds.: W. Skorupa, H. Schmidt), Springer Series in Materials Science, 2014.[3] Y. Shuai, S. Zhou, D. Bürger, M. Helm, H. Schmidt, J. Appl. Phys., 109, 124117 (2011)

DS 3.10 Mon 12:00 H8

Structural characterization of epitaxial trigonal Ge-Sb-Te grown by MOVPE — •Martin Schuck[1], Sally Riess[1], Hongchu Du[2], Manuel Bornhöfft[3], Gregor Mussler[1], Martina von der Ahe[1], Alexander Schwedt[2], Joachim Mayer[2,3], Hilde Hardtdegen[1], and Detlev Grützmacher[1] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-9), JARA, 52425 Jülich, Germany — [2]Forschungszentrum Jülich GmbH, Ernst Ruska Centre for Microscopy and Spectroscopy with Electrons (ER-C), JARA, 52425 Jülich, Germany — [3]RWTH Aachen University, Central Facility for Electron Microscopy (GFE), JARA, 52074 Aachen, Germany

Recently, we reported on the successful deposition of trigonal monocrystalline $Ge_1Sb_2Te_4$ on Si by MOVPE. The deposited material bears structural analogies to interfacial Phase-Change Memories (iPCM), where induced switching in the crystalline phase has been reported in highly textured crystalline $(Sb_2Te_3)_x(GeTe)_y$ super-lattices. Therefore trigonal Ge-Sb-Te may act as a model material for iPCM to elucidate the underlying switching effect.

Here we present the structural characterization of epitaxial trigonal $Ge_1Sb_2Te_4$ and $Ge_2Sb_2Te_5$ films on Si (111) deposited by MOVPE. The morphology, structure and composition was investigated using SEM, XRD, HAADF-STEM, EBSD and EDS. STEM investigations reveal highly ordered septuple and nonuple layers, respectively, separated by van der Waals gaps. The structural correlation between monocrystalline Ge-Sb-Te and iPCM will be discussed.

DS 3.11 Mon 12:15 H8

Metalorganic vapour phase deposition of indium-antimony-tellurium nanostructures — •Kristof Keller, Martin Schuck, Martina von der Ahe, Gregor Mussler, Hilde Hardtdegen, and Detlev Grützmacher — Forschungszentrum Jülich GmbH, Peter Grünberg Institute (PGI-9), JARA, 52425 Jülich, Germany

In the search for future non-volatile memories, phase change materials (PCM) are a promising prospect due to their fast switching speeds and high scalability. Alloys from the ternary system germanium-antimony-tellurium are mostly used commercially, so far. Compared to these materials, indium-antimony-tellurium, also a PCM, has advantages including higher crystallization and melting temperatures, leading to enhanced retention at elevated temperatures. Also lower reset currents and the capability of multilevel data storage were reported. Nanostructures like nanowires are called for as they are self-heating elements, thus facilitating the switching mechanism. They also reduce the volume of the switched material.
Here, we present the MOCVD growth of In-Sb-Te nanostructures on a Si substrate using dimethylaminopropyldimethyl-indium (DADI), trimethylindium (TMIn), triethylantimony (TESb) and diethyltellurium (DETe) as precursors and pure N_2 as carrier gas. The deposited nanostructures were characterized by means of scanning electron microscopy, energy dispersive X-ray spectroscopy and X-ray diffraction. The influence of reactor pressure, growth temperature and gas composition on the growth of the nanostructures will be presented in this contribution.

DS 3.12 Mon 12:30 H8

Phase transformation in epitaxial GST thin films grown on Si (111) by Pulsed Laser Deposition — •Isom Hilmi, Andriy Lotnyk, Erik Thelander, Jürgen W. Gerlach, Philipp Schumacher, and Bernd Rauschenbach — Leibniz Institut für Oberflächenmodifizierung (IOM); Leipzig

GeTe-Sb2Te3-based material has been widely applied as a phase change data storage media. Recently, a superlattice GeTe-Sb2Te3 system has been proven to have improved switching characteristics [1,2]. It leads to an investigation of deposition of more ordered or epitaxial Ge-Sb-Te based layers. In this work, the epitaxial layers of Ge2Sb2Te5 (GST) were deposited on Si (111) substrates using pulsed laser deposition (PLD) technique. The crystal structures of the post-annealed epitaxial films were studied by means of x-ray diffraction, energy dispersive and Cs-corrected scanning transmission electron microscopy. The surface morphology was observed by AFM in a taping mode. The as-deposited GST film contains both cubic and hexagonal (h-GST) grain structures. The significant structure change towards h-GST is observed for samples with longer post-annealing up to 7 h, which is, however, also accompanied by loss of Ge.

[1] R. E. Simpson et al., Nat. Nano. 6, 501, (2011). [2] F. Katmis et al., Cryst. Growth Des. 11, 4606, (2011)

DS 3.13 Mon 12:45 H8

Ab initio Simulations of Liquid Phase-Change Materials — •Mathias Schumacher[1], Hans Weber[2,3], Ivan Kaban[2,3], Riccardo Mazzarello[1,4], and Pal Jovari[5] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [2]IFW Dresden, Institute for Complex Materials, Dresden, Germany — [3]Institute of Materials Science, TU Dresden, Germany — [4]JARA FIT and JARA HPC, RWTH Aachen, Germany — [5]Department of Complex Fluids, Institute for Solid State Physics and Optics, Wigner RCP of the H.A.S., Hungary

Phase-Change materials (PCMs) undergo fast and reversible transitions between the amorphous and crystalline phase at high temperature. This property is exploited in non-volatile phase-change memories and rewritable optical disks. The liquid state plays a role in both directions of the switching process: the amorphization occurs upon rapid quenching from the liquid state, whereas fast crystallization takes place from the supercooled liquid. Hence, detailed knowledge of the properties of liquid PCMs is crucial for the understanding of the switching phenomenon. Here we present large scale ab initio molecular dynamics (AIMD) simulations of liquid and supercooled liquid PCMs. We consider large models of GeTe, $Ge_2Sb_2Te_5$ and Ag, In-doped Sb_2Te containing about 500-600 atoms and carry out long simulations (of the order of 100 ps) at different temperatures, below and above the melting temperature. We extract structural and dynamic properties from these trajectories, including radial and angle distribution functions and viscosities. The results are in fair agreement with recent experiments.

DS 3.14 Mon 13:00 H8

Dielectric properties and AC conductivity of amorphous phase change materials — •chao chen[1], hanno volker[1], peter jost[1,2], marvin kaminski[2], and matthias wuttig[1,2] — [1]I.

Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA-FIT, RWTH Aachen University, Germany

Chalcogenide-based phase-change materials (PCMs) are popular for their widespread potential applications in both optical and electrical data storage devices [1]. These applications depend on the pronounced contrast of physical properties between the amorphous and crystalline phases and the ability to rapidly switch between these two phases. PCMs are non-volatile, with fast switching velocity (10 ns) and excellent endurance (10^{10} cycles), which ensures significant potential application for switches. Although the properties of crystalline PCMs have been intensively studied, the phenomena of electrical drift [2] and threshold switching [3] in the amorphous phase are still not well understood, which hampers the development of PCM-based electrical devices and multilevel storage. Several mutually incompatible models about electric transport, such as the small polaron model by Emin [4], the Poole Frenkel model [5], and a band transport model [6] have been developed to explain the behavior of amorphous PCMs. To provide crucial input parameters that should help to derive a unique model, the AC conductivity and dielectric constants of several amorphous PCMs have been studied to determine properties trends and develop a more systematic understanding.

DS 4: Organic Thin Films I

Time: Monday 9:30–12:45 Location: H11

Invited Talk DS 4.1 Mon 9:30 H11

Controlling and tailoring molecular thin film growth — •Stefan Kowarik — Institut für Physik, Humboldt Universität Berlin, Newtonstr. 15, 12489 Berlin

Organic thin films are widely used in applications ranging from (opto-) electronic devices such as OLEDs to functional coatings e.g. in biosensors. Tailoring the thin film properties, such as molecular orientation, crystal structure and phase purity, surface roughness and grain size for a given application is therefore an important challenge. Here we demonstrate different strategies to tailor film growth and showcase important analytical tools to control film growth with in situ X-ray scattering and X-ray spectroscopy (XRR, GISAXS, NEXAFS) as well as UV-vis spectroscopy. We will discuss how micro-kinetic models of growth are starting to become available to predict the influence of the important parameters temperature and growth rate in determining (non-equilibrium) thin film structures. We will discuss how lattice matching with the substrate can be used to change the molecular orientation and how slight chemical modification of molecules can be used to alter the growth mode. Finally we will highlight novel ways to control molecular film growth e.g. by fast temperature cycles to separately control nucleation and coalescence in each monolayer or using laser light to increase phase purity in thin films.

DS 4.2 Mon 10:00 H11

Ultra-robust thin film devices from self-assembled metal-terpyridine wires — •Florian von Wrochem[1], Frank Scholz[1], William Ford[1], Zoi Karipidou[1], Maria Rampi[2], Barbara Branchi[2], Wolfgang Wenzel[3], and Velimir Meded[3] — [1]Sony Deutschland GmbH, Stuttgart, Germany — [2]Department of Chemistry, Ferrara University, Italy — [3]Institute of Nanotechnology, Karlsruhe Instutute of Technology, Germany

Considerable efforts have been undertaken within the past decades to shift organic-based thin-film devices from basic research to the application level. A major hurdle towards the practical realization of large area, thin film circuits is however given by the thermal deposition of the metal electrodes, which remained elusive due to the damage and the electrical shorts experienced by the fragile molecular layers.

Here, we show that large area molecular junctions of outstanding electronic properties and robustness can be realized using densely packed molecular wires consisting of FeII-terpyridine complex oligomers, despite a conventional fabrication process involving top electrode evaporation directly on the molecular layer. Surprisingly, these oligomer-based devices are stable for over 2 years under regular current-voltage cycling, withstanding a wide range of temperatures (150-360 K) and applied voltages (3 V). Electrical studies in conjunction with ab-initio calculations reveal that charge transport occurs via electron (hopping) conduction and is limited by the charge injection through a Shottky barrier of 0.72 eV, following Richardson-Schottky injection.

DS 4.3 Mon 10:15 H11

Patterning functional organic molecules based on the liquid behavior — •Hong Wang, Wenchong Wang, and Lifeng Chi — Physikalisches Institut and Center for Nanotechnology (CeNTech), Universität Münster, 48149 Münster, Germany

Small organic molecules were reported to have the probability to perform like liquid on a surface under vacuum condition, which enable us to fabricate functional organic patterns through focusing on the liquid behavior of it. Here we demonstrate the versatility of the technique in vacuum chamber to create organic hetero-patterns on hierarchically pre-pattern surface through temple-directed growth to locate N,N'-Di[(N-(3, 6-di-tbutyl-carbazyl)ndecyl] quinacridone (DtCDQA) at predefined area firstly, and then anneal at optimized temperature to tune the pattern in situ. Meanwhile, the controlling of organic liquid can also be taken in ambient condition. By using N -ethyl- d -glucamine (NEDG) as the liquid source, we succeeded to pattern organic films on Au stripes directly through self-driven microfluidics. Furthermore, the fluid can be used to transport other functional molecules, e.g., dye molecules, creating multicolored patterns in one step.

DS 4.4 Mon 10:30 H11

Domain size distribution of PTCDA on KCl(100) determined by SPA-LEED and optical spectroscopy — •Christian Marquardt[1], Alexander Paulheim[1], Alexander Eisfeld[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Noethnitzer Str. 38, 01187 Dresden, Germany

The organic dye molecule 3,4,9,10-perylenetetracarboxylicacid dianhydride (PTCDA) forms a monolayer with a commensurate $(2\sqrt{2}\times2\sqrt{2}\ R45^\circ)$ brickwall structure on the KCl(100) surface. Within this structure, the molecules arrange in a head-to-tail configuration forming two-dimensional J-aggregates with optical properties correlated to the size of the exciton delocalization [1]. Under real growth conditions and at cryogenic temperatures, the exciton delocalization is mainly limited by the size of the PTCDA domains. Here, we present a combined SPA-LEED and optical spectroscopy study, to demonstrate the huge impact of the present domain size distribution on the obtained spectral features in optical fluorescence (FL) and FL excitation spectra. Supported by DFG.

[1] M. Müller et al., J. Chem. Phys. 139 044302 (2013).

DS 4.5 Mon 10:45 H11

Origin of F1s NEXAFS Dichrosim in oriented perfluorinated acenes — •Michael Klues[1], Paul Jerabek[1], Tobias Breuer[1], Martin Oehzelt[2], Robert Berger[1], and Gregor Witte[1] — [1]Uni. Marburg, Marburg, Germany — [2]Helmholtz Zentrum Berlin, Berlin, Germany

NEXAFS is a widely used technique to determine molecular orientations on surfaces. Especially for planar molecules with extended π-systems the analysis of angle-dependent intensity variations (dichroism) is straightforward. Surprisingly the analysis of NEXAFS data of fluorinated aromatic molecules measured at the F1s-edge has led to misleading results in the past. In a recent theoretical study [1] this has been attributed to an unexpected overlap of π and σ resonances in the energy region of interest. To further investigate this phenomenon highly ordered multilayers of Perfluoropentacene (PFP) were grown on HOPG and SiO2. PFP crystallizes flat lying respectively nearly upright standing on these substrates. This structural difference results in diverging dichroisms, enabling a detailed assignment of underlying excitations. To gain detailed insights into the nature of these excitations the NEXAFS-signature was calculated using the StoBe-code. Thereby, relaxation effects turned out to be of central importance. To cover this effects the computational approach was improved to determine excitation energies as well as oscillator strength within a ΔSCF-method. Finally these results were able to reproduce not only the signature but also the angle dependants of the experimental spectra.

[1] Oteya et al. Phys. Rev. B 2012, 86, 075469.

DS 4.6 Mon 11:00 H11

Monolayer phases of a dipolar perylene derivative on Au(111) and surface potential built-up in multilayers — •Jens Niederhausen[1,2], Heath R. Kersell[3], Christos Christodoulo[1,2], Georg Heimel[1], Henrike Wonneberger[4], Klaus Müllen[5], Jürgen P. Rabe[1], Saw-Wai Hla[3], and Norbert Koch[1,2] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Humboldt-Universität zu Berlin, Institut für Physik & IRIS Adlershof, Berlin, Germany — [3]Ohio University, Physics & Astronomy Department, Ohio, USA — [4]BASF SE, Ludwigshafen, Germany — [5]Max Planck Institut für Polymerforschung, Mainz, Germany

The molecular self-assembly and the electronic structure of a strongly polar perylene derivative on Au(111) was elucidated with room temperature scanning tunneling microscopy and spectroscopy in combination with ultraviolet and X-ray photoelectron spectroscopies. The molecular arrangements and the increase of the average number of molecules per unit cell via ripening indicate a significant influence of the dipole moment on the molecular assembly. Applying an electric field with the STM tip is found to induce a phase change that can alter the anisotropy of the molecular film. Multilayer molecules arrange with a slightly preferred out-of-plane orientation, inducing a surface potential of up to 1.2 eV. This resembles the giant surface potential effect that was reported before for other polar molecules and deemed applicable for data storage. Notably, the surface potential in the present case can in part be *reversibly* removed by visible light irradiation.

15 min. break.

DS 4.7 Mon 11:30 H11

Evolution of Crystalline C_{60} Films: Influence of the Subjacent Pentacene Layer — •Andrea Karthäuser, Tobias Breuer, and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7, D-35032 Marburg, Germany

A key process in organic photovoltaic devices is the charge transfer that takes place at the heterojunction between molecular donors and acceptors. In many cases, however, an intermixture of both materials hampers detailed studies of the elementary optoelectronic excitations and their structure interrelation. Here we report on the hetero-growth of Buckminster-Fullerene (C_{60}) films on Pentacene (PEN, $C_{22}H_{14}$) bottom layers. While C_{60} deposition on SiO_2 yields amorphous films only, crystalline islands are formed when the substrate is precoated with a PEN buffer layer [1]. Using atomic force microscopy in combination with x-ray diffraction we show that the thickness of the PEN buffer layer is decisive for the crystallinity of the resulting C_{60} films, which can be explained by an interplay of diffusion and nucleation of the impinging C_{60} molecules.

[1] Itaka K. et. al. Adv. Mater. (2006), 18, 1713

DS 4.8 Mon 11:45 H11

Structure and thermal stability of dithiol SAM on Au(111) — •Johannes Völkner and Gregor Witte — AG Molekulare Festkörperphysik, Philipps-Universität Marburg

Self-assembling monolayers (SAMs) are commonly used for molecular modification of metal surfaces. It results in a variation of surface properties such as wetting behavior, friction, reactivity and biocompatibility. In this study an Au(111) surface is functionalized with aromatic trans-stilbene dithiol by means of wet-chemical preparation. While one thiol moiety binds to the surface under thiolate formation the opposite one stays intact. Latter terminates the self-assembling monolayer and thus enables binding events on top of the film. This was for instance recently exploited in a biosensor application based on photoexcitation of quantum dots [1].

Efficient coupling of additional layers however requires high stability and packing density of the film. We prepared stilbene dithiol SAMs under different conditions and verified intactness of the terminating group by means of XPS. Complementary, structural order was investigated in NEXAFS measurements. A clear alteration of the films upon annealing was identified and related to thermal desorption spectra.

[1] N. Sabir et al., Small 11, 5844 (2015)

DS 4.9 Mon 12:00 H11

1,4-phenylene diisocyanide adsorption on metals : from single crystals to supported nanoparticles — •ahmed ghalgaoui, nassar doudin, and martin sterrer — Institute of Physics, University of Graz, Universitätsplatz 5, A-8010 Graz, Austria

We have investigated the adsorption of PDI on single crystal metal surfaces and metal nanoparticles supported by an insulting layer (Au\FeO\Pt(111)). Both, gas-phase and liquid-phase deposition methods were applied. The role of PDI concentration and Au nanoparticle size on the surface structure/adsorption mode of PDI has been investigated by STM and Sum Frequency Generation (SFG) Spectroscopy. The PDI molecule adsorbs either with both - NC groups interacting with the surface, leading to flat adsorption geometry, or by only one - NC group, assuming a vertical adsorption structure. SFG measurements in the -NC stretching region show that PDI deposited from the gas-phase always binds with both - NC groups to Au(111), independent of surface coverage. In the case of liquid-phase deposition, PDI molecules adsorb in the flat adsorption geometry at low concentration, but change to the vertical geometry upon increasing the concentration. This concentration dependence is absent on Pt(111), where PDI exclusively adsorbs in the vertical geometry. Finally, the influence of Au particle size on the adsorption structure of PDI will be discussed.

DS 4.10 Mon 12:15 H11

A novel strategy for enhancing layer-by-layer growth of organic thin films: Temperature variation during individual monolayer growth — •Laura Bogula, Linus Pithan, Anton Zykov, and Stefan Kowarik — Inst. für Physik, Humboldt-Universität zu Berlin, Germany

We investigate the influence of a time dependent substrate temperature on the thin film growth of the organic semiconductor PTCDI-C_8. We show that varying the substrate temperature during the growth of each monolayer allows one to control the nucleation and coalescence regimes and to enhance layer-by-layer growth. We analysed the PTCDI-C_8 films with *in situ* X-ray reflectivity at the Anti-Bragg point and post-growth atomic force microscopy and consistently found smoother films when the dynamic heating method was applied as compared with static substrate temperatures. We thus demonstrate a novel method to induce enhanced layer-by-layer growth of organic molecules, which is highly relevant for applications in organic electronics.

DS 4.11 Mon 12:30 H11

3-D hybrid inorganic-organic structures: metallic nanoparticles self-assembled in organic molecular crystall — •Olga Molodtsova[1,2], Sergey Babenkov[1], Irina Aristova[3], Denis Vyalikh[4], Oleg Vilkov[4], Maxim Tchaplyguine[5], Ralf Nyholm[5], Karina Schulte[5], Andrei Hloskovsky[1], and Victor Aristov[1,3,6] — [1]DESY, Hamburg, Germany — [2]ITMO, Saint Petersburg, Russia — [3]ISSP RAS, Chernogolovka, Russia — [4]BESSY, Berlin, Germany — [5]Max-lab, Lund, Sweden — [6]TU Bergakademie, Freiberg, Germany

The evolution of the morphology and the electronic properties of the hybrid organic-inorganic systems composed of metallic nanoparticles distributed in semiconductor organic matrix (FxCuPc, x=0,4,16), as a function of nominal metal content was studied by transmission electron microscopy and by surface- and bulk sensitive photoelectron spectroscopy. This work supported by the RFBR Grant No. 13-02-00818 and the BMBF-Project No. 05K12GU2, PSP-Element No. U4606BMB1211

DS 5: Two-dimensional Materials (Joint session of DS and HL, organized by HL)

Time: Monday 9:30–13:00 Location: H16

DS 5.1 Mon 9:30 H16

Boundary conditions for transition-metal dichalcogenide monolayers in the continuum model — •Csaba Géza Péterfalvi, Andor Kormányos, and Guido Burkard — Department of Physics, University of Konstanz, D-78464 Konstanz, Germany

We derive the boundary conditions for $\mathrm{MoS_2}$ and similar transition-metal dichalcogenide honeycomb (2H polytype) monolayers with the same type of $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian within the continuum model around the K points. [1] In an effective 2-band description, the electron-hole symmetry breaking quadratic terms are also taken into account. We model the effect of the edges with a linear edge constraint method that has been applied previously to graphene. Focusing mainly on zigzag edges, we find that different reconstruction geometries with different edge-atoms can generally be described with one scalar parameter varying between 0 and 2π. We analyze the edge states and their dispersion relation in $\mathrm{MoS_2}$ in particular, and we find good agreement with the results of previous density functional theory calculations for various edge types.

[1] Cs. G. Péterfalvi, A. Kormányos, G. Burkard, arXiv:1509.00184 (2015).

DS 5.2 Mon 9:45 H16

High Q-factor in WSe2 Nano-electromechanical resonator — •Antoine Reserbat-Plantey[1], Nicolas Morell[1], Ioannis Tsioutsios[1], Kevin Schädler[1], François Dubin[2], Frank Koppens[1], and Adrian Bachtold[1] — [1]ICFO, The Insitutue for Photonic Sciences, Barcelona, ES — [2]INSP, Université Paris 6, Paris, FR

Atomically thin nano-electromechanical systems (2D-NEMS) combine extremely low mass resonators having resonant frequencies in the MHz-GHz range, wide tunability, low damping and exotic non-linearities. Atomically thin 2D semi-conductors such as transition metal dichalcogenides (TMD) have extremely rich optical properties (direct band gap, spin valley, embedded quantum emitters), which are intrinsically linked to their low dimensionality. Optical and electronic properties of WSe2, an emblematic TMD, have been intensively studied while there is no extensive nanomechanical investigation of this system. Here we show a new generation of semiconductor 2D-NEMS made of monolayer of WSe2. We record mechanical and photoluminescence spectra of WSe2 nanoresonators down to cryogenic temperatures. We measure mechanical quality factor Q>47000 at T=3.5 K, which is the highest value reported so far for 2D-NEMS in this temperature range. Combining ultra-low dissipation resonators with the very rich optical properties of TMD, paves the way for novel type of optomechanical experiments with 2D materials.

DS 5.3 Mon 10:00 H16

Landau levels and Shubnikov-de Haas oscillations in monolayer transition metal dichalcogenide semiconductors — •Andor Kormányos[1], Péter Rakyta[2], and Guido Burkard[1] — [1]Physics Department, University of Konstanz — [2]Department of Theoretical Physics, Budapest University of Technology and Economics

We study the Landau level (LL) spectrum using a multi-band $\mathbf{k}\cdot\mathbf{p}$ theory in monolayer transition metal dichalcogenide semiconductors [1]. We find that in a wide magnetic field range the LL can be characterized by a harmonic oscillator spectrum and a linear-in-magnetic field term which describes the valley degeneracy breaking. The effect of the non-parabolicity of the band-dispersion on the LL spectrum is also discussed. Motivated by recent magnetotransport experiments, we use the self-consistent Born approximation and the Kubo formalism to calculate the Shubnikov-de Haas oscillations of the longitudinal conductivity. We investigate how the doping level, the spin-splitting of the bands and the broken valley degeneracy of the LLs affect the magnetoconductance oscillations. We consider monolayer $\mathrm{MoS_2}$ and $\mathrm{WSe_2}$ as concrete examples and compare the results of numerical calculations and an analytical formula which is valid in the semiclassical regime. Finally, we briefly analyze the recent experimental results [Cui et al., Nat. Nanotechnol. **10**, 534 (2015)] using the theoretical approach we have developed.

[1] New J. Phys. **17**, 103006 (2015).

DS 5.4 Mon 10:15 H16

Second-harmonic generation in MoS2 monolayers coupled to resonant nanoantennas — •Franz Johannes Friedrich Löchner[1], Stefan Fasold[1], Antony George[2], Paul Douglas Harrison[1], Christoph Menzel[1], Andrey Turchanin[2], Isabelle Staude[1], Falk Eilenberger[3], Frank Setzpfandt[1], and Thomas Pertsch[1] — [1]Institute of Applied Physics, Abbe Center of Photonics , Friedrich-Schiller-Universität Jena, 07743 Jena, Germany — [2]Institute of Physical Chemistry, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany — [3]Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

Two-dimensional monolayers of transition metal dichalcogenides (TMDs), a new class of direct band-gap semiconductors, recently have attracted a lot of attention due to their pronounced excitonic emission lines and strong second-order nonlinearity.

Coupling TMDs to resonant nanoantennas allows to further enhance these effects by concentrating the exciting optical field into a small volume. Such enhancement has been shown for excitonic emission using plasmonic nanoantennas. However, nonlinear optical effects in TMD-nanoantenna systems have not been studied yet.

In our contribution, we report on experimental investigations of second-harmonic generation in molybdenum disulfide (MoS2) monolayers coupled to nanoantennas, resonant at the exciting fundamental-harmonic wavelength. Polarization resolved measurements show the profound impact which the presence of the nanoantenna has on the second-harmonic radiation generated by the MoS2-monolayer.

DS 5.5 Mon 10:30 H16

Electrochemical growth and characterization of molybdenum sulfide layers for thin film transistors — •Talha Nisar, Torsten Balster, and Veit Wagner — Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany

Molybdenum disulfide has attracted considerable interest for its great potential in the field of nanoelectronics due to its semiconducting and 2D nature. It has been successfully deposited by the Scotch tape method resulting in high-mobility transistors with an area of a few square microns. The state-of-the-art method for the growth of crystalline molybdenum disulfide single and multilayers is chemical vapor deposition.

In our study we use electrochemical deposition as an alternative approach to grow large area molybdenum sulfide layers. For this purpose, ammonium tetrathiomolybdate (ATTM) has been used as precursor material for the electrodeposition in cathodic regime with respect to Ag/AgCl reference electrode. The obtained layers are amorphous as could be confirmed by Raman measurements. In addition, in the UV-VIS spectra of the MoS_x (x=2..3) layer a transition at 2.4 eV is visible, which could be related to oxygen contamination. Further annealing steps in an $\mathrm{Ar/H_2}$ atmosphere with an additional sulfur source at temperatures above 600°C are necessary to remove the oxygen and to convert the layer into crystalline $\mathrm{MoS_2}$. The converted layer has to be transferred onto $\mathrm{SiO_2/Si}$ substrates for thin film transistor applications.

30 min. Coffee Break

Invited Talk DS 5.6 Mon 11:15 H16

Epitaxial paradigms of van der Waals bonded chalcogenide materials — •Raffaella Calarco — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

In recent years it has become clear that materials with covalent bonding in only two dimensions (2D) have attractive properties for devices. The bonding in the third dimension, which is between individual layers, occurs by van der Waals (vdW) forces, which are weaker if compared to the covalent bonding. Materials used in conventional devices are instead characterized by covalent bonding in three dimensions (3D). In the present contribution, I shed some light on understanding the mechanisms that determine the interface structure between 2D and 3D or 2D materials. To study possible options for altering the bonding configurations of the 2D-3D interface GeTe-Sb2Te3 layers are deposited by molecular beam epitaxy on top of five different surface reconstructions-passivation of the Si(111). The 2D-2D interface is best studied using graphene as a substrate. Finally, I address the most crucial issue:

The realization of vdW epitaxy in Sb2Te3-GeTe superlattices. Such superlattices, if compared to their alloy counterpart, show impressive performances highly attractive for future non-volatile memory applications.

DS 5.7 Mon 11:45 H16

Transparent Conducting Materials: Insights from High-Throughput — •Pino D'Amico[1,2], Alice Ruini[1,2], Alessandra Catellani[2], Arrigo Calzolari[2], Marco Fornari[3,5], and Marco B. Nardelli[4,5] — [1]FIM-UNIMORE, Modena, Italy — [2]CNR-NANO S3, Modena, Italy — [3]Central Michigan Univ., Mt. Pleasant, USA — [4]Univ. of North Texas, Denton, USA — [5]Duke Univ., Durham, USA

Good electrical conductivity and optical transparency in the visible domain are the physical properties required in order to have Transparent Conducting Material (TCM). Various semiconductors becomes TCM when doped and up to now their discovery has followed an a-posteriori path: take a material and investigate its physical properties in order to see if it is a good TCM. Thanks to the large amount of data available in the AFLOWLIB repository[1], we use instead an inverse-design approach in order to search for new possible TCMs: starting from the paradigmatic case of ZnO[2] we have identified the physical descriptors representing a TCM and extracted from the database a list of materials having the required characteristics using highthroughput techniques. We investigated doped structures of resulting materials inserting substitutional elements in a systematic way with a given concentration. We will present an accurate study of both conductivity and optical properties of the doped structures obtained by means of a newly developed numerical tool based on Boltzmann theory and dielectric function calculations[3] and reliyng on an efficient ab-initio tight-binding representation of the lattice structures[4]. [1]www.aflowlib.org; [2]ACS Photonics 1, 703 (2014); [3]preprint(2015); [4]arXiv:1509.02558 (2015).

DS 5.8 Mon 12:00 H16

Investigating the Potential of TMD Monolayers as Photodetectors — •Maja Feierabend[1], Gunnar Berghäuser[2], and Ermin Malic[2] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden

Transition metal dichalcogenides (TMDs) are promising materials for technological application in the area of optoelectronics. Due to the direct band gap and the extraordinarily strong Coulomb interaction, TMDs exhibit efficient light-matter coupling and tightly bound excitons [1]. As atomically thin materials, they are very sensitive to changes in the surrounding environment. This motivates a functionalisation approach, where external molecules are non-covalently attached to the material surface to control its optical properties.

Here, we theoretically investigate functionalized TMDs based on the density matrix formalism combined with tight-binding wave functions. Considering exemplary spiropyran molecules exhibiting a strong dipole moment, we predict pronounced spectral red-shifts and the appearance of an additional side-peak in the absorption spectrum of functionalized TMDs. Interestingly, we also observe a further peak splitting due to the intervalley coupling between the high-symmetry K/K' points. The predicted pronounced changes in optical spectra of TMDs show their potential for technological application in photodetectors.

[1] G. Berghäuser and E. Malic, PRB 89, 125309 (2014)

DS 5.9 Mon 12:15 H16

Investigation of excitonic resonances in monolayer MoSe2 for strong coupling experiments at room temperature — •Nils Lundt[1], Aleksander Maryński[2], Grzegorz Sek[2], Oliver Iff[1], Sefaattin Tongay[3], Sven Höfling[1,4], and Christian Schneider[1] — [1]Chair for Apllied Physics, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of Physics, Wrocław University of Technology, Wybrzeze Wyspiańskiego 27, 50-370 Wrocław, Poland — [3]School for Engineering of Matter, Transport, and Energy, Arizona State University, Tempe, Arizona 85287, United States — [4]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY 16 9SS, United Kingdom

We studied the temperature evolvement of the reflectivity of a MoSe2 monolayer. From this investigation we deduced the dependence of linewidth and oscillator strength on temperature. The results were used for transfer matrix simulations of strong coupling reflectivity spectra, expected if the MoSe2 monolayer is integrated into a micro-cavity. These calculations should evaluate, if strong coupling can be observed in MoSe2 monolayers at room temperature. Calculations were conducted for different cavity designs such as an open cavity approach, a monolithic cavity and for the coupling to a Tamm Plasmon. Moreover, we present results of excitation power dependent photoluminescence studies on MoSe2 monolayers.

DS 5.10 Mon 12:30 H16

Localized states from WSe$_2$ as promising candidates for new single-photon sources — •Sven Borghardt[1], Jhih-Sian Tu[1], Florian Winkler[2], Detlev Grützmacher[1], and Beata Kardynal[1] — [1]PGI-9, Forschungszentrum Jülich, Jülich, Germany — [2]ER-C, Forschungszentrum Jülich, Jülich, Germany

An emission of single photons from WSe$_2$ monolayers (ML) has been recently demonstrated but the origin of the emission is still not clear. The aim of our research is to understand its origin and then control the localized emission in this material to harvest the unique properties of the material for new applications in quantum photonics.

Samples prepared by exfoliation from synthetic crystals and also grown with CVD are measured using polarization resolved μ-photoluminescence (PL) as well as time-resolved PL.

Our results show linearly polarized emission doublet lines with an energy splitting of up to a few meV. The samples show a high density of such lines close to the sample edges. We attribute the linear polarization of the localized states to a mixing of K- and K'-states. There is an evidence of an alignment of the polarization of emission with the crystal lattice. PL from the localized states decays faster with the temperature than the one from the free exciton states. Chemical modification of the samples is further used in an attempt to manipulate the emission from the localized states.

DS 5.11 Mon 12:45 H16

Theoretical studies of transition metal dichalcogenides for the use in electron holography — •Sven Borghardt[1], Zeila Zanolli[4], Matthieu Verstraete[3], Florian Winkler[2], Juri Barthel[2], Rafal Dunin-Borkowski[2], and Beata Kardynal[1] — [1]PGI-9, Forschungszentrum Jülich, Jülich, Germany — [2]ER-C, Forschungszentrum Jülich, Jülich, Germany — [3]PCPM, Université Catholique de Louvain, Louvain-la-Neuve, Belgium — [4]PGI-2 and IAS, Forschungszentrum Jülich, Jülich, Germany

Few-layer transition metal dichalcogenides (TMDs) represent a new family of materials with promising properties for new optoelectronic nano-devices. Their well-known and tailorable thickness render them an ideal system for quantitative electron holography.

Here, we present the simulation of the effect of charge reorganisation due to bonding on the phase acquired by electrons passing through few layer TMD structures in electron holography experiments. This is done by simulating the phases for potentials from density functional theory calculations in comparison with ones obtained from the independent-atom approximation. The results show in an impressive way that neglecting the atomic bonding and the associated small change in the overall charge distribution leads to an overestimation of the average electron phase by approximately 5% for the analyzed materials. Comparison with experimental data confirms this conclusion.

Building on the results for pristine materials, we present calculations for single defects and heterostructures composed of different materials from the transtition-metal dichalcogenide family.

DS 6: Graphene: Theory (Joint session of DS, DY, HL, MA, O and TT organized by HL)

Time: Monday 9:30–12:30 Location: H17

DS 6.1 Mon 9:30 H17

Instantaneous Quantum Time Reversal Mirror in Graphene — •Phillipp Reck[1], Cosimo Gorini[1], Arseni Goussev[2], Mathias Fink[3], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Department of Mathematics and Information Sciences, Northumbria University, Newcastle Upon Tyne, UK — [3]Ecole Supérieure de Physique et Chimie Industrielle, CNRS, PSL Research University, Paris, France

The physicists' fascination for time inversion goes back a long time, as testified by the famous 19th-century argument between Loschmidt and Boltzmann concerning the arrow of time. Both metaphysical and practical considerations intrigued generations of scientists, who have ever since strived to devise and implement time-inversion protocols – in particular, different forms of "time mirrors" for classical waves such as sound- and electromagnetic-waves (see e.g. [1-2]), and recently an instantaneous time mirror for water waves [3].

Here we propose the realization of instantaneous Time Mirrors for quantum systems. These are controlled time discontinuities acting on wavefronts as mirrors in time and leading to distinct wavefunction echoes. More precisely, our Quantum Time Mirror exploits up to now unrelated concepts of wavefront time inversion and population reversal in two-level systems, the latter quintessential to spin echoes. It can be implemented in a relativistic Dirac-like system, e.g. graphene.

[1]M. Fink , IEEE Trans. Ultr. Ferroel. Freq. Control, 39, 555, (1992)

[2]G. Lerosey, et al., Phys. Rev. Lett. 92, 193904 (2004)

[3]V. Bacot, et al., preprint (2015)

DS 6.2 Mon 9:45 H17

Plasmon signature in Dirac-Weyl liquids — •Johannes Hofmann — TCM Group, Cavendish Laboratory, University of Cambridge, UK

I shall discuss theoretically as a function of temperature the plasmon mode arising in three-dimensional Dirac liquids, i.e., systems with linear chiral relativistic single-particle dispersion, within the random phase approximation. It is found that whereas no plasmon mode exists in the intrinsic (undoped) system at zero temperature, there is a well-defined finite-temperature plasmon with superlinear temperature dependence, rendering the plasmon dispersion widely tunable with temperature. The plasmon dispersion contains a logarithmic correction due to the ultraviolet-logarithmic renormalization of the electron charge, manifesting a fundamental many-body interaction effect as in quantum electrodynamics. The plasmon dispersion of the extrinsic (doped) system displays a minimum at finite temperature before it crosses over to the superlinear intrinsic behavior at higher temperature, implying that the high-temperature plasmon is a universal feature of Dirac liquids irrespective of doping. This striking characteristic temperature dependence of intrinsic Dirac plasmons along with the logarithmic renormalization is a unique manifestation of the three-dimensional relativistic Dirac nature of quasiparticle excitations and serves as an experimentally observable signature of three-dimensional Dirac materials.

DS 6.3 Mon 10:00 H17

Finite temperature and electric field effects in the RKKY interaction in graphene and bilayer graphene — •Nicolas Klier[1], Sangeeta Sharma[2], Oleg Pankratov[1], and Sam Shallcross[1] — [1]Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7-B2, 91058 Erlangen — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction in Bernal stacked bilayer graphene [1,2] is shown to have a particularly rich dependence on temperature and a layer symmetry breaking electric field. Depending on whether we consider the chemical potential or particle number as the fixed variable we find that an electric field may tune the RKKY between ferromagnetic (FM) and anti-ferromagnetic (AFM) coupling, or an oscillatory and AFM coupling.

[1] N. Klier, S. Shallcross, and O. Pankratov, *P*hys. Rev. B **90**, 245118, 2014.

[2] N. Klier, S. Shallcross, S. Sharma, and O. Pankratov, *P*hys. Rev. B **92**, 205414, 2015.

DS 6.4 Mon 10:15 H17

The Electronic Structure of Graphene from Dyson-Schwinger Equations with Partially Screened Coulomb Interactions — •Manon Bischoff[1], Katja Kleeberg[2], Dominik Smith[2], Lorenz von Smekal[2], and Björn Wellegehausen[2] — [1]Johannes Gutenberg Universität, Mainz, Deutschland — [2]Justus Liebig Universität, Gießen, Deutschland

We have studied the possibility of a semimetal-insulator transition via spin-density or charge-density wave formation with partially screened Coulomb interactions in graphene from the coupled Dyson-Schwinger equations (DSEs) for the electronic excitations and their Lindhard screening on the honeycomb lattice. In the limit of purely static Lindhard screening these DSEs close on themselves and no further truncation is necessary. With appropriate boundary conditions they can then be solved numerically by fixed-point iteration. This is particularly efficient on graphical processing units (GPUs). After validating the static approximation from Monte-Carlo simulations on smaller lattices with appropriate boundary conditions, it allows to study much larger sheets than in the ab-initio simulations, e.g., to search for Miransky scaling, and to include cases where the latter break down because of a fermion-sign problem as for charge-density wave formation, for example.

DS 6.5 Mon 10:30 H17

Ab-initio lattice Monte-Carlo simulations of the Neck-disrupting Lifshitz transition in mono-layer graphene — •Michael Koerner, Dominik Smith, and Lorenz von Smekal — Institut fuer Theoretische Physik, Justus-Liebig-Universitaet Giessen

We study the effects of inter-electron interactions on the neck-disrupting Lifshitz transition, which is characterized by a change of topology of the Fermi surface. The Lifshitz transition is known to occur within a pure tight-binding description of mono-layer graphene when an external chemical potential drives the Fermi surface away from half-filling and across the saddles at the M-points. At these Van Hove singularities the density of states diverges logarithmically without interactions. We employ ab-intio Monte-Carlo simulations, which account for the full many-body physics of interacting electrons. We choose a partially screened Coulomb potential which combines the screening from localized electron states at short distances with the unscreened long-range Coulomb tails characteristic of graphene at half filling. Our goal is to determine whether interactions change the character of the topological transition, such that a real phase transition in the thermodynamic sense may occur, possibly in combination with chiral superconductivity.

DS 6.6 Mon 10:45 H17

Tight-binding description of spin-orbit coupling in graphene due to adatoms — •Susanne Irmer, Denis Kochan, Klaus Zollner, Martin Gmitra, Tobias Frank, and Jaroslav Fabian — University of Regensburg, Regensburg, Germany

We present realistic effective tight-binding models for proximity spin-orbit coupling in graphene due to adatoms at top, bridge, and hollow positions. The models are built from symmetry arguments and fitted to ab initio calculations for a variety of adsorbants, such as H [1], F [2], Cu, and CH3 [3]. For each of these adatoms we provide magnitudes for orbital couplings to the adsorbants, as well as the intrinsics, Rashba, and pseudospin-inversion asymmetry (PIA) couplings. Our models can be used to study spin relaxation, spin Hall effect, and spin transport using quantum transport models.

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

[1] M. Gmitra, D. Kochan, J. Fabian, Phys. Rev. Lett. 110, 246602 (2013)

[2] S. Irmer, T. Frank, S. Putz, M. Gmitra, D. Kochan, J. Fabian, Phys. Rev. B 91, 115141 (2015)

[3] K. Zollner, T. Frank, S. Irmer, M. Gmitra, D. Kochan, J. Fabian, arXiv:1507.02820

30 min. Coffee Break

DS 6.7 Mon 11:30 H17

Ab initio studies of excitations in monolayer black phosphorus — •Tobias Frank[1], Marcin Kurpas[1], Martin Gmitra[1], Rene Derian[2], Ivan Stich[2], and Jaroslav Fabian[1] — [1]Universität Regensburg, Regensburg, Germany — [2]Slovak Academy of Sciences, Bratislava, Slovakia

Monolayer black phosphorus, or phosphorene, represents an ideal system to study many-body electron-electron and electron-hole interactions due to its strong anisotropy driven 1d electronic nature. In particular, the size of the fundamental band gap value and excitonic binding energies remain unresolved given the different gap values of 1.6 to 2.4 eV [1] obtained by many-body GW calculations. We present our contribution to this issue studying excitations in phosphorene employing quantum monte carlo (QMC) calculations. We show the evolution of finite size effects of the fundamental and optical gap, with respect to relatively large supercell sizes in the theoretical framework of diffusion monte carlo (DMC) explicitly including electronic correlations. Our studies point to a significant influence of electron correlation on the fundamental gap as well as to a strong anisotropic nature of the excitonic state. Furthermore we address the question of a multiconfigurational ground state in monolayer black phosphorus. This work is supported by the DFG GRK 1570, SFB 689, and European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

[1] A. N. Rudenko, Shengjun Yuan, and M. I. Katsnelson, Phys. Rev. B 92 085419 (2015)

DS 6.8 Mon 11:45 H17

Phase structure of graphene from Hybrid Monte-Carlo simulations — •Pavel Buividovich[1], Lorenz von Smekal[2], Dominik Smith[2], and Maksim Ulybyshev[1] — [1]Regensburg University, Institute for Theoretical Physics, D-93053 Regensburg, Universitatstr. 31 — [2]Giessen University, Institute for Theoretical Physics, D-35392 Gießen, Heinrich-Buff-Ring 16

We study the phase structure of monolayer graphene in the parametric space of on-site and nearest-neighbour interactions using the Hybrid Monte-Carlo algorithm similar to those used in lattice QCD simulations. Our simulation code allows us to perform ab-initio simulations on lattices as big as 36x36 unit cells. We numerically determine the boundaries of the charge density wave, spin density wave and the Kekule distortion phases. We also confront the results with analytic studies based on Schwinger-Dyson equations, which allow to reach even larger lattice sizes, up to 5000x5000 unit cells.

DS 6.9 Mon 12:00 H17

Quantum Monte-Carlo study of graphene in external magnetic field — •Maksim Ulybyshev — Institute of Theoretical Physics, University of Regensburg, D-93053 Germany, Regensburg, Universitatsstrasse 31

Recent experimental results indicate that graphene turns into insulator in sufficiently strong magnetic field. However, the exact nature of this state is still elusive and there are some discrepancies between theoretical predictions and experimental results. To resolve this discrepancies extensive simulations of graphene in external magnetic field were performed using Hybrid Monte Carlo algorithm. Insulating state was observed in agreement with experiment. Mass gap and various order parameters were measured.

DS 6.10 Mon 12:15 H17

Interaction-induced conductance from zero modes in a clean magnetic graphene waveguide — •Laura Cohnitz[1], Wolfgang Häusler[2,3], Alex Zazunov[1], and Reinhold Egger[1] — [1]Institut für Theoretische Physik, Heinrich-Heine-Universität, D-40225 Düsseldorf, Germany — [2]Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany — [3]Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany

We consider a waveguide formed in a clean graphene monolayer by a spatially inhomogeneous magnetic field. The single-particle dispersion relation for this waveguide exhibits a zero-energy Landau-like at band, while finite-energy bands have dispersion and correspond, in particular, to snake orbits. For zero-mode states, all matrix elements of the current operator vanish, and a finite conductance can only be caused by virtual transitions to finite-energy bands. We show that Coulomb interactions generate such processes. In stark contrast to finite-energy bands, the conductance is not quantized and shows a characteristic dependence on the zero-mode filling. Transport experiments thereby offer a novel and highly sensitive probe of electron-electron interactions in clean graphene samples. We argue that this interaction-driven zero-mode conductor may also appear in other physical settings and is not captured by the conventional Tomonaga-Luttinger liquid description.

DS 7: Graphene: Transport
(Joint session of DS, DY, HL, MA, O and TT organized by HL)

Time: Monday 14:45–17:45 Location: H17

Invited Talk DS 7.1 Mon 14:45 H17

Advances in Raman Spectroscopy of Graphene and Layered Materials — •Andrea C. Ferrari — Cambridge Graphene Centre, University of Cambridge, Cambridge, CB3 OFA, UK

Raman spectroscopy is an integral part of graphene research [1]. It is used to determine the number and orientation of layers, the quality and types of edges, and the effects of perturbations, such as electric and magnetic fields, strain, doping, disorder and functional groups[2,3]. I will review the state of the art, future directions and open questions in Raman spectroscopy of graphene and related materials, focussing on the effect of disorder[3,4], doping[5,6] and deep UV laser excitation[7]. I will then consider the shear [8] and layer breathing modes(LBMs)[9], due to relative motions of the planes, either perpendicular or parallel to their normal. These modes are present in all layered materials[10,11]. Their detection allows one to directly probe the interlayer interactions [10,11]. They can also be used to determine the elastic constants associated with these displacements: the shear and out-of-plane elastic moduli[12]. This paves the way to the use of Raman spectroscopy to uncover the interface coupling of two-dimensional hybrids and heterostructures[10-12].

1. A. C. Ferrari et al. Phys. Rev. Lett. 97, 187401 (2006) 2. A.C. Ferrari, D.M. Basko, Nature Nano. 8, 235 (2013) 3. A.C. Ferrari, J Robertson, Phys. Rev. B 61, 14095 (2000) 4. G. Cancado et al. Nano Lett. 11, 3190 (2011) 5. M. Bruna et al. ACS Nano 8, 7432 (2014) 6. A. Das et al. Nat. Nanotechnol. 3, 210 (2008) 7. A.C. Ferrari, S. Milana, P. H. Tan, D. M. Basko, P. Venezuela, submitted (2016) 8. P. H. Tan et al. Nature Materials 11, 294 (2012) 9. X. Zhang et al. Phys. Rev. B 87, 115413 (2013) 10. J. B. Wu et al. Nature Comms. 5, 5309 (2014) 11. J.B. Wu et al. ACS Nano, 9, 7440 (2015) 12. S. Milana et al. submitted (2016)

DS 7.2 Mon 15:15 H17

Landau Quantization in Twisted Bilayer Graphene — •Johannes C. Rode, Dmitri Smirnov, Christopher Belke, Hennrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

The bandstructure of bilayer graphene is highly sensitive to rotational mismatch between layers. At large angles, the twisted bilayer effectively behaves like two decoupled monolayers, while the dispersions merge in low-energy van Hove singurities for small interlayer twist[1]. Whereas the regime of large rotational mismatch has been extensively studied in transport experiments[2], there have been few reports on small angle samples[3,4] and none for the transition between the two angular regimes so far. We here examine the magnetotransport behavior across this transition, closing the gap in experimental evidence. The results are discussed with respect to theory[5] and and under special consideration of gate-induced layer asymmetries.

[1] Lopes dos Santos, J. M. B., Perez, N. M. R., Castro Neto, A. H. *Phys. Rev. Lett.* **99**, 25682.
[2] Schmidt, H. *et al. Appl. Phys. Lett.* **93**, 172108.
[3] Schmidt, H., Rode, J. C., Smirnov, D., and Haug, R. J. *Nat. Commun.* **5**, 5742.
[4] Lee, D. *et al. Phys. Rev. Lett.* **107**, 216602.
[5] de Gail, R., Goerbig, M. O., Guinea, F., Montambaux, G., Castro Neto, A. H. *Phys. Rev. B* **84**, 045436.

DS 7.3 Mon 15:30 H17

Magnetic exchange coupling across a graphene layer — •Alessandro Barla[1], Valerio Bellini[2], Stefano Rusponi[3], Paolo Ferriani[4], Marina Pivetta[3], Fabio Donati[3], François Patthey[3], Luca Persichetti[5], Sanjoy K. Mahatha[1], Marco Papagno[6], Cinthia Piamonteze[7], Simon Fichtner[4], Stefan Heinze[4], Pietro Gambardella[5], Harald Brune[3], and Carlo Carbone[1] — [1]Istituto di Struttura della Materia, CNR, I-34149 Trieste, Italy — [2]S3-Istituto di Nanoscienze-CNR, I-41125 Modena, Italy — [3]Institute of Condensed Matter Physics, EPFL, CH-1015 Lausanne, Switzerland — [4]Institute of Theoretical Physics and Astrophysics, University of Kiel, D-24098 Kiel, Germany — [5]Department of Materials, ETH Zürich, CH-8093 Zürich, Switzerland — [6]Dipartimento di Fisica, Universitá della Calabria, I-87036 Arcavacata di Rende, Italy — [7]Swiss Light Source, PSI, CH-5232 Villigen PSI, Switzerland

In order to access the potential of graphene in spintronic devices, its ability to mediate magnetic exchange interactions has to be verified. We present the results of our investigations of the magnetic coupling between Co atoms and Ni(111) mediated by epitaxial graphene. Experimental and theoretical calculations reveal that individual Co atoms occupy two distinct adsorption sites, with different magnetic coupling to the underlying Ni(111) surface. We further report a transition from an antiferromagnetic to a ferromagnetic coupling with increasing Co coverage. Our results highlight the extreme sensitivity of the exchange interaction mediated by graphene to the adsorption site and to the inplane coordination of the magnetic atoms.

DS 7.4 Mon 15:45 H17

Transport studies in laterally density-modulated graphene-boron nitride-heterostructures — •Martin Drienovsky[1], Christian Baumgartner[1], Felix Simbürger[1], Takashi Taniguchi[3], Kenji Watanabe[3], Ming-Hao Liu[2], Fedor Tkatschenko[2], Klaus Richter[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik Universität Regensburg, 93053 Regensburg — [2]Institut für Theoretische Physik Universität Regensburg, 93053 Regensburg — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

We report on ballistic transport in graphene-boron nitride heterostructures with a tunable charge carrier density profile. Employing a dry van-der-Waals stacking method, we prepare high mobility graphene devices, where the charge carrier mean free path can exceed the lattice period of the induced multibarrier system by several times. These potential barriers are generated by multiple local top gate electrodes and a global back gate, and yield a pronounced Fabry-Pérot interference pattern in the bipolar transport regime. The extended ballistic length - in comparison to former samples - gets us within reach of the superlattice effect, which we highlight by matching the experimental data to a model calculation. We additionally apply a high, perpendicular magnetic field to our multibarrier systems and observe mode-mixing in the Quantum-Hall-regime of a 4-point measurement setup. By comparing samples with different top gate periods and separately controllable top electrodes, we study adiabatic and equilibrated unipolar edge channel transmission and suppression of equilibration at bipolar junctions.

15 min. Coffee Break

Invited Talk DS 7.5 Mon 16:15 H17

Thermodynamic picture of ultrafast conduction in graphene — •Dmitry Turchinovich[1], Zoltan Mics[1], Klaas-Jan Tielrooij[1,2], Ivan Ivanov[1], Xinliang Feng[1], Klaus Müllen[1], and Mischa Bonn[1] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]ICFO, 08860 Barcelona, Spain

Graphene has very high steady-state conductivity, which, however, does not hold in the regime of ultrafast, sub-picosecond electric fields corresponding to the terahertz (THz) frequencies. Here we show that in graphene, the electron conduction on an ultrafast timescale is determined by a simple thermodynamic balance maintained within its electronic system acting as a thermalized electron gas [1]. The energy of ultrafast electric currents passing trough graphene is near-instantaneously converted into the thermal energy of its entire charge carrier population, thereby raising the electronic temperature and reducing the chemical potential. The interplay between electron heating and cooling dynamics in graphene ultimately defines its ultrafast conductivity. We demonstrate that this simple thermodynamic picture describes very well the THz linear, nonlinear, and photo-induced conductivity of this remarkable material [1-3].

[1] Z. Mics, K.-J. Tielrooij, K. Parvez, S. A. Jensen, I. Ivanov, X. Feng, K. Müllen, M. Bonn, and D. Turchinovich, Nat. Commun. 6, 7655 (2015). [2] S. A. Jensen, Z. Mics, I. Ivanov, H. S. Varol, D. Turchinovich, F. H. L. Koppens, M. Bonn, and K. J. Tielrooij, Nano Lett. 14, 5839 (2014). [3] I. Ivanov, M. Bonn, Z. Mics, and D. Turchinovich, EPL - Europhys. Lett. 111, 67001 (2015).

DS 7.6 Mon 16:45 H17

Magnetotransport in graphene antidot arrays: semiclassics and moiré lattices — •Andreas Sandner[1], Tobias Preis[1], Christian Schell[1], Paula Giudici[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]NIMS, 1-1 Namiki, Tsukuba, Japan

Embedding graphene into a heterostructure with hexagonal boron nitride (hBN) on both sides was shown to be an efficient way of achieving a high bulk mobility. However, nanopatterning graphene can add extra damage and drastically degrade the intrinsic properties by edge disorder. But graphene encapsulated between hBN is protected during a top-down fabrication procedure. In this way, we can prepare graphene-based antidot lattices where the high mobility is preserved.

We performed magnetotransport experiments in monolayer-graphene antidot lattices with lattice periods down to 50 nm. We observe pronounced commensurability features in ρ_{xx} stemming from ballistic orbits around one or several antidots. Due to the short lattice period in our samples, we can explore the boundary between the semiclassical and the quantum transport regime, as the Fermi wavelength of the electrons approaches the smallest length scale of the artificial potential.

Additionally, we study the interplay between a moiré and the imposed antidot superlattice potential in several of our samples. There is a gradual suppression of the classical commensurability features by approaching the satellite Dirac points of the moiré potential.

DS 7.7 Mon 17:00 H17

Influence of disordered edges on transport properties in graphene — Dmitri Smirnov[1], Galina Yu. Vasileva[1,2,3], •Christopher Belke[1], Johannes C. Rode[1], Yurij B. Vasilev[2], Yurij L. Ivanov[2], and Rolf J. Haug[1] — [1]Institut fuer Festkoerperphysik, Leibniz Universitaet Hannover — [2]Ioffe Institute, Russian Academy of Sciences, St. Petersburg — [3]Peter the Great Polytech University, St. Petersburg

The influence of plasma etched edges on electrical transport and doping on graphene devices is studied. Mono- and bilayer samples were fabricated into a specific Hall bar geometry with differing width. The fabrication was done via transfer on a Si/SiO$_2$ substrate and structuring and contacting via plasma oxygen etching and e-beam lithography. The specific shape allows to investigate the influence of edge disorder on the overall doping and the effective mobility.

The doping concentration, calculated from the charge neutrality point, differs for every region and an inverse dependence on the region width was observed. The sample edge was determined as a strong p-doping source, dominating the bulk doping component and the edge doping contribution and efficiency was obtained.

A further study of the mobility for different regions was used to quantify the edge scattering. We find, that for decreasing region width the mobility decreases as well. This behavior can be attributed to the samples edge, establishing it as a further scattering mechanism.

DS 7.8 Mon 17:15 H17

Acoutoelectric currents in coated graphene on SiC — •Alberto Hernández-Mínguez, Abbes Taharoui, Marcelo Lopes, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Surface acoustic waves (SAWs) provide useful mechanisms for the dynamic modulation and transport of carriers in two-dimensional semiconductor heterostructures. In the case of graphene, we have recently shown that the piezoelectric fields accompanying SAWs can induce unipolar electric currents in lithographically patterned graphene layers grown on SiC. Due to the weak piezoelectricity of SiC, however, the interaction between SAW and carriers in graphene is relatively small. Future applications of the acoustic transport require the generation of strong SAWs for their efficient coupling to graphene, as well as the control of the density and type of carriers transported by the SAW. In this contribution, we study structures for efficient generation of high frequency acoustic transport (> 1 GHz) in graphene grown on SiC that are also compatible with top gates for the electric control of the carrier density. Several Rayleigh modes with frequencies up to 7 GHz are efficiently generated in our structure, inducing acoustic currents for the fundamental frequency that are 300 times larger than the ones reported in our previous devices. These results are an important step towards the dynamic control of carriers in graphene at the sub-micrometer regime, as well as for the dynamic manipulation of the electron spin by strain-induced gauge fields.

15 min. Coffee Break

DS 8: Thin Film Characterisation: Structure Analysis and Composition I

Time: Monday 15:00–16:30 Location: H8

Invited Talk DS 8.1 Mon 15:00 H8

Materials characterization at the nanoscale by X-ray spectrometry — •Burkhard Beckhoff — Physikalisch-Technische Bundesanstalt (PTB), Abbestraße 2-12, 10587 Berlin, Germany

The development of efficient nanoscaled materials requires the correlation of the materials functionality with their chemical and physical properties. To probe these properties, analytical methods that are sensitive at the nanoscale are required. The reliability of most analytical methods is based on the availability of reference materials or calibration samples, the spatial elemental composition of which is as similar as possible to the matrix of the specimens of interest. However, there is a drastic lack of reference materials at the nanoscale. PTB addresses this challenge by means of an X-ray analytical method where all instrumental and experimental parameters are determined with known contributions to the uncertainty of the analytical results. This first-principle based approach does not require any reference materials but a complete characterization of the instrumental characteristics and, in addition, of the X-ray fundamental parameters related to the elements composing the sample. X-ray spectrometric methods allow for the variation of the analytical sensitivity, selectivity, and information depth needed to effectively reveal the spatial, elemental, and chemical specimen parameters of interest. Examples of interfacial speciation, elemental depth profiling, as well as layer composition and thickness characterizations in various materials will be given. Recent instrumental achievements provide access to liquid-solid interfaces as well as towards the in-situ speciation of battery materials.

DS 8.2 Mon 15:30 H8

Determination of growth quality of thin films by In-situ GISAXS during the deposition process — •Jörg Wiesmann[1], Peter Siffalovic[2], Karol Vegso[2], and Martin Hodas[2] — [1]Incoatec GmbH, Geesthacht, Germany — [2]Inst. of Physics, Slovak Acad. of Sci., Bratislava, Slovakia

We present how the growth of thin films can be investigated during the deposition by means of grazing incidence small angle X-ray scattering (GISAXS). These experiments are typically done only at synchrotrons. They are now also feasable in the home-lab by using modern microfocus sources like the air cooled IμS.

The IμS is explained in more detail. It is a high-brilliance X-ray source for diffractometry and available with Cr, Co, Cu, Mo, and Ag anodes. It is equipped with a 2-dim beam shaping multilayer optic. We can form either a collimated beam with low (below 0.5 mrad) or a focusing beam with higher divergence (up to 10 mrad) and very small focal spots below 100 μm.

In our presentation we give an overview of experiments and results demonstrating the potential of the IμS in in-situ GISAXS studies. We present 2 applications in detail:

1) Multilayers deposited by ion beam assisted deposition: This experiment was done only at synchrotrons. With an IμS it becomes feasible in the home-lab.

2) Growth of thin metallic layers on graphene: The difference between production by PVD and Thermal Deposition is discussed.

DS 8.3 Mon 15:45 H8

Real-Time Investigation at Metal-Polymer-Interfaces during Sputter Deposition. — •Matthias Schwartzkopf[1], Oleksandr Polonskyi[2], Alexander Hinz[2], Thomas Strunskus[2], Franziska Löhrer[3], Volker Körstgens[3], Peter Müller-Buschbaum[3], Franz Faupel[2], and Stephan V. Roth[1] — [1]DESY, Photon Science, Notkestr. 85, 22607 Hamburg — [2]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, Kaiserstr.2, 24143 Kiel — [3]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

The reproducible low-cost fabrication of functional metal-polymer-nanocomposites remains a major issue in applied nanotechnology. In order to obtain full control over the nanostructural evolution at the metal-polymer interface, we employed the combination of in-situ time-resolved GISAXS [1] and GIWAXS with in-situ ellipsometry during sputter deposition of gold on thin polystyrene films. We correlate the evolution of the metallic layer morphology with changes in the key scattering features. This enabled us to identify the impact of different deposition rates on the growth regimes with their specific thresholds and permits a better understanding of the growth kinetics of gold clusters on polymer substrates. 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).

DS 8.4 Mon 16:00 H8

Ion beam sputter deposition (IBSD) of cubic MgO and NiO — •Martin Becker, Robert Hamann, Mario Gies, Fabian Michel, Angelika Polity, and Martin Eickhoff — 1st Physics Institute, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Ion beam sputter deposited MgO and NiO thin films were grown on (0001) (c-cut), ($01\bar{1}2$) (r-cut), ($11\bar{2}0$) (a-cut) and ($10\bar{1}0$) (m-cut) sapphire substrates. A pure Ni metallic target and a MgO ceramic target were processed with different gas mixtures of argon and oxygen at elevated substrate temperatures. X-ray photoelectron spectroscopy (XPS) and energy dispersive X-ray spectroscopy (EDX) were used to identify composition and stoichiometry. It is shown, that elevated temperatures favor crystallization in preferential orientations. The determined out-of-plane relationships were $XO(111)\|Al_2O_3(0001)$ (c-cut), $XO(111)\|Al_2O_3(11\bar{2}0)$ (a-cut) and $XO(110)\|Al_2O_3(10\bar{1}0)$ (m-cut) for $X = Mg/Ni$, whereas on $Al_2O_3(01\bar{1}2)$ (r-cut) no significant out-of-plane intensity was observed. XRD rocking curves indicated small full width at half maximum (FWHM) around 10-100 arcsec. X-ray pole figures and reciprocal space mapping (RSM) indicated distinct epitaxial in-plane relationships. The morphology was studied by scanning electron microscopy (SEM) and atomic force microscopy (AFM), which reveal smooth and homogeneous surfaces for thin layers, enabling their use as appropriate buffer layers for established IBSD-sputtered materials like cuprous oxide and stannic oxide.

DS 8.5 Mon 16:15 H8

Determing the optical constants of NiO with Resonant X-Ray Reflectivity — •Katrin Fürsich[1], Volodymyr B. Zabolotnyy[1], Christian Schüssler-Langeheine[2], Maurits W. Haverkort[3], and Vladimir Hinkov[1] — [1]University Würzburg, Am Hubland, 97074 Würzburg — [2]HZB, Albert-Einstein-Str. 15, 12489 Berlin — [3]MPI for CPfS, Nöthnizer Straße 40, 01187 Dresden

NiO has been serving as the model system to study electronic correlations and antiferromagnetism of transition-metal oxides, mostly because of its appealing properties like large bandgap and high Néel temperature. Nevertheless, it is still a challenge to describe NiO theoretically as common methods such as DFT and LDA+U are known to fail. We use Resonant X-Ray Reflectivity (RXR) in combination with cluster calculations to study the optical properties of NiO. RXR is a non-destructive technique with a probing depth >100 nm and sub-nm spatial resolution. Thus RXR provides an excellent opportunity to extract layer-resolved optical constants, which are directly related to physical properties like crystal field effects and spin-orbit interactions. However, because of the screening effects it is hard to determine these parameters theoretically. This results in uncertainties in the calculations. We perform RXR measurements on *in situ* grown NiO thin films of different thicknesses and on cleaved NiO bulk crystals to overcome these problems and to tune unknown variables in the state of the art cluster calculation. The analysis combines theory and experiment in order to give remarkable insight into the physical properties of correlated electron systems.

DS 9: Organic Thin Films II

Time: Monday 15:00–16:45 Location: H11

DS 9.1 Mon 15:00 H11

Investigation of phase separation in bulk heterojunction organic solar cells — •Vladislav Jovanov, Arne Hendel, Nivedita Yumnam, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Performances of bulk heterojunction organic solar cells strongly depend on their ability to dissociate photo-generated excitons. Efficient exciton dissociation is crucial for achieving high short circuit currents and energy conversion efficiencies. A volume distributed junction between donor and acceptor material is needed to obtain efficient dissociation, since exciton dissociation occurs only at their interface. Furthermore, the domain sizes of donor and acceptor material should be at nanometer length scale, so that excitons can reach the interface before they recombine. In this study, a phase separation of bulk heterojunction organic solar cells based on a blend mixture of PTB7 (donor) and PCBM (acceptor) material is investigated. To record the phase separation, an atomic force microscopy (AFM) has been used. The phase image measured by AFM depends on the energy dissipated by a cantilever tip to a material at the surface of a sample. Consequently, the phase contrast observed in the phase image is influenced by different materials present at the sample surface. By identifying the phase of donor and acceptor material, the phase separation and its dependence on preparation conditions can be determined from AFM phase image.

DS 9.2 Mon 15:15 H11

Charge transport and trap dynamics investigations in organic solar cells via MIS structures — Nivedita Yumnam, Hippolyte Hirwa, and •Veit Wagner — Jacobs University, Campus Ring 1, 28759 Bremen, Germany

The charge transport in organic bulk heterojunction solar cells is a critical process affecting the performance of the solar cell. Investigating the charge transport dynamics in the solar cell allows determination of the relevant transport parameters. The mobility of the charge carriers can be determined in the short time regime (up to 1ms). While the longer time regime allows to study the density of trap states. For our characterization we have prepared metal insulator semiconductor (MIS) devices based on Si/SiOx substrate and bulk heterojunction semiconductor mixture of P3HT and PCBM. The mobility of charge carriers is determined by using MIS-CELIV (metal insulator semiconductor- charge carrier extraction by linearly increasing voltage) [1]. For the investigation of trap states in our device, we have employed our recently developed transient current measurement technique which does not need light illumination [2]. This illumination-free transient current (IFTC) technique offer insights on the capture time of the trapping states, their density of states and the attempt-to-escape frequency of trapped carriers. [1] A.Armin et al., Advanced Energy Materials, 2014, 4, 1300954.[2] H.Hirwa, V.Wagner, Organic electronics, Vol. 25, 2015, 112*120

DS 9.3 Mon 15:30 H11

Investigation of Solution-Processable Electron Injection Layers in Organic Light-Emitting Diodes — •Florian Ullrich[1,2,3], Sebastian Stolz[1,3], Michael Scherer[1], Malte Jesper[4], Manuel Hamburger[1,4], Gerardo Hernandez-Sosa[1,3], and Eric Mankel[1,5] — [1]InnovationLab GmbH, Heidelberg — [2]University of Heidelberg, Kirchhoff-Institute for Physics — [3]Karlsruhe Institute of Technology, Light Technology Institute — [4]University of Heidelberg, Organisch-Chemisches Institut — [5]TU Darmstadt, Material-Wissenschaft, Surface Science

One crucial obstacle for the realization of efficient organic light-emitting diodes (OLEDs) produced by high-throughput printing technologies is the poor injection of electrons since typical low work-function cathode layers like calcium or barium are highly reactive and cannot be solution-processed.

In this work, we investigate alkali metal stearates as solution processable electron injection layers in OLEDs. We fabricated yellow emitting OLEDs with different concentrations of Cs, Rb and K stearate and studied the influence on device performance, e.g. efficiency and efficacy. Values of about 9 cd/A and 10 lm/W were reached equalling the respective values of reference devices. The results were correlated to topography studies using atomic force microscope. The electronic interaction of the alkali metal stearates with the emitting layer and the aluminum top contact was examined by various photoelectron spectroscopy measurements.

DS 9.4 Mon 15:45 H11

Thermoelectric characterization of doped organic semiconductors — •Bernhard Nell and Koen Vandewal — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

The introduction of p- and n-doped layers into the device structure of opto-electronic devices plays a crucial role in improving device performance. In this way, the charge carrier extraction or injection from or into the organic photo-active layer is improved and ohmic losses are reduced. Molecular doping of organic host materials increases the conductivity of the transport layers and moves the Fermi level to the appropriate position enabling electron or hole selectivity. In this work, we use thermovoltage (Seebeck effect) and temperature-dependent conductivity measurements to determine the dominating type of charge carriers introduced by the dopant and to gain insight into the position of the transport level with respect to the Fermi level. The investigation of fullerene dopants with a different degree of fluorination in various amorphous host materials allows us to tune the energy level offsets between host and dopant and study their influence on the Fermi level position and overall doping efficiency systematically.

DS 9.5 Mon 16:00 H11

Computer simulation of self-assembled monolayers of alkanethiols on liquid mercury — •Anton Iakovlev[1], Dmitry Bedrov[2], and Marcus Müller[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [2]Department of Materials Science & Engineering, University of Utah, Salt Lake City, 84112, UT, USA

The defectless, high-tension surface of liquid mercury facilitates the creation of high-quality self-assembled monolayers (SAMs) of organic molecules. SAMs of alkanethiols on liquid mercury are widely used in organic electronics to study the properties of metal-SAM-metal and metal-SAM-semiconductor junctions, where the liquid mercury is usually utilized as the second electrode. Recent experiments have revealed the coexistence of densely packed standing and flat-lying alkanethiols on the surface of liquid mercury and proposed rectangular unit cells for both, the head groups and tails, in the standing phase. Earlier, an oblique unit cell has also been considered to be a possible arrangement of alkanethiols on liquid mercury. In this report we present the first study of the phase coexistence and structure of SAM of alkanethiols on mercury by means of large-scale Molecular Dynamic simulation. We have developed a model of the SAM of alkanethiol on mercury, that allows us to reproduce the experimentally observed coexistence of the standing and lying molecules and to gain additional insights (eg. tilting of the tails) into the structure of alkanethiol SAMs on mercury. Our results indicate the oblique arrangement of thiols to be the preferred one.

DS 9.6 Mon 16:15 H11

Tip-induced gating of carbene-based molecular circuits — Giuseppe Foti and •Hector Vazquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

In this talk I will discuss N-heterocyclic carbene-based (NHC) molecules on gold [1] and explore their adsorption, mechanical and transmission properties by means of first-principles simulations based on DFT and NEGF.

First, I will examine the adsorption properties of NHCs on Au(111). NHCs bind selectively to the Au atop sites through a strong Au-C bond. I will then address the mechanical properties of NHCs through simulations where the metal-molecule junction is stretched. Upon elongation, the strong Au-C bond induces rearrangements of the Au surface and ultimately a Au-Au bond, and not the Au-C bond, breaks. Finally, I will discuss the conducting properties of NHC-based molecular junctions. We consider several tip structures and find a strong dependence of the position of the NHC molecular levels with the atomistic structure of the tip [2]. The LUMO position changes by almost 0.8 eV with tip shape. This is understood in terms of the net charge transfer, electron redistribution and work function for each tip structure. The differences in the LUMO position effectively gate the molecular levels and result in large conductance variations. These findings open the way to modulating the conductance of NHC-based molecular circuits through the controlled design of the tip atomistic structure.

[1] C.M. Crudden et al., Nature Chemistry 6 409 (2014).

[2] G. Foti and H. Vazquez (under review).

DS 9.7 Mon 16:30 H11

Magnetic transition metal phthalocyanine thin films, tuning of electronic properties via alkali metal doping — •Olga Molodtsova[1,2], Sergey Babenkov[1], Ralf Nyholm[3], Karina Schulte[3], Denis Vyalikh[4], Oleg Vilkov[4], Volodymyr Maslyuk[5], Ingrid Mertig[5], Thomas Bredow[6], and Victor Aristov[1,7,8] — [1]DESY, Hamburg, Germany — [2]ITMO, Saint Petersburg, Russia — [3]Max-lab, Lund, Sweden — [4]BESSY, Berlin, Germany — [5]Uni Halle, Germany — [6]Uni Bonn, Germany — [7]ISSP RAS, Chernogolovka, Russia — [8]TU Bergakademie, Freiberg, Germany

The evolution of electronic structure of the MTM-Pc*s intrinsic and with potassium doping has been studied by means of photoemission spectroscopy, near-edge X-ray absorption fine structure and DFT calculations. The DFT calculations and detailed analysis of the core-level spectra permit us to suggest possible lattice sites for the potassium ions. The data disclosed filling of the lowest unoccupied molecular orbital upon doping and associated changes of the core level absorption spectra. None of the films prepared in our studies showed a finite electronic density of states at the Fermi level. This work was supported by the RFBR Grant No. 13 -02-00818 and the BMBF-Project No. 05K12GU2, PSP-Element No. U4606BMB1211

DS 10: Transport: Topological Insulators - 2D (Joint session of DS, HL, MA, O and TT, organized by TT)

Time: Monday 15:00–17:45 Location: H18

DS 10.1 Mon 15:00 H18

Probing the spin texture of generic helical edge states with an antidot — •Alexia Rod[1,2], Giacomo Dolcetto[1], Thomas L. Schmidt[1], and Stephan Rachel[2] — [1]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [2]Institut für Theoretische Physik, TU Dresden, Germany

Edge states of time-reversal topological insulators are generally described as helical edge states, where the spin-axis symmetry is conserved. However, this symmetry is usually not guaranteed in experimental realizations. In its absence, the most general model to describe edge states is called generic helical liquid. Using this framework, a rotation of the spin quantization axis has been predicted, independently of the microscopic model and of the considered geometry [1, 2].

Here we propose a scheme to probe the spin texture of the edge states on a transport device. We investigate the transport properties of generic helical edge states in a two-dimensional topological insulator bar with an antidot in its center. We show that the conductance is implicitly dependent of the spin texture in the case of uniform bulk or structural inversion asymmetry. We also study sequential tunneling and cotunneling in presence of Coulomb interaction due to electron confinement on the antidot.

[1] T.L. Schmidt, S. Rachel, F. von Oppen, L. Glazman, PRL **108**, 156402 (2012).

[2] A. Rod, T.L. Schmidt, S. Rachel, PRB **91**, 245112 (2015).

DS 10.2 Mon 15:15 H18

Electron quantum optics in 2d topological insulators — •Andrea Spichtinger, Sven Essert, Viktor Krückl, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Besides conventional quantum Hall systems [1], 2d topological insulators (TIs) are ideal systems providing ballistic channels for guiding charge carriers along edge states allowing for the study of two-particle interferometric effects. Employing wave-packet approaches we investigate correlations between indistinguishable spin pairs at opposite quantum spin Hall edges. Interconnecting opposite edges at TI constrictions or through quantum dots acting as ”beam splitter” allows for realizing fermionic analogues of the famous photonic Hong-Ou-Mandel (HOM) effect. In particular, we will consider generalizations of the HOM effect since the dwell time of the quantum dot enters as a new timescale into HOM physics.

[1] E. Bocquillon et al., Ann. Phys. **526**, 1 (2014)

DS 10.3 Mon 15:30 H18

Transport in quantum spin Hall systems in parallel magnetic fields — •Michael Wimmer[1], Rafal Skolasinski[1], Dmitry Pikulin[2], and Jason Alicea[3] — [1]TU Delft, The Netherlands — [2]University of British Columbia, Canada — [3]Caltech, US

Edge states in quantum spin Hall (QSH) systems are protected by time-reversal symmetry, resulting in a qunatized conductance. A magnetic field breaks that protection, and should lead to a deviation from perfect quantization. We will discuss generic features of semiconductor-based QSH systems (such as HgTe/CdTe and InAs/GaSb) that affect the magnetic field dependence of edge state conductance, focusing on the effect of an in-plane field.

DS 10.4 Mon 15:45 H18

Spectral functions of the correlated topological insulator — •Damian Zdulski and Krzysztof Byczuk — Faculty of Physics, Institute of Theoretical Physics, University of Warsaw, ul.Pasteura 5, PL-02-093 Warsaw, Poland

In our recent paper [1], we have studied the influence of electron correlations on topological insulators (TIs) at finite temperatures. The correlated TI was represented by the Kane-Mele model with the interaction term as in the Falicov-Kimball model and it was examined within the Hartree and the Hubbard I approximations. In this talk, we will present extension of that analysis by investigating properties of the system within the dynamical mean field approximation. Our findings show that dynamical correlations yield totally new structures, which are seen in the the momentum dependent spectral functions. Namely, we see: 1) widening of Dirac nodes over finite range of $\mathbf{k}$ points in the Brillouin zone (BZ), 2) creation of almost flat subbands in a finite range of the BZ, 3) appearance of kinks, and 4) splitting of kinks with formation of overlapping bands.

[1] D. Zdulski, K. Byczuk, PRB **92**, 125102 (2015)

DS 10.5 Mon 16:00 H18

The topological Anderson insulator phase in the Kane-Mele model — Christoph P. Orth[1], •Tibor Sekera[1], Christoph Bruder[1], and Thomas L. Schmidt[2] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [2]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg

It has been proposed that adding disorder to a topologically trivial mercury telluride/cadmium telluride (HgTe/CdTe) quantum well can induce a transition to a topologically nontrivial state. The resulting state was termed topological Anderson insulator and was found in computer simulations of the Bernevig-Hughes-Zhang model.

We show that the topological Anderson insulator is a more universal phenomenon and also appears in the Kane-Mele model of topological insulators on a honeycomb lattice. We numerically investigate the interplay between the parameters characterizing intrinsic spin-orbit coupling, extrinsic Rashba spin-orbit coupling and staggered sublattice potential. We establish the parameter regimes in which the topological Anderson insulator is found. For weak enough disorder, a calculation based on the lowest-order Born approximation reproduces the numerical data. Our results thus considerably increase the number of candidate materials for the topological Anderson insulator phase.

15 min. break

DS 10.6 Mon 16:30 H18

Interplay of topology and interactions in the quantum Hall regime of topological insulators: spontaneous symmetry breaking, tunable strongly interacting Luttinger liquid — •Stefan Jürgens, Maxim Kharitonov, and Björn Trauzettel — Institute of Theoretical Physics, University of Würzburg, Germany

We consider a class of two-dimensional topological insulators, in which the single-particle edge states are preserved in the presence of the magnetic field by a symmetry (such as crystalline) other than time-reversal, relevant to such materials as HgTe-type heterostructures.

We focus on the vicinity of the topological crossing point between two Landau levels. At half-filling, Coulomb interactions lead to the formation of the quantum Hall "ferromagnetic" many-body state with gapped charge excitations in the bulk. We derive and analyze the σ-model that describes the low-energy properties of this strongly interacting state, including the effect of the edge. We obtain the bulk phase diagram and find three phases, two with preserved and one with spontaneously broken U(1) symmetry. We study the collective edge charge excitations of these phases.

We demonstrate that in one of the phases with preserved U(1) symmetry, the edge charge excitations are gapless and described by a highly tunable, strongly interacting Luttinger liquid. When U(1) symmetry is broken in this phase, edge excitations become gapped and are described by a sine-Gordon model. Our main conclusion is that continuous U(1) symmetry is a necessary condition for the existence of the gapless edge excitations in this strongly interacting system.

DS 10.7 Mon 16:45 H18

Terahertz properties of Dirac electrons and holes in HgTe films with critical thickness — •Uladzislau Dziom[1], Alexey Shuvaev[1], Nikolai Mikhailov[2], Ze Don Kvon[2], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Novosibirsk State University, Novosibirsk 630090, Russia

We present and discuss properties of mercury telluride (HgTe) films with critical thickness in far-infrared (THz) spectral range. Density of charge carriers is controlled, using contact-free optical gating by visible light. Transmission measurements in applied magnetic field demonstrate switching from hole to electron-like behavior, as illumination time increases. The cyclotron mass of the electrons, extracted from the data, shows a square root dependence upon the charge concentration in a broad range of parameters. This can be interpreted as a clear proof of a linear dispersion relations, i.e. Dirac-type charge carriers.

DS 10.8 Mon 17:00 H18

Topological Edge States with Zero Hall Conductivity in a Dimerized Hofstadter Model — •Alexander Lau[1], Carmine Ortix[1,2], and Jeroen van den Brink[1,3] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [2]Institute for Theoretical Physics, Utrecht University, The Netherlands — [3]Department of Physics, TU Dresden, Germany

The Hofstadter model is one of the most celebrated models for the study of topological properties of matter and allows the study of the quantum Hall effect in a lattice system. Indeed, the Hofstadter Hamiltonian harbors the topological chiral edge states that are responsible for the quantized Hall conductivity.

Here, we show that a lattice dimerization in the Hofstadtermodel opens an energy gap at half-filling. What is more, we demonstrate that even if the ensuing insulator has a Chern number equal to zero, concomitantly a doublet of edge states appear that are pinned to specific momenta. We show that the presence of these states can be understood from the topological properties of lower dimensional cuts of the system, using a mapping of the Hofstadter Hamiltonian to a collection of one-dimensional Aubry-Andre-Harper (AAH) models. A sub-set of AAH chains in this collection preserve inversion symmetry. This guarantees the presence of topologically protected doublets of end modes to which the edge states are pinned. To explicitly prove the robustness of the emerging edge states, we define and calculate the topological invariant that protects them, which turns out to be an integer invariant for inversion-symmetric AAH models.

DS 10.9 Mon 17:15 H18

Disorder induced zero Landau level in topological insulator nanowires and its signature in conductance fluctuations — •Emmanouil Xypakis and Jens H Bardarson — Max-Planck-Institut f. Physik komplexer Systeme Noethnitzer Str. 38, 01187 Dresden, Germany

In this talk I will discuss the quantum transport properties of a disordered topological insulator in a strong magnetic field. The focus is on the case when the chemical potential is close to the Dirac point, where the transport is dominated by induced chiral modes. Disorder has a drastic role in the system electrical response by revealing a zero Landau level, which is absent for clean topological insulators. We study the dependence of the zero Landau level energy window on the system parameters, such as system size, disorder and magnetic field strength.

DS 10.10 Mon 17:30 H18

Time-resolved pure spin fractionalization and spin-charge separation in helical Luttinger liquid based devices — •Giacomo Dolcetto[1,2], Matteo Carrega[2], Alessio Calzona[2,3], and Maura Sassetti[2,3] — [1]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [2]SPIN-CNR, Genova, Italy — [3]Dipartimento di Fisica, Università di Genova, Italy

Helical Luttinger liquids, appearing at the edge of two-dimensional topological insulators, represent a new paradigm of one-dimensional systems, where peculiar quantum phenomena can be investigated [1]. Motivated by recent experiments on charge fractionalization [2], we propose a setup based on helical Luttinger liquids that allows one to time-resolve, in addition to charge fractionalization, also spin-charge separation and pure spin fractionalization. This is due to the combined presence of spin-momentum locking and interactions. We show that electric time-resolved measurements can reveal both charge and spin properties, avoiding the need of magnetic materials [3, 4]. Although challenging, the proposed setup could be achieved with present-day technologies, promoting helical liquids as interesting playgrounds to explore the effects of interactions in one dimension.

[1] G. Dolcetto, M. Sassetti, and T. L. Schmidt, arXiv preprint arXiv:1511.06141

[2] H. Kamata, N. Kumada, M. Hashisaka, K. Muraki, and T. Fujisawa, Nat. Nanotechnol. **9**, 177 (2014)

[3] A. Calzona, M. Carrega, G. Dolcetto, and M. Sassetti, Physica E **74**, 630 (2015)

[4] A. Calzona, M. Carrega, G. Dolcetto, and M. Sassetti, PRB **92**, 195414 (2015)

DS 11: Hybrid and Perovskite Photovoltaics I (Joint session of CPP, DS and HL, organized by CPP)

Time: Monday 15:00–17:30 Location: H38

DS 11.1 Mon 15:00 H38

Effect of phase transition on photoluminescence polarization of single perovskite nano-objects — •Daniela Täuber[1], Alexander Dobrovolsky[1], Rafael Camacho[1,2], and Ivan Scheblykin[1] — [1]Chemical Physics, Lund University, Lund, Sweden — [2]Department of Chemistry, University of Leuven, Leuven, Belgium

We use 2D polarization resolved microscopy to study the polarization of single $CH_3NH_3PbI_3$ perovskite nano-objects in excitation and emission at 295, 152 and 77 K. Depending on size and shape, polarization of up to 70% was observed at 77 K in emission, while it is in general smaller in excitation, and it decreases with increasing temperature. For wire-shaped objects the polarization is along the long axis, which points to contributions from antenna effects and crystal growth direction in combination with asymmetric crystal structures. The difference seen in excitation and emission may be caused by the band structure and the excitation wavelength at 448 nm.

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

DS 11.2 Mon 15:15 H38

Energy Levels at Perovskite/Electron Transport Layer Interfaces — •Fengshuo Zu[1], Johannes Frisch[1], Liangsheng Liao[2], and Norbert Koch[1] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 6, 12489 Berlin, Germany — [2]FUNSOM,Soochow University, Jiangsu 215123, China

organometal halide perovskites attract substantial attention for high-efficiency thin film solar cells. Numerous studies are focused on film processing and device configuration variation in order to further improve device efficiency, but the fundamental physics in particular regarding interfacial energy level alignment with charge transport materials (e.g., fullerene derivatives) are yet poorly understood. It is generally believed that perovskites form type-II p-n junctions with C60 or PCBM, which would favor the charge separation process at the interface. To substantiate this proposition, we performed TRPL and UPS measurements to investigate the interface energy levels and the charge separation process at perovskite/fullerene junctions. However, contrary to the common believe, our measurements show that both junctions exhibit n-n type-I level alignment. TRPL results show no different decay channels with or without fullerene layers, which indicates the perovskite/fullerene interface does not provide a driving force for charge separation. Nonetheless, our solar cells with PCBM junctions show reasonable performance, with a power conversion efficiency of 9.30%. In constrast, the perovskite/C60 solar cells show much lower efficiency, which we attribute to upward band bending within perovskite when in contact with C60.

DS 11.3 Mon 15:30 H38

The influence of hole transporting materials on the charge transport in stacked perovskite-based systems — •Kathrin Bader[1,2], Michiel Petrus[1,2], Thomas Bein[1,2], Pablo Docampo[1,2], Matthias Handloser[1,2], and Achim Hartschuh[1,2] — [1]Department of Chemistry and CeNS, LMU Munich — [2]Nanosystems Initiative Munich (NIM)

Hybrid metal halide perovskites have become a focal point of the photovoltaic community as promising candidates for next-generation solar cells. Extremely fast progress in this field has taken efficiencies to over 20 % [1] and lead to the development of a large variety of material compositions, preparation techniques and device structures [2]. Although the fabrication of the perovskite absorber itself is comparably cheap, latest device architectures incorporate the expensive hole transporting material (HTM) spiro-OMeTAD. To reduce the overall production costs for perovskite-based devices alternative organic HTMs have been developed [3]. Here we use a contact-less technique based on time-resolved laser scanning confocal microscopy [4] to visualize the influence of different HTMs on $\mathrm{CH_3NH_3PbI_3}$ thin films. We investigate charge carrier transport properties and photoluminescence lifetimes of individual HTM layers as well as stacked perovskite/HTM systems and identify potential candidates to replace the expensive spiro-OMeTAD in the device structure. [1] Green, M. A. et al., Prog. Photovolt: Res. Appl. 2015, 23, 805-812. [2] Green, M. A. et al., Nature Photon. 2014, 8, 506-514. [3] Petrus, M. L. et al., J. Mater. Chem. A 2015, 3, 12159-12162. [4] Bader, K. et al., ACS Photonics 2015, under review.

DS 11.4 Mon 15:45 H38

Substrate-dependent electronic structure and film formation of MAPbI3 perovskites — •Selina Olthof and Klaus Meerholz — University of Cologne, Institute for Physical Chemistry, Luxemburger Straße 116, 50939 Köln, Germany

Hybrid organic / inorganic perovskite materials have attracted significant attention in the past years. However, little is known so far about the electronic structure and, more importantly, the energetic alignment at interfaces. Here, we present the investigation of the interface formation between the perovskite MAPbI3 and various substrate materials. The perovskite films are incrementally evaporated in situ while the electronic structure is evaluated using photoelectron spectroscopy (PES). The results show a deviation from the commonly assumed flat band condition, and that dipole formation and band bending dominate the interfaces. More importantly, we find a deviation from the expected perovskite stoichiometry at the interface due to a wide variety of chemical interaction taking place, which are highly dependent on the nature of the substrate material. On metal oxides the perovskite film formation is hindered and it takes up to 30 nm for the density of states of perovskite to emerge in the PES measurements. Therefore, the nature of the substrate not only changes the energetic alignment of the perovskite, but can hinder film formation and introduce gap states as well.

DS 11.5 Mon 16:00 H38

In-Situ Investigation of Optoelectronic Properties during One-Step Synthesis of $\mathbf{MAPbI_{3-x}Cl_x}$ Perovskite — •Klara Suchan, Justus Just, Martin Kärgell, Dan R. Wargulski, Pascal Becker, and Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Organometal halide perovskites have emerged as promising absorber materials for solid state solar cells since 2012. With the fast improvement in power conversion efficiency to over 20 %, perovskites have high prospects for low-cost, high efficiency solar cell production. $CH_3NH_3PbI_{3-x}Cl_x$ layers are prepared by a one-step solution based process using $PbCl_2$ and MAI precursors dissolved in DMF. Since solution based processes do not need cost intensive vacuum technology and no high-temperature annealing steps, they yield high potential for industrial implementation. However, little is known about the exact mechanisms during synthesis, leading to poor reproducibility. Employing in-situ photoluminescence and reflection imaging as well as spectroscopy we monitor the growth process. The evolution of optoelectronic properties for various temperature profiles and annealing durations is analysed. Additional X-ray diffraction measurements during various stages of the process are used to evaluate structural changes occurring during film formation.

DS 11.6 Mon 16:15 H38

Reversible Laser induced Amplified Spontaneous Emission from Coexisting Tetragonal and Orthorhombic Phases in Hybrid Lead Halide Perovskites — •Fabian Panzer[1,2,3], Sebastian Baderschneider[2,4], Tanaji Gujar[5], Thomas Unger[1,2], Heinz Bässler[2], Ralf Moos[3], Mukundan Thelakkat[5], Richard Hildner[2,4], and Anna Köhler[1,2] — [1]Experimental Physics II — [2]Bayreuth Institute of Macromolecular Research (BIMF) — [3]Department of Functional Materials — [4]Experimental Physics IV — [5]Applied Functional Polymers, Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany

Organic-inorganic mixed halide perovskites received enormous attention over the last few years due to their outstanding performances when used as absorber material in solar cells or in light emitting devices, while offering the possibility for low cost production, e.g. by solution-processing. Furthermore it is known that most halide perovskite materials can exist in different crystal structures, depending on environmental conditions such as temperature. Here we show that a coexistence of tetragonal and orthorhombic phases within the same crystalline grain can be optically induced into the halide perovskite $\mathrm{CH_3NH_3PbI_3}$ at low temperatures, leading to amplified spontaneous emission simultaneously at two distinct wavelengths. The emission feature associated with the tetragonal phase can be reproducibly written, read-out, and erased at 5 K by choosing appropriate laser fluences or raising the temperature. Finally we show to which extend our findings can be exploited for use as an all optical data storage device.

15 min. break

DS 11.7 Mon 16:45 H38

Iodine Migration and its Effect on Hysteresis in Perovskite Solar Cells — Cheng Li[1], Steffen Tscheuscher[2], Fabian Paulus[3], Paul Hopkinson[3], Johannes Kiessling[1], Anna Köhler[2], Yana Vaynzof[3], and •Sven Hüttner[1] — [1]Organic and Hybrid Electronics, Makromol. Chemie I, Universität Bayreuth — [2]Experimentalphysik II, Universität Bayreuth — [3]Centre for Advanced Materials, Universität Heidelberg

Solution-processed organic-inorganic hybrid perovskite solar cells (e.g. $\mathrm{CH_3NH_3PbI_3}-x\mathrm{Cl}_x$) currently exhibit promising performances. However, the origin of the observed hysteresis in the current-voltage (J-V) curves, i.e. the sweeping-history-dependent electrical current, is still not sufficiently understood. To investigate its origin we employ electroabsorption (EA) spectroscopy to explore the built-in potential in working photovoltaic devices. Furthermore, we study the temperature dependent dynamic processes in perovskite solar cells by characterizing their current-voltage behavior at different temperatures. The electrical current relaxation process during temperature dependent J-V measurements provides the evidence of the migration of ions. In order to investigate the nature of these ions, we further present X-ray photoemission spectroscopy (XPS) experiments which shows the elemental redistribution after applying an electrical bias. The results give a concise picture that mainly iodide ions can be driven by an external electrical field and then accumulate at the respective perovskite/electrode interfaces. The migration and accumulation of iodide ions create a modulation of the respective interfacial barriers which is the origin of the hysteresis.

DS 11.8 Mon 17:00 H38

The Importance of Hydrogen Defect Migration in Organic-Inorganic Perovskites — •David A. Egger[1], Leeor Kronik[1], and Andrew M. Rappe[2] — [1]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel — [2]The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323, USA

Solar cells based on organic-inorganic perovskites have been proven to be remarkably efficient in recent years. However, they exhibit hysteresis in the current-voltage curves, and their stability properties, especially in the presence of water, are problematic. Both issues are possibly related to ionic diffusion phenomena occurring in the hybrid perovskite material. Using first-principles calculations based on density functional theory, we study the properties of an important defect in hybrid perovskites - interstitial hydrogen.[1] We show that differently charged defects occupy different sites in the hybrid perovskite crystal, which allows for an ionization-enhanced defect migration following the Bourgoin-Corbett mechanism. Our analysis further highlights the structural flexibility of organic-inorganic perovskites, where successive displacements of iodide combined with hydrogen bonding enables proton diffusion with low migration barriers. These findings indicate that hydrogen species can be highly mobile in hybrid perovskite solar cells and thus relevant for their performance.
[1] Angew. Chem. Int. Ed. 54, 12437 (2015)

DS 11.9 Mon 17:15 H38

Humidity-induced hydration of methylammonium lead iodide perovskite: Understanding and prevention — •Yinghong Hu[1], Pablo Docampo[1], Aurélien Leguy[2], and Piers Barnes[2] — [1]Department of Chemistry, Ludwig-Maximilians-Universität, 81377 München, Germany — [2]Physics Department, Imperial College, London, SW7 2AZ, United Kingdom

The long-term stability of hybrid metal halide perovskite solar cells is of paramount importance for the future of this emerging technology. In particular, solar cells composed of methylammonium lead iodide (MAPI) are notorious for their sensitivity to moisture. Here, we elucidate the humidity-induced degradation mechanisms occurring within the perovskite material and report on the development of a novel interlayer which improves the moisture stability of perovskite solar cells. Our results show that MAPI undergoes a stepwise transformation into two species of hydrated MAPI crystal phases upon exposure to moist air at room temperature. However, we show that this hydration process can be reversed when the material is subsequently dried in nitrogen. In contrast to water vapor, the presence of liquid water directly leads to the irreversible decomposition of MAPI to form lead iodide. Our developed functional moisture barrier significantly enhances the stability of the perovskite solar cells towards cycles of hydration and dehydration. We believe that our results open new possibilities for the design of moisture resistant, highly efficient perovskite solar cells.

DS 12: Postersession DS

Presenters are kindly requested to be near their poster for at least one hour during poster session or leave a note about their availability for discussions.

Time: Monday 17:00–19:00 Location: Poster A

DS 12.1 Mon 17:00 Poster A

Ultrathin multilayers grown by pulsed laser deposition — •Bea Jaquet, Christian Eberl, Florian Döring, and Hans-Ulrich Krebs — Institute for Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The physical properties of multilayers with layer periods in the nanometer range (way below 5 nm) crucially depend on the chosen material combination, their crystalline or amorphous state, heat of mixing of the chosen system, and amount of intermixing. For this, ultrathin multilayers consisting of different materials (metals, oxids, semiconductors) are grown by pulsed laser deposition (PLD) with layer periods of high quality. The structure, microstructure and interface roughness of the different multilayers were characterized by x-ray reflectivity (XRR), x-ray diffraction (XRD) and (high resolution) transmission electron microscopy (TEM). In this contribution we discuss the properties of the multilayers with respect to the used material combinations.

DS 12.2 Mon 17:00 Poster A

Long term XPS analysis of Fe/GaAs(001) — •Karim Shamout[1,2], Dominique Krull[1,2], Philipp Espeter[1,2], Christoph Keutner[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]TU Dortmund, Dortmund, Deutschland — [2]DELTA, Dortmund, Deutschland

The III-V compound semiconductor gallium arsenide is an applicable substrate for spintronic multi-layer systems due to its electronic und magnetic properties. The structure of the 3-layers the system MgO/Fe/GaAs(100) has already been discussed in detail and it has been shown that the Ga-rich surface reconstruction of GaAs(4x2) can be investigated beneath the MgO and Fe layer by x-ray photoelectron diffraction (XPD) [1]. Since these XPD measurements last several hours and iron is highly reactive even at pressures $p < 2\cdot10^{-10}$ mbar this study focuses on the long term oxidation of an Fe-film prepared on GaAs(001). Within this work, we demonstrate that XPD measurements of samples with terminating FE layers at the surface must be carried out as quickly as possible in order to avoid oxidation levels.

[1] D. Handschak, T. Lühr, F. Schönbohm, S. Döring, C. Keutner, U. Berges and C. Westphal. Phys. Rev. B, 88:045313, 2013

DS 12.3 Mon 17:00 Poster A

Bi atoms mobility-driven self-organized circular domains at the Bi/InAs(111) interface — •Maria Christine Richter[1,2], Abdoul Gafoor[1], Laurent Nicolaï[1,2,3], Jan Minar[3,4], Jürgen Braun[3], Hubert Ebert[3], Uros Djukic[1], Olivier Heckmann[1,2], Jean-Michel Mariot[5], Nick Barett[2], Vitaly Feyer[6,7], Claus M Schneider[6], and Karol Hricovini[1,2] — [1]LPMS, Université de Cergy-Pontoise, Cergy-Pontoise, France — [2]DSM/IRAMIS/SPEC, CEA Saclay, Gif-sur-Yvette, France — [3]LMU Munich, Munich, Germany — [4]University of West Bohemia, Czech Republic — [5]LCP-MR, Université P et M Curie, Paris, France — [6]Peter Grünberg Institute (PGI-6), JARA-FIT, Research Center Jülich, Jülich, Germany — [7]NanoESCA beamline, Sincrotrone Trieste, Area Science Park, Basovizza, Italy

30 ML Thick Bi film deposition on the InAs(111)-A side and subsequent annealing at 600 K leads to self-organized circular structures with the diameter of several μm. Spatial analysis by PEEM of Bi 5d, In 4d and As 3d core-level photoemission spectra shows that the circular patterns are composed of the unaltered InAs substrate coverd by a thin Bi layer. The spots in the middle of the circles are Bi cristallites and the region in between them are In-poor and As-rich ternary compounds. From the k-resolved PEEM spectra along the Γ-M line we estimate that the medium thickness of the Bi-layer is approximately one monolayer. The InAs(111)-B side shows no particular morphology but stronger chemical shifts of the core-level spectra evidencing Bi-As bonds.

DS 12.4 Mon 17:00 Poster A

Texture Optimization of the Binary Compound Sb_2Te_3 by Using UHV DC Magnetron Sputter Deposition — •Artur Romanov, Carolin C. Jacobi, Matthias M. Dück, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Aachen, Germany

The binary compound Sb_2Te_3 exhibits extraordinary thermoelectric properties. These are desirable for a range of industrial applications, e.g. for solid state refrigerators. Additional to its applicability, Sb_2Te_3 is of high fundamental scientific interest since it was identified as a topological insulator (TI). In order to develop the surface states, that enable the topological properties, a high texture quality of the deposited thin film is needed. Highly textured films are usually produced with elaborate methods like Molecular Beam Epitaxy (MBE). However, recently textured films were successfully produced using the sputter deposition method. In contrast to MBE, sputter deposition offers benefits for industrial applications like convenient scalability and high deposition rates. The choice of process parameters was found to influence the quality of the deposited thin film heavily. Accompanied by the growth type, changes can occur in texture and electrical properties. The limit of texture optimization is not yet achieved and requires further investigation. Goal of this project is to establish an efficient and fast method to produce Sb_2Te_3 in a texture similar to MBE. The film's texture is determined by x-ray diffraction (XRD), in particular employing measurements of Rocking Curves and measurements using Bragg-Brentano geometry.

DS 12.5 Mon 17:00 Poster A

RBS-Investigations of Mo-doped $BiVO_4$ thin films deposited by reactive magnetron sputtering — •Marie Mende[1], Emanuel Schmidt[1], Fuxian Wang[2], Klaus Ellmer[2], and Elke Wendler[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 3, 07743 Jena, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Bismuth vanadate ($BiVO_4$) has recently emerged as a promising material for the use as photoanode in solar water splitting applications. However, the performance of $BiVO_4$ as photoanode material is strongly limited by its intrinsically slow electron and hole transport.

In order to overcome these limitations, novel doping strategies have been developed. To benefit from these modification and fabrication methods an extensive control of the composition and the dopant concentration must be guaranteed.

In this work we investigate molybdenum doped thin film samples of $BiVO_4$ deposited on glassy carbon or (100) yttria-stabilized zirconia (YSZ) substrates with different dopant contents by reactive magnetron sputtering from a Bi and a V target. Rutherford-Backscattering-Spectroscopy (RBS) is used to determine the structure (epitaxial growth) and composition of these layers for assisting further investigations regarding the dependence of photocatalytic activity on the material composition and doping.

DS 12.6 Mon 17:00 Poster A

Twins and Strain in magnetron sputtered epitaxial perovskite oxide films — •Immo Bahns, Patrick Thiessen, Jörg Hoffmann, and Christian Jooss — Uni Göttingen

Because of the large acoustic mismatch multilayers composed of the perovskites SrTiO3 (STO) and Pr0.65Ca0.35MnO3 (PCMO) are interesting model systems for phonon blocking structures. However, the thermal conductivity is significantly affected by strain effects due to the lattice mismatch and preparation-caused defects. In addition, PCMO films are commonly highly twined because of the cubic-to-orthorhombic phase transition. In this contribution we investigate the homoepitaxial growth of STO films on (100) STO substrates and the heteroepitaxial growth of PCMO on STO. The about 200 nm thick films were prepared by magnetron-sputtering of the oxide targets in an argon/oxygen gas mixture. The deposition temperatures were varied between 600 and 800 °C. Phase formation, lattice constants and therefore the strain state are deduced from X-ray inspections. Since PCMO belongs to the class of manganites with a pronounced Colossal Magneto-Resistance effect (CMR) and the CMR is very sensitive with respect to point-like disorder, magnet field dependent resistivity measurements were performed. We also discuss the influence of the deposition parameters on the formation of the 6 twin domains.

DS 12.7 Mon 17:00 Poster A

evaluation of structure and mechanical properties of Ni-rich/ Ti-rich NiTi thin film — •Maryam Mohri[1,2], Mahmoud Nili-ahmadabadi[2], Julia Ivanisenko[1], and Horst Hahn[1] — [1]Karlsruhe Institute of Technology, Institute of Nanotechnology, 76021 Karlsruhe, GermanyKarlsruhe Institute of Technology, Institute of Nanotechnology, Karlsruhe, Germany — [2]School of Metallurgy and Materials Engineering, College of Engineering, University of Tehran, Tehran, Iran.

NiTi alloys have received more attraction for a wide range of smart designs and innovative applications due to shape memory effect and pseudo elasticity. In this paper, the gradient structure and mechanical properties of a martensitic/austenitic (Ni49Ti/Ni51Ti (at.%)) bi-layered thin film with 1000nm thickness deposited using DC magnetron sputtering on Si substrate and subsequent annealing were studied. The structure, transformation temperatures and mechanical properties of the bi-layer were analyzed using grazing incidence X-ray diffraction (GIXRD), scanning transmission electron microscopy, differential scanning calorimetry (DSC) and nanoindentation. The X-ray diffraction results indicated that the bi-layer was composed of austenitic and martensitic layers. The bi-layered thin film exhibited a combined pseudo elastic behavior and shape memory effect specific to the austenitic and martensitic thin films, respectively. The combination of pseudo elastic effect with shape memory leads to a two-way shape memory effect with a reduced hysteresis in the bi-layers.

DS 12.8 Mon 17:00 Poster A

Control of octahedral rotations in LaNiO3/LaGaO3 superlattices via octahedral connectivity at heterointerfaces — •Haoyuan Qi[1], Michael Kinjanjui[1], Xiaodan Chen[1], Johannes Biskupek[1], Dorin Geiger[1], Eva Benckiser[2], Hanns-Ulrich Habermeier[2], Bernhard Keimer[2], and Ute Kaiser[1] — [1]University of Ulm, Central Facility of Electron Microscopy, Electron Microscopy Group of Materials Science, Albert Einstein Allee 11, D-89081 Ulm, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

For ABO3 perovskites, octahedral rotations and distortions couple strongly to the functional properties. However, precise control of the octahedral rotations in ABO3 heterostructures remains challenging. By using aberration-corrected HRTEM, we investigated the local octahedral rotations in [(4 unit cell (u.c.)//4 u.c.)*8] and [(1 u.c.// 4 u.c.)*13] LaNiO3/LaGaO3 superlattices grown on tensile-strain inducing (001) SrTiO3 substrates. For the [(4 u.c.// 4 u.c.)*8] LaNiO3/LaGaO3 superlattice, the NiO6 octahedral rotations were found to be relaxed to bulk value near the surface of the superlattice indicating that epitaxial strain alone is not enough to stabilize certain octahedral rotational magnitudes throughout the entire superlattice. For the [(1 u.c.// 4 u.c.) *13] LaNiO3/LaGaO3 superlattice, the NiO6 octahedral rotations have the same magnitudes as the neighboring GaO6 octahedra due to interfacial octahedral connectivity. Our study has demonstrated that octahedral rotations in ABO3 heterostructures can be precisely controlled via octahedral connectivity at heterointerfaces.

DS 12.9 Mon 17:00 Poster A

Ultrafast structural deformation studied by time-resolved x-ray diffraction — •Mathias Sander[1], Azize Koc[2], Christelle Kwamen[2], Matthias Reinhardt[2], Wolfram Leitenberger[1], Peter Gaal[2,3], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24/25 14476 Potsdam — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Wilhelm-Conrad-Röntgen Campus, Bessy II, Albert-Einstein-Str. 15, 12489 Berlin — [3]Institute for Nanostructure and Solid State Physics, University of Hamburg, Jungiusstr. 11c/352, 20335 Hamburg

We investigate the ultrafast dynamics of coherent acoustic phonons in a photo-excited thin film. The excitation of the sample with an ultrashort laser pulse triggers coherent expansion and compression waves within the thin layer, which modulate the diffraction efficiency of an x-ray probe pulse on the picosecond timescale. A novel sample structure extinguishes the diffraction background from the laser deposited heat which is essential for repetition rates of 200kHz. The structure can be employed as ultrafast switchable mirror to shorten bursts of hard x-rays emitted from synchrotron storage rings. In addition, we study the in-plane sample dynamics by intersecting two optical pump pulses at the sample surface. The generated transient grating is characterized by x-ray reflection under grazing incidence and by reciprocal space mapping. The diffraction efficiency of the thermal grating can be tuned by the incoming laser fluence.

DS 12.10 Mon 17:00 Poster A

A critical look at the resolution function of a TOF neutron reflectometer and why we should care when we do GISANS experiments — •Jean-François Moulin and Sebastian Busch — German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH, Lichtenbergstr. 1, 85747 Garching bei München, Germany

Grazing incidence small angle neutron scattering (GISANS) is increasingly used to characterize the structure of thin films. This method makes it possible to detect lateral correlations over a broad range of length scales (from nm to μm). Because the probing wave is evanescent one can tune the depth from which the scattering originates. This makes it in theory possible to perform structural depth profiling, but unfortunately the penetration depth is a very steep function of the wavelength (or incident angle) which means that high resolution measurements are needed or at the very least that a good knowledge of the resolution function is fundamental. We will show a detailed analysis of the resolution function of a time-of-flight neutron reflectometer and illustrate how the data binning scheme as well as the primary wavelength spectrum shape can affect the accuracy of penetration depth measurements. The influence of these resolution effects in the case of conventional reflectivity measurements will also be discussed.

DS 12.11 Mon 17:00 Poster A

Towards Imaging of Defects in Diamond by High-Resolution TEM — •Robert Leiter[1], Haoyuan Qi[1], Johannes Biskupek[1], Boris Naydenov[2], Fedor Jelezko[2], and Ute Kaiser[1] — [1]Electron Microscopy Group of Materials Science, University of Ulm, Albert-Einstein Allee 11, 89081 Ulm, Germany — [2]Institute for Quantum Optics, University of Ulm, Albert-Einstein Allee 11, 89081 Ulm, Germany

Nitrogen-vacancy (NV), Silicon-vacancy (SiV) and other colour centres in diamond have been of rising interest in recent years due to their potential applications, such as quantum information processing[1] and fluorescent labelling in biology. For biological applications, NV and SiV centres can be created in nanodiamonds with sizes down to less than 10 nm[2,3]. Although structural characterisation of NV-centres has been done by optical and magnetic resonance methods, structure of other colour centres often remain uncovered. By using aberration-corrected high-resolution transmission electron microscopy (HRTEM), atomic resolution can be achieved. However, the imaging conditions necessary to directly image the structure of an SiV, GeV and other new centres remain unclear. Here we explore the imaging conditions that are suitable for this problem by means of image simulations and subsequent testing using an FEI TITAN image-side aberration corrected TEM operated at 80 kV and 300 kV.

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[2] J. Tisler et al., ACS Nano 3, 1959-1965 (2009)

[3] I. Vlasov et al., Nature Nanotechnology 9, 54-58 (2014)

DS 12.12 Mon 17:00 Poster A

Kavitationserosion als Haftungstest für chromdotierte Aluminiumoxidschichten auf unterschiedlichen Substraten — •Ingo Erdmann[1], Friederike Deuerler[1], Ali Haligür[2] und Volker Buck[2] — [1]Fakultät 7, Fachgebiet Werkstofftechnik, Bergische Universität Wuppertal — [2]Falkultät für Physik, AG Dünnschichttechnologie, Universität Duisburg-Essen

Die Signalintensität thermographischer Phosphore ist proportional zu ihrem Volumen und hängt damit bei dünnen Schichten von der Schichtdicke ab. Da die mechanischen Spannungen in einer dünnen Schicht in der Regel proportional zur Schichtdicke ansteigen, führt dieser Effekt oft zu einem Abplatzen der Schicht, wenn eine spezifische Dicke erreicht wird, wodurch die maximal erreichbare Schichtdicke begrenzt wird. Die untersuchten chromdotierten Aluminiumoxidschichten wurden in einem plasmaunterstützten CVD-Prozess mit unterschiedlichen Beschichtungszeiten (d.h. unterschiedlichen Schichtdicken) auf Silizium- und Edelstahlsubstraten abgeschieden. Es zeigte sich, dass bis zu Dicken von etwa 20 Mikrometern (wo ausreichende Intensität der Phosphoreszenz gegeben ist) kein Abplatzen der Schichten beobachtet werden konnte. Die Schichten wurden anschließend einer Kavitationserosion gemäß ASTM G32-98 ausgesetzt und der Grad des Schichtversagens nach unterschiedlichen Kavitationszeiten optisch erfasst und quantifiziert, woraus sich die jeweilige Kavitationsrate ergab. Hierbei zeigte sich eine deutlich geringere Kavitationsrate der Schichten auf den Siliziumsubstraten im Vergleich zu den verwendeten Edelstahlsubstraten, was einer signifikant höheren Schichthaftung auf Silizium entspricht.

DS 12.13 Mon 17:00 Poster A

Drastic deviations from stoichiometry transfer during pulsed laser deposition — •Christina Klamt, Arne Dittrich, Christian Eberl, Susanne Schlenkrich, Felix Schlenkrich, Florian Döring, and Hans-Ulrich Krebs — Institute for Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In common, one of the most characteristic properties of pulsed laser deposition (PLD) is the stoichiometry transfer between target and substrate, which has been used heavily for many complex systems. In this contribution we show that it is yet possible to obtain drastic deviations from stoichiometry transfer in a binary system by just varying the fluence during laser deposition. In the W-Cu system, the W-concentration of films grown from either a W60Cu40 or a W80Cu20 target (wt. %) can indeed continuously be changed over an unprecedented large range of 0 to 75 wt. % W. Close to the deposition threshold, pure Cu-films are formed due to the much higher vapor pressure of Cu. At higher laser fluences, more and more W-rich W-Cu alloy samples are obtained, since ion implantation and intermixing processes occur. These alloys can reach W-contents even higher than that of the target because of enhanced resputtering and reflection of the lighter Cu atoms at the film surface. Stoichiometric films are only obtained at laser fluences around $3\,J/cm^2$, when the strong Cu evaporation from the target and reflection and resputtering effects of Cu at the film surface are in balance.

DS 12.14 Mon 17:00 Poster A

Phonon, structural and magnetic properties of ordered double perovskite $\mathbf{A_2BMnO_6}$ (A = La, Pr, Nd, Sm, Gd, Y, B = Co, Ni) thin films — •Christoph Meyer, Bernd Damaschke, Konrad Samwer, and Vasily Moshnyaga — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

B-site ordered double perovskites A_2BMnO_6 (A =rare earth; B = Co, Ni) with monoclinic $P12_1/n1$ structure are promising materials for spintronic applications due to ferromagnetic ordering, magnetodielectric coupling and multiferroic behavior. To study the influence of A- and B-site cations, we grew series of A_2BMnO_6 (A=La, Pr, Nd, Sm, Gd, Y; B=Co, Ni) thin films on $SrTiO_3$(111), $SrTiO_3$(100) and MgO (100) substrates by metalorganic aerosol deposition. The films were analyzed by X-ray diffraction (XRD), magnetization measurements (SQUID) and far-field Raman and tip-enhanced Raman spectroscopy (TERS). All films are epitaxially and obey monoclinic $P12_1/n1$ structure with superlattice reflections in the cubic [111] direction due to high degree of B-site ordering. Ferromagnetic ordering with high T_C and a strong A_g symmetry mode of B/MnO_6 octahedral stretching at $\sim 630 - 670$ cm^{-1} in the TERS and far-field Raman spectra were detected. Enhanced T_C and A_g mode frequency values for A_2NiMnO_6 compared to A_2CoMnO_6 and a systematic reduction of T_C and the stretching mode frequency by decreasing the A-site cation size were observed. Financial support by the DFG via project SFB 1073/B04 is gratefully acknowledged.

DS 12.15 Mon 17:00 Poster A

Raman spectroscopy of crystal field excitations and vibration modes in $\mathbf{CePt_5}$ surface layers — •Benedikt Halbig[1], Utz Bass[1], Martin Zinner[2], Kai Fauth[2], and Jean Geurts[1] — [1]Universität Würzburg, Exp. Physik III, Würzburg, Germany — [2]Universität Würzburg, Exp. Physik II, Würzburg, Germany

The rare-earth compound $CePt_5$ is highly relevant for heavy-fermion quasiparticles and Kondo physics. The Ce 4f electron energy levels are split by the crystal field of their neighbor atoms by about 20 meV. We report on the detection of this splitting by Raman spectroscopy from electron crystal field excitations (CFE) in $CePt_5$ surface layers with thicknesses between 2 and 16 unit cells, grown in UHV by annealing-induced alloying on Pt(111) substrates. For reference, $LaPt_5$ layers were employed, i.e. without 4f electrons. The crystal lattice consists of alternating $CePt_2$- ($LaPt_2$-) and Pt-kagome layers, whereas the surface is a hexagonal Pt layer. Depending on the $CePt_5$ layer thickness, up to three peaks in the $in-situ$ UHV Raman spectra at T≈20K are identified as CFE of the 4f electron because of their absence for the $LaPt_5$ reference samples. Their energies are 17meV, 23meV and 25meV. From their individual thickness-dependent intensity behavior, we assign them to CFE transitions at the Pt(111)-$CePt_5$ interfaces, in the $CePt_5$ layer, and at the $CePt_5$-Pt surface layer, respectively. Besides, we observe three additional Raman peaks: one is assigned to the E_{2g} vibration mode of the $CePt_5$ lattice, the other two to the near-surface part of the $CePt_5$ layer, whose symmetry is reduced by shifted Pt layers. Equivalent vibration peaks occur for the $LaPt_5$ reference.

DS 12.16 Mon 17:00 Poster A

Evaluation of graphite defects by microscopic ellipsometry — •Shun Okano[1], Jana Kalbacova[1], Constance Schmidt[1], Christoph Günther[1], Raul D. Rodriguez[1], Elias Garratt[2], Babak Nikoobakht[2], Ovidiu D. Gordan[1], Angela Hight Walker[3], and Dietrich R. T. Zahn[1] — [1]Technische Universität Chemnitz Semiconductor Physics, Chemnitz, 09126 — [2]Materials Measurement Science Division, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA — [3]Semiconductor and Dimensional Metrology Division, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

Carbon materials, for instance graphite, graphene, or CNTs, are interesting for many modern applications. Therefore it is important to investigate defects in these materials. Since defects have a great effect on the properties of the material, like the refractive index, we focused on the investigation of defects by microscopic ellipsometry and compare the results with those from micro-Raman spectroscopy which is an established method for the characterization of defects. Defects on highly ordered pyrolytic graphite were produced by a focused Ga^+ ion beam with ion fluence ranging from $3{\cdot}10^{10}$ to 10^{15} ions/cm^2 in areas of 5×5 μm^2. The sample was investigated using an ellipsometry mapping, with an Accurion Nanofilm EP4 setup. With this we can visualize the defects the Ψ and Δ maps and determine the changes of refractive index and optical constants.

DS 12.17 Mon 17:00 Poster A

Raman spectroscopic investigations of Sr_2IrO_4 epitaxial thin films — •Cameliu Himcinschi[1], Chengliang Lu[2], Jens Kortus[1], and Marin Alexe[3] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — [3]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

5d material systems, as Sr_2IrO_4 oxides, have interesting properties due to the strong spin-orbit coupling. Epitaxial Sr_2IrO_4 thin films were grown on $SrTiO_3$, $DyScO_3$ and $LaAlO_3$ substrates by pulsed laser deposition. The films were investigated using temperature dependent Raman spectroscopy. The larger compressive strain of the film deposited on $LaAlO_3$ induced a blue shift of the Sr_2IrO_4 Raman active modes. On the other hand, by using different excitation wavelengths the conditions for resonant Raman effect in Sr_2IrO_4 material have been probed.

DS 12.18 Mon 17:00 Poster A

Influence of Graphene on Charge Transfer between CoPc and Metals: The Role of Graphene-Substrate Coupling — Johannes Uihlein[1], Małgorzata Polek[1], Mathias Glaser[1], Hilmar Adler[1], David Balle[1], Ruslan Ovsyannikov[2], •Milutin Ivanovic Ivanovic[1], Alexei B. Preobrajenski[3], Alexander V. Generalov[3], Thomas Chassé[1], and Heiko Peisert[1] — [1]University of Tübingen, Institute of Physical and Theoretical Chemistry, 72076 Tübingen, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany — [3]Lund University, MAX-Laboratory, 22100 Lund, Sweden

The electronic structure of cobalt phthalocyanine (CoPc) on Pt(111), graphene/Pt(111) and Au-intercalated graphene/Ni(111) is investigated by photoemission and X-ray absorption spectroscopy. For CoPc on metal substrates, significant changes of the shape of the spectra indicate a charge transfer from the substrate to the Co ion of CoPc. The disturbance of the graphene electronic structure by interaction with underlying substrate accompanied by a doping of graphene has been found to affect electronic properties of adsorbed CoPc considerably.

DS 12.19 Mon 17:00 Poster A

Controlling the energetics at the interface of p-doped low band gap polymer — •Milutin Ivanović, Heiko Peisert, and Thomas Chassé — University of Tübingen, Institute of Physical and Theoretical Chemistry, 72076 Tübingen, Germany

Polymer/fullerene based organic photovoltaic cells (OPVCs) have been extensively investigated as a promising technology for the rising energy demand, in particular due to their low cost production potential. One approach to achieve more efficient OPVCs is the molecular p-doping of the polymer in thin films affecting the energy level alignment between the donor and both the acceptor and the electrode.1, 2 We studied interfaces with substrates and the fullerene C60, of thin films of prototype low bandgap polymer PCPDTBT, doctor blade casted on substrates with wide span of work functions. We employ X-ray and Ultraviolet photoelectron spectroscopy to investigate interface properties of the pure and F4TCNQ doped polymer. It is found that p-doping can be useful tool for tuning/controling energetics at both polymer interfaces.

References: 1.*Bao, Q. et al. Advanced Materials Interfaces 2015, 2, n/a-n/a. 2.*Yu, S. et al. Applied Physics Letters 2015, 106, 203301.

DS 12.20 Mon 17:00 Poster A

3D conformal deposition of ceramic layers on complex metallic tools and injection molds via chemical vapor deposition — •Tatiana Fedosenko-Becker[1], Friederike Deuerler[1], Gregor Fornalczyk[2], and Frank Mumme[2] — [1]University of Wuppertal, School of Mechanical Engineering and Safety Engineering, Material Technology, Wuppertal, Germany — [2]Gemeinnuetzige KIMW Forschungs-GmbH, Luedenscheid, Germany

Chemical vapor deposition (CVD) is a well-known process to produce high quality thin coatings, such as films with specific properties to protect metallic tools and injection molds from wear, corrosion, and others. However, it can be difficult to obtain a high-performance coating on complicated three-dimensional surfaces of some tools. It needs understanding of the formation of solid material from a gaseous phase, containing complex molecules of volatile matter; research of metalorganic precursors, which decompose at low temperatures (500 °C) and allow the deposition of conformal layers into narrow cracks and holes; and the detailed research of the 3D substrate materials to clarify the influence of the steel alloy on the adhesion of the layers.

The aim of this study is the deposition of CVD layers for three-dimensional zirconia coatings on metallic tools and injection molds. At the present stage of the research the way of deposition and characterization of the coatings on 3D surfaces is developed, the experimental parameters for successful deposition of zirconia layers are found and physical and geometrical properties of the substrate materials are investigated.

DS 12.21 Mon 17:00 Poster A

Scribing of CIGS thin film solar cells with 1550 nm nanosecond laser radiation — •Martin Ehrhardt, Klaus Zimmer, Pierre Lorenz, and Lukas Bayer — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany

Microstructuring of thin functional films without affecting the functionality is a great challenging for laser-assisted methods. The laser pattering experiments of copper indium gallium selenide (CIGS) solar cells with a 1.55 μm laser source with a pulse length of 6 ns is present. It will be shown that two different material removal processes were found in dependence on the specific laser parameter used. For high laser repetition rate a material ablation starting from the front side of the samples was observe. By using a low laser repetition rate the laser pulse penetrate the CIGS material and were absorbed in the interface between the CIGS and the Mo causing a delamination lift-off process of the CIGS from the Mo back contact. The morphology and size of the resultant pattern were studied by scanning electron microscopy (SEM). The composition of the sample material after the laser treatment was analyzed by energy dispersive X-ray spectroscopy (EDX) and micro Raman spectroscopy. Furthermore, the different removal processes was simulated using finite element method (FEM) where the laser-solid interaction was approximately described by a heat equation.

DS 12.22 Mon 17:00 Poster A

Magnetoresistance of devices directly written using a focused ion beam — •Vico Liersch[1], Tobias Warnatz[1], Sebastian Wintz[1,2], Gregor Hlawacek[1], Steffen Cornelius[1], Kay Potzger[1], Jürgen Lindner[1], Jürgen Fassbender[1,3], Artur Erbe[1], and Rantej Bali[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Deutschland — [2]Paul-Scherrer Institut, Villigen, Schweiz — [3]Technische Universität Dresden, Deutschland

Magnetoresistance (MR) effects are widely studied in multilayered structures, where the current flows perpendicular to the substrate plane. These devices involve complex lithography steps for achieving the required layered structure and electrical contacting. Here we present a different approach, where the magnetic layers are directly embedded onto a current carrying wire template via lateral focused ion beam writing. It is known that ferromagnetism in an ordered (paramagnetic) Fe60Al40 alloy can be induced by ion beam irradiation [1]. We use this phase transition to create a pattern with alternating ferromagnetic and paramagnetic regions [2]. Due to shape anisotropy it is possible to obtain stable states where the neighboring ferromagnetic regions are of either parallel or antiparallel alignment respectively. Respective resistance of parallel or antiparallel alignment states under the influence of a swept magnetic field was observed. First MR measurements of such patterned structures at low temperatures will be shown. [1] J. Fassbender, et al. Physical Review B 77 (2008). [2] R. Bali, et al. Nano letters 14.2 (2014).

DS 12.23 Mon 17:00 Poster A

Magnetoresistance of devices directly written using a focused ion beam — •Vico Liersch[1,2], Tobias Warnatz[1], Sebastian Wintz[1,3], Gregor Hlawacek[1], Steffen Cornelius[1], Kay Potzger[1], Artur Erbe[1], Jürgen Lindner[1], Jürgen Fassbender[1,4], Wieland Zahn[2], and Rantej Bali[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Deutschland — [2]Westsächsische Hochschule Zwickau, Deutschland — [3]Paul-Scherrer Institut, Villigen, Schweiz — [4]Technische Universität Dresden, Deutschland

Magnetoresistance (MR) effects are widely studied in multilayered structures, where the current flows perpendicular to the substrate plane. These devices involve complex lithography steps for achieving the required layered structure and electrical contacting. Here we present a different approach, where the magnetic layers are directly embedded into a current carrying planar wire via a focused ion beam. Ferromagnetism in an ordered (initially paramagnetic) $Fe_{60}Al_{40}$ alloy can be induced by ion beam irradiation [1]. We deployed a ~ 2 nm diameter beam of Ne^+ at 20 - 30 keV to induce a pattern with alternating ferromagnetic and paramagnetic stripes in a 40 nm thick $Fe_{60}Al_{40}$ wire [2]. The stripe geometry consisted of two different alternating stripe widths separated by a narrow paramagnetic spacer, and showed a two stepped reversal curve due to parallel and antiparallel magnetization configurations. MR measurements of such patterned structures, with different stripe geometries will be shown. [1] J. Fassbender, et al. Physical Review B 77 (2008). [2] R. Bali, et al. Nano letters 14.2 (2014).

DS 12.24 Mon 17:00 Poster A

Photo-induced dynamics in combined magnonic and phononic multilayer systems — •Markus Müller[1], Dennis Meyer[1], Henning Ulrichs[1], Maria Mansurova[1,3], Florian Döring[2], Jakob Walowski[3], and Markus Münzenberg[3] — [1]I. Physikalisches Institut Georg-August Universität, Göttingen, Germany — [2]Institut für Materialphysik Georg-August Universität, Göttingen, Germany — [3]Physikalisches Institut Ernst Moritz Arndt Universität, Greifswald, Germany

We present investigation of elastic dynamics in periodic and aperiodic thin film multilayers. In particular we discuss dynamics in samples combining alternating layers of tungsten and polycarbonate, grown by pulsed laser deposition. Experiments were carried out by means of time-resolved all-optical pump-probe spectroscopy. The findings are supported by simulations, and suggest the possibility to block a wide range of phonons. Downscaling of the design principle should enable the realization of a thermally insulating medium.

Further functionalization was obtained by incorporating ferromagnetic layers. We discuss how magneto-elastic coupling can be exploited in order to excite spin waves simultaneously with the elastic modes.

DS 12.25 Mon 17:00 Poster A

Elastic dynamics in CoFeB/MgO multilayers: Excitation and suppression of THz phonons — •Dennis Meyer[1], Markus Müller[1], Henning Ulrichs[1], Maria Mansurova[1,2], Jakob Walowski[2], and Markus Münzenberg[2] — [1]I. Physikalisches Institut, Georg-August Universität Göttingen — [2]Institut für Physik, Ernst Moritz Arndt Universität Greifswald

When thin films are impinged by a laser pulse, the thermal stress induced at the surface triggers coherent elastic waves which subsequently propagate through the sample. We present a combined experimental and numerical investigation of such dynamics in a CoFeB/MgO multilayer. Experiments were carried out by time-resolved pump-probe spectroscopy. The main finding is the appearance of a 0.5 THz phonon mode, which is a Bloch-like eigenmode of the system. By breaking the translational symmetry of the superlattice, this mode can be effectively suppressed. These findings are supported by numerical simulations, which in addition provide spatial information inaccessible by experiment. Besides being a building block for photo-induced THz phononics, we will discuss in how far such phonon blocking structures can be utilized for controlling heat flow in thin films.

DS 12.26 Mon 17:00 Poster A

Tunnel diodes—A method to picture quantum correlations in disordered tellurides — Dominik Gholami Bajestani[1], •Henrik Padberg[1], Tobias Schäfer[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA-FIT, RWTH Aachen University, Germany

Phase change materials (PCMs) are promising candidates for a new generation of fast and non-volatile memories unifying flash and DRAM properties. Besides the fast electrical (or optical) switching between amorphous and crystalline phase, storage of additional information in the crystalline state becomes possible because of the resistivity being tunable over several orders of magnitude. The variation of the resistivity stems from different degrees of disorder in the PCM and is linked to quantum correlations. Both effects are known to alter the density of states (DoS). A method to measure the DoS are tunnel diodes, which make use of the tunnel effect and consist of a layer stack with a metal and the PCM separated by a thin oxide layer.

In this study, we investigate changes in disorder and quantum correlation in the PCM $Sn_1Sb_2Te_4$ (SST) using tunnel diodes. As magnetron-sputtering and subsequent annealing are the best way to control the PCM's disorder, we have developed an in situ sputter process to guarantee a high quality layer stack. Besides characterization studies of the diodes, the DoS of SST has been examined for different annealing states to link band structure phenomena to the material properties. To probe the DoS ($\propto \frac{dI}{dV}$), an AC-voltage signal is applied to a biased tunnel diode, at liquid helium temperatures.

DS 12.27 Mon 17:00 Poster A

Nanoparticle gradient composites for resistive switching — •Alexander Vahl[1], Julian Strobel[2], Thomas Strunskus[1], Lorenz Kienle[2], and Franz Faupel[1] — [1]Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Multicomponent Materials, Kaiserstr. 2, 24143, Kiel, Germany — [2]Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Synthesis and Real Structure of Solids, Kaiserstr. 2, 24143, Kiel, Germany

Resistive Switching has been reported in various material systems and recently attracted increasing attention. Composite materials comprising of a gradient of nanoparticles within an insulating matrix are of particular interest for analog resistive switching without filament formation. In focus of this work is the preparation (DC magnetron quasi-cosputtering) and morphological examination of vertical gradients of silver nanoparticles in an amorphous silicon matrix for further investigation of resistive switching. The silver nanoparticles were either formed by self-organization onto the surface or within a gas aggregation cluster source. Deposition time evolution of self-organization of nanoparticles was studied by TEM and compared to nanoparticles generated by gas aggregation cluster source. Nanocomposite samples were characterized by TEM, SEM, Raman spectroscopy and electrical hysteresis measurements. Electron diffraction shows polycrystalline silver nanoparticles and amorphous silicon matrix. SEM cross section images indicate the successful formation of nanoparticle gradients.

DS 12.28 Mon 17:00 Poster A

Using direct laser writing for photonic crystal structures in nanocrystal solar cells — •Stephan Dottermusch[1], Aina Quintilla[2], Guillaume Gomard[2], and Bryce Richards[1,2] — [1]Institut für Mikrostrukturtechnik (IMT), Karlsruher Institut für Technologie (KIT), Karlsruhe, Deutschland — [2]Lichttechnisches Institut (LTI), Karlsruher Institut für Technologie (KIT), Karlsruhe, Deutschland

In recent years light trapping in thin-film solar cells using photonic crystal (PC) based structures has found an increasing interest. Many different types of textures and structures have been proposed. Whereas the fabrication of 1D and 2D PCs has been shown using conventional top-down etching methods or bottom-up self-assembly methods, 3D PCs are rarely seen do to a lack of fabrication techniques. Direct laser writing (DLW) is an emerging technology with the capacity of 3D structuring polymers on a sub-micrometer scale. In this work, PCs were created using DLW and infiltrated with CIS nanocrystals. Light trapping in these structures was investigated using simulations, and observed by measuring the absorption spectrum. Absorption peaks were identified by comparing the spectrum of a flat reference layer.

DS 12.29 Mon 17:00 Poster A

Investigation of thermoelectric properties of thin film chalcogenides — •Matteo Cagnoni[1] and Matthias Wuttig[1,2] — [1]Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA-FIT, RWTH Aachen University, Germany

Future strategies for energy supply are going to demand an increasing use of renewable, clean and sustainable energy sources. The chance of recycling waste heat through thermoelectric generators and the employment of solid-state Peltier coolers in refrigerators are very attractive. Therefore, the interest of the scientific community into thermoelectric properties of materials has experienced a continuous revival from the 90s, after the proof that high efficiencies can be obtained.

The finding of new high-efficiency thermoelectric materials, characterized by large Seebeck coefficients and high electrical conductivity, and small thermal conductivity, is a very difficult task because of the interplay of a multitude of different physical phenomena that govern thermoelectric behavior. Research driven by physical intuition and trial and error has allowed placing materials classes such as skutterudites and chalcogenides in the Olympus of thermoelectrics.

In this project, the behavior of thin film chalcogenides has been investigated in relation to stoichiometric and structural changes, in order to unravel the link between physical properties and thermoelectric performances.

DS 12.30 Mon 17:00 Poster A

Thermal Transport of Phase Change Materials and related Chalcogenides — •Daniel Führen[1], Matteo Cagnoni[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA-FIT, RWTH Aachen University, Germany

Phase change materials (PCMs) are a unique class of materials combining interesting physical properties such as large electronic and optical contrast between the amorphous and crystalline states. One remarkable feature of those materials is the fast reversible switching between their states on a timescale of nanoseconds. This combination of properties is used to store information in rewritable optical data storage applications. The chalcogenide GeTe was the first investigated PCM which shows good optical contrast and fast recrystallization. Many compositions with Ge have been found as PCMs and are applied in commercial products like rewritable DVDs.

Thermal properties of materials play an important role for an efficient switching behavior between the two states. PCMs may be promising candidates for thermoelectric devices because of their specific characteristic of low thermal conductivity in the crystalline state. Here, we present thermal properties of phase change alloys measured between room temperature and 120 °C. The samples are produced as thin films via sputter deposition and are analyzed by 3-omega technique, which has a high accuracy and applicability in a large temperature range, to determine the thermal conductivity.

DS 12.31 Mon 17:00 Poster A

Thermal Electron Emission from LaB$_6$ und BaO in a Thermionic Set-Up — •Michael Hohage[1], Michael Schneiderbauer[2], Mariella Denk[1], Anna Steiner[1], Markus Gusenbauer[1], and Peter Zeppenfeld[1] — [1]Institut für Experimentalphysik, Abt. für Atom- und Oberflächenphysik, Johannes Kepler Universität Linz, Altenbergerstraße 69, 4040 Linz, Austria — [2]te+, Quellenweg 33, 4203 Altenberg, Austria

Thermionic emission is a promising approach to convert heat into electric energy at temperatures reached by burning wood or fossil fuels. We have studied the electron emission from the materials LaB$_6$ and BaO at temperatures up to 1550 K. The cathode and anode surfaces are coplanar for the purpose of a systematic study of the electron emission yield as a function of distance. The electrode temperatures are measured by thermocouples and an infrared pyrometer.

We show the dependence of the thermionic emission current on temperature, distance and on the activation procedure of the BaO electrode. A simple model of the magnitude of the space charge and its influence on thermal electron emission will be introduced. Concepts to lower the space charge and its effect on the thermal emission will be presented and tested against simulations and experiments. In particular, the role of the geometry and macrostructure of the electrodes as well as the influence of external electric and magnetic fields will be discussed.

DS 12.32 Mon 17:00 Poster A

Thermal Characterisation of Ultrathin Complex Oxide Multilayers by the 3ω-Method — •Patrick Thiessen[1], Felix Rieger[1], Vladimir Roddatis[1], Immo Bahns[1], Christian Jooss[1], Oleg Shapoval[2,3], Alexandr Belenchuk[2,3], and Vasily Moshnyaga[2] — [1]Institut für Materialphysik, Universität Göttingen — [2]1. Physikalisches Institut, Universität Göttingen — [3]Institute of Applied Physics,Chisinau(Republic of Moldova)

The present work evaluates the thermal conductivity of ultrathin complex oxide superlattices. Three different deposition methods - Metal Aerosol Deposition (MAD), Pulsed Laser Deposition (PLD) and Ion Beam Sputtering (IBS) - were used to epitaxially grow periodic superlattices consistent of La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO) and SrTiO$_3$ (STO) respectively Pr$_{0.7}$Ca$_{0.3}$MnO$_3$ (PCMO) and STO on STO(100) substrates with varying individual layer thickness and number of layers. The goal of this work was to investigate the influence of the interfaces in dependence of the superlattice periodicity on the thermal conductivity - i.e. the phonon propagation and scattering. The manganite-STO system serves as a model system for acoustic impedance missnatch (AIM) due to the high difference in its elastic properties and its good epitaxial grow. XRay- and TEM-studies are included in order to distinguish between interface related effects and changes in the lattice strain or in the point defect density.

DS 12.33 Mon 17:00 Poster A

In-plane thermal conductivity of thin films measured by steady-state infrared thermography — •Anton Greppmair[1], Caroline Gerstberger[1], Benedikt Stoib[1], Nitin Saxena[2], Peter Müller-Buschbaum[2], Martin Stutzmann[1], and Martin S. Brandt[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [2]Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Strasse 1, 85748 Garching, Germany

We demonstrate a simple and quick method for the measurement of the in-plane thermal conductance of thin films via steady-state IR thermography. The films are suspended above a hole in an opaque substrate and heated by a homogeneous visible light source. The temperature distribution of the thin films is captured via infrared microscopy and fitted to the analytical expression obtained for the specific hole geometry in order to obtain the in-plane thermal conductivity. For thin films of poly(3,4-ethylenedioxythiophene):polystyrene sulfonate post-treated with ethylene glycol and of polyimide we find conductivities of 1.0 W/(mK) and 0.3 W/(mK) at room temperature, respectively. These results are in very good agreement with literature values, validating the method developed.

DS 12.34 Mon 17:00 Poster A

Improving Thermoelectric Performance of TiNiSn by insertion of NiMnSb in the Half Heusler Structure — •Tanya Berry, Siham Ouardi, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.

TiNiSn n-type semiconductors are promising thermoelectric material due to their high power factor. TiNiSn and NiMnSb are Half Heusler alloys that are economic and in high abundance in nature. In this work, we improved the thermoelectric properties of TiNiSn by insertion of NiMnSb in the Half Heusler Structure. The samples were prepared using arc melting technique. As caste and annealed samples were characterized using powder X-ray diffraction patterns, energy-dispersive X-ray spectroscopy, and differential scanning calorimetry to determine the phases and microstructure of the samples. Full Heusler phases were observed in samples with higher substitution amount of NiMnSb. Compared to TiNiSn, the power factor of substituted compounds is enhanced and the thermal conductivity is reduced. Further results will be discussed in the poster.

DS 12.35 Mon 17:00 Poster A

Relation between the symmetry of diperiodic atomic crystals and the existence of Dirac cones in their energy spectrum — •Vladimir Damljanovic and Rados Gajic — Institute of Physics Belgrade, Belgrade, Serbia

We have determined [1] sufficient conditions for the appearance of s=1/2 Dirac cones in any diperiodic, non-magnetic atomic crystal in which the spin-orbit coupling is negligible. Our group theoretical analysis of all 80 diperiodic groups, shows that combined time-reversal and crystal symmetry allows the existence of Dirac cones in the vicinity of K-points in the Brillouin zone, for systems belonging to certain hexagonal diperiodic groups. We have illustrated our results by a tight-binding example.

[1] V. Damljanović, R. Gajić: "Existence of Dirac cones in Brillouin zone of diperiodic atomic crystals according to group theory", arXiv: 1510.09065v1

DS 12.36 Mon 17:00 Poster A

Atomic layer engineering of tunnel barriers in manganite based spin valves — •Vitaly Bruchmann-Bamberg[1], Vasily Moshnyaga[1], Alexander Belenchuk[2], and Oleg Shapoval[2] — [1]I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Pl. 1, 37077 — [2]IIEN, Academy of Science of Republic, Moldova, Academia 3/3, MD-2028 Chinisau, Republic of Moldova

We have prepared La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO)-electrode based spin valves by means of metalorganic aerosol deposition. SrTiO$_3$ (STO) is a well-known insulator used as a tunnel barrier and for magnetic decoupling of both electrodes. Unfortunately, it creates so called dead layers at the valence-mismatched interface to LSMO, reducing the tunnel magnetoresistance significantly [1]. In order to improve the interface by following recent reports [2], atomic layer deposition of interfacial SrO similar to Ruddlesden Popper STO as well as other manganite insulators as tunnel barriers were examined.

[1] H. Yamada et al., Science 305, 646 (2004).

[2] M. Matvejeff et al., Appl. Phys. Lett. 107, 141604 (2015).

DS 12.37 Mon 17:00 Poster A

Growth of continuous hexagonal boron nitride on smooth Ni films — •Siamak Nakhaie, Joseph M. Wofford, Manfred Ramsteiner, Carsten Pfüller, Marcelo J. Lopes, and Henning Riechert — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Hexagonal boron nitride (h-BN) has recently been the subject of an extensive ongoing research effort. This has in large part been driven by the suitability of h-BN for integration into heterostructures with other 2-dimensional materials, such as graphene [1]. However, a scalable synthesis method which combines high-crystalline quality with absolute thickness control remains elusive. We report the synthesis of atomically thin, continuous h-BN on smooth crystalline Ni films using molecular beam epitaxy (MBE). The presence of well-ordered, crystalline h-BN films on Ni (which were grown on MgO(111) substrates) was confirmed using Raman spectroscopy, which revealed a sharp and narrow optical-phonon peak at 1361 cm^{-1}. The width of the Raman peak of the MBE grown h-BN is comparable to that obtained from single-crystalline mechanically exfoliated h-BN. The ubiquity of wrinkle structures in numerous atomic force microscopy scans, together with the uninterrupted observation of the h-BN Raman signal, offer strong evidence that the h-BN films are continuous. Furthermore, the smoothness of the Ni surface allowed for a detailed morphological study of the grown h-BN. This includes the observation of h-BN buckling even on single atomic steps of the underlying Ni. [1] C.R. Dean et al., Nat. Nanotechnol. 5 (2010) 722

DS 12.38 Mon 17:00 Poster A

Resistive switching phenomenon and hole wind effect in YBCO thin films — Martin Truchly[1], •Elena Zhitlukhina[2], and Tomas Plecenik[1] — [1]Department of Experimental Physics, Comenius University, 84248 Bratislava, Slovak Republic — [2]Donetsk Institute for Physics and Engineering, 03680 Kyiv, Ukraine

We present an overview of our experimental and theoretical activities aimed to clarify the mechanism of resistive memory effects in YBCO thin layers. The phenomenon was studied by scanning spreading resistance microscopy (SSRM) and scanning tunneling microscopy (STM) techniques. The most striking feature uncovered (in contrast to previous experiments on planar bilayers with YBCO films) was the opposite voltage-bias polarity of the switching effect in all SSRM and a number of STM measurements. Observed hysteresis in current-voltage characteristics is interpreted as a movement of oxygen vacancies in the vicinity of the tip-YBCO contact. Since the charge distribution in YBCO samples is expected to be strongly inhomogeneous, the balance between the direct electrostatic force on activated oxygen ions and that caused by momentum exchange with the current carriers (holes) hitting them determines direction in which the oxygen vacancies are moving. We propose a minimalist model with the only fitting parameter that accounts for the resistance hysteresis phenomenon in the YBCO films studied.

DS 12.39 Mon 17:00 Poster A

MgO barrier parameter and TMR of PLD grown magnetic tunnel junctions with zinc ferrite electrodes — •Michael Bonholzer, Daniel Splith, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für experimentelle Physik II, Linnéstr. 5, 04103 Leipzig

We built zinc ferrite (ZnFe$_2$O$_4$) based magnetic tunnel junctions (MTJs) with an epitaxial MgO barrier and investigated their electrical properties.

A multilayer of TiN/ZnFe$_2$O$_4$/MgO/Co was deposited on (100)-MgO substrates by PLD. MTJs, lateral size ranging from 5×5 to $30\times30\,\mu\mathrm{m}^2$, were defined by argon ion etching. A high quality, epitaxial TiN layer [1] is used to reduce series resistance. RHEED intensity oscillations, visible during PLD-growth of MgO, show the high structural quality of the barrier and allow an accurate determination of barrier thickness. With that, other barrier parameters were determined out of I-V measurements by a modified BDR-model [2]. Since the original BDR-model neglects the influence of lateral thickness variations, we introduced the barrier roughness as new parameter modelled by a Gaussian distribution of thickness and fixed the mean thickness to the value determined by RHEED. The new model gives reasonable values for roughness and height of the MgO barrier.

Magnetic field-dependent resistance measurements carried out on these structures show a TMR of 1% at 200 K.

[1] M. Bonholzer *et al.*, Phys. Status Solidi A **211**, 2621 (2014)
[2] W.F. Brinkman *et al.*, J. Appl. Phys. **41**, 1915 (1970)

DS 12.40 Mon 17:00 Poster A

Investigations of defects in weakly damaged ion implanted GaAs — •Sascha Creutzburg[1], Emanuel Schmidt[1], Ingo Uschmann[2], and Elke Wendler[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Institut für Optik und Quantenelektronik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

In case of room temperature ion implantation of GaAs, a saturation of defects at a rather low level without amorphization is observed, the microstructure of which is not yet understood. The aim of the present work is to investigate this state of weak damage in GaAs by RBS-channelling, optical, TEM, XRD and in-situ stress measurements. Undoped <100> oriented GaAs wafers were implanted with 1 MeV Si$^+$ at room temperature to ion fluences between $1\cdot10^{13}$ cm^{-2} and $3\cdot10^{15}$ cm^{-2} with constant ion flux. The energy dependence of the minimum yield as measured by RBS-channelling indicates the presence of correlated displaced atoms. This is in agreement with previously performed temperature dependent RBS-channelling measurements. The near edge absorption coefficient K shows an exponential behaviour of the photon energy $\hbar w$ according to $K \sim \exp(\hbar w/E)$ with the tailing energy $E = (0.36 - 0.51)$ eV depending on the ion fluence. Theoretical considerations have shown that the range of tailing energy can be explained assuming a high concentration of antisite defects and vacancies. Further information about lattice strain within the implanted layers will be obtained by ex-situ XRD rocking curve measurements and by in-situ measurements of the sample curvature.

DS 12.41 Mon 17:00 Poster A

Secondary Ion Mass Spectrometry (SIMS) in Helium and Neon Ion Microscopy — David Dowsett, •Florian Vollnhals, Jean-Nicolas Audinot, and Tom Wirtz — Advanced Instrumentation for Ion Nano-Analytics (AINA), MRT Department, Luxembourg Institute of Science and Technology (LIST), 41 rue du Brill, L-4422 Belvaux, Luxembourg

Helium Ion Microscopy (HIM) was introduced a few years ago as an imaging tool with a lateral resolution below 1 nm. The addition of Neon as a working gas in the Orion NanoFab (Zeiss) has opened up new possibilities in high resolution nano-machining and FIB applications.

We developed instrumentation to combine the HIM with Secondary Ion Mass Spectrometry (SIMS). In SIMS, the sample is sputtered by a primary beam, e.g., the highly focused He or Ne ion beam of a HIM, while the secondary ion emission is recorded. This combination takes advantage of both probe size of the He/Ne beam and sensitivity of the SIMS analysis, allowing for high resolution correlative microscopy. In addition, the HIM-SIMS combination has very promising prospects regarding in-situ process control during nano-machining.

We will discus instrumental and method development, including theoretical and experimental aspects, e.g., He and Ne ion beam interaction with sample surfaces.[1] He and Ne ion beams will be shown to be viable primary species for successful imaging SIMS, approaching the physical resolution limits of <20 nm.[2]

[1] D. Dowsett et al., J. Vac. Sci. Technol. B 30 (2012), 06F602
[2] T. Wirtz et al., Nanotechnology 26 (2015), 434001

DS 12.42 Mon 17:00 Poster A

Implementation of a setup for ion energy and ion mass selective hyperthermal ion-beam assisted deposition of ultrathin nitride films — •Philipp Schumacher[1], Jürgen W. Gerlach[1], Stephan Rauschenbach[2], and Bernd Rauschenbach[1] — [1]Leibniz-Institut für Oberflächenmodifizierung, Leipzig — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart

Ion-beam assisted deposition (IBAD) is a widely used deposition technique to produce high-quality thin films of different kind. For this study, an already existing system for hyperthermal nitrogen ion-beam assisted molecular-beam epitaxy (IBA-MBE) of GaN was equipped with a quadrupole mass filter setup in order to perform the deposition process with ions of a certain preselected mass (N^+ or N_2^+) as well as with a preselected kinetic ion energy in the hyperthermal energy range up to about 100 eV. This way, the influence of the ion species on the growth process of GaN and on the properties of the produced ultrathin films can be investigated. The respective influence of the kinetic energy of the ions is to be studied as well. Here, the quadrupole setup in combination with a hollow-anode plasma-source is described and its performance is presented. Mass separation is demonstrated and the relevant properties of the ion beam, such as ion energy distribution, ion current density distribution and ion beam profile, are presented in regard to ion-beam assisted film growth. Finally, preliminary results on GaN film deposition by applying this setup are shown.

DS 12.43 Mon 17:00 Poster A

Intense Electrospray Ionization Sources/Atmospheric Pressure Interfaces for Ion Beam Deposition — •Stephan Rauschenbach[1], Laurent Bernier[2], Matthias Pauly[3], and Julius Reiss[2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Technical University Berlin, Germany — [3]University Strasbourg, ICS-CNRS, France

Reactive or soft-landing molecular ion beam deposition requires high fluence ion beams, which present soft ionization sources, such as electrospray ionization (ESI), cannot deliver. In principle, electrospray ionization can generate ion currents in the microamp range, however, the ion transport in the atmospheric interface, i.e. the transfer of ions trough a capillary or pinhole from atmospheric pressure to vacuum, is extremely inefficient. The particle transport is governed by electric forces, diffusion and by the flowing background gas. The gas flow can be laminar or turbulent and is strongly compressible. Its interplay with ions can strongly influence the efficiency of the source, which is however not fully understood. We present the experimental and numerical analysis of the ion transport behavior in a confined, flowing gas and show that highly efficient ion sources can be conceived.

DS 12.44 Mon 17:00 Poster A

Phase transition of pulsed laser deposition-deposited $Ge_2Sb_2Te_5$ films induced by nano- and femtosecond single laser pulse irradiation — •Xinxing Sun[1], Martin Ehrhardt[1], Andriy Lotnyk[1], Erik Thelander[1], Jürgen W. Gerlach[1], Tomi Smausz[2], Ulrich Decker[1], and Bernd Rauschenbach[1,3] — [1]Leibniz Institute of Surface Modification, Permoserstr. 15, D-04318, Leipzig, Germany — [2]University of Szeged, Dóm tér 9. H-6720 Szeged, Hungary — [3]Institute for Experimental Physics II, Leipzig University, Linnéstr.5, D-04103 Leipzig, Germany

Fast phase transformation of $Ge_2Sb_2Te_5$ (GST) materials is a vital requirement for devices based on phase change materials. In this present work, the crystallization process of pulsed laser deposition (PLD)-deposited GST films irradiated by nano- and femtosecond single pulses at a wavelength of 248 nm with varied laser fluences is compared. Detailed structural information about the phase transformation is elucidated by x-ray diffraction and high resolution transmission electron microscopy (TEM). A high optical reflectivity contrast (25%) between amorphous and completely crystallized GST films was achieved by fs laser single pulse irradiation induced at a fluence between 13 and 16 mJ/cm^2 and by ns laser single pulse irradiation induced at a fluence between 67 and 130 mJ/cm^2. Finally, the fluence dependent increase of the reflectivity is discussed in terms of each photon involved into the crystallization process for ns and fs pulses, respectively.

DS 12.45 Mon 17:00 Poster A

Electronic Tuning in Phase Change Materials using Ionic Liquid Gating — •Bo Thöner, Hanno Volker, Tobias Schäfer, Peter Jost, Artur Romanov, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University

Phase change materials (PCM), which are renowned for their pronounced optical and electrical property changes upon crystallization, receive renewed interest because of their potential applications in novel electronic storage devices.

Since disorder strongly affects their properties, PCMs are an obvious choice to examine the competing impact of electron correlation and disorder-induced localization, which both can explain metal-insulator transitions (MITs). In the scope of Anderson's theory, the MIT is achieved by moving the so-called mobility edge with respect to the Fermi energy. On the one hand, the mobility edge can be shifted by thermal annealing. On the other hand, it is reasonable to assume that a transition due to a shift of the Fermi energy by applying an electric field is also possible. This could allow for a more precise and reversible crossing of the MIT and a better understanding of the process. Hence, we have investigated the feasibility of using ionic liquid gating as a method to induce the MIT.

The use of ionic liquids as the gating electrolyte enables a potentially larger number of induced charge carriers compared to conventional gating which increases the range in which the Fermi energy can be shifted.

DS 12.46 Mon 17:00 Poster A

Spectroscopic near-field investigation of trigonally symmetric contrasts on solvothermally grown Sb_2Te_3 platelets in the mid-infrared. — •Lars Mester[1], Martin Lewin[1], Tobias Saltzmann[2], Ulrich Simon[2], and Thomas Taubner[1] — [1]I. Physikalisches Institut A, RWTH Aachen — [2]Institut für Anorganische Chemie, RWTH Aachen

Chemical syntheses could provide a cheap alternate approach to conventional nanofabrication as e.g. gas-phase deposition techniques [1]. Solvothermally synthesised Sb_2Te_3 platelets of $2-3\,\mu m$ size grown under various synthesis conditions are spectroscopically investigated via scanning near-field microscopy (SNOM) at various mid-infrared wavelengths. In SNOM measurements, laser light is focused on an AFM tip which is scanned in tapping mode over the sample. Backscattered light from the tip is influenced by near-fields of the sample and enables microscopy and spectroscopy beyond the diffraction limit with lateral resolution in the order of the AFM tip radius ($\approx 25\,\mathrm{nm}$) [2].

The investigated single-crystalline Sb_2Te_3 platelets show unexpected domains of several 100 nm lateral extent with different optical response. By modeling the response with the Drude model and Finite Dipole Model, Hauer *et al* attributed the domains to regions of two different charge carrier concentrations [3]. Further analysis of the Drude characteristics is made with SNOM spectroscopy between $900-1900\,\mathrm{cm}^{-1}$.

[1] Saltzmann et al, Angew. Chem. Int. Ed. 54, pp. 6632-6636 (2015)

[2] Taubner et al, J. of Microsc., 210, Pt 3, pp. 311-314 (2003)

[3] Hauer et al, Nano Lett. 15, pp. 2787-2793 (2015)

DS 12.47 Mon 17:00 Poster A

Spectroscopic near-field investigation of trigonally symmetric contrasts on solvothermally grown Sb_2Te_3 platelets in the mid-infrared. — •Lars Mester[1], Martin Lewin[1], Tobias Saltzmann[2], Ulrich Simon[2], and Thomas Taubner[1] — [1]I. Physikalisches Institut A, RWTH Aachen — [2]Institut für Anorganische Chemie, RWTH Aachen

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[2] Taubner et al, J. of Microsc., 210, Pt 3, pp. 311-314 (2003)

[3] Hauer et al, Nano Lett. 15, pp. 2787-2793 (2015)

DS 12.48 Mon 17:00 Poster A

Characterization of Ta_2O_5 and $BaTiO_3$ based memristive systems — •Lauritz Schnatmann[1], Norman Shepheard[1], Stefan Niehörster[1], and Andy Thomas[1,2] — [1]Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — [2]IFW Dresden, IMW, Helmholtzstrasse 20, 01069 Dresden, Germany

We prepared thin film resistive tunnel junctions based on Ta_2O_5 and $BaTiO_3$ by magnetron sputtering and defined the junctions by optical lithography in sizes between 10 μm and 25 μm. We looked into the memristive switching behaviour based on Chua et al. [1], where he theoretically described it in 1976. He predicted the change of the switching with a variation of the measurement frequencies. To do this, we read out the current at a fixed bias voltage during a whole loop.

Di Ventra et al. [2] described two different types of memristors: Type I and type II. These two types show a crossing or non-crossing behavior at 0 V in the hysteresis loop and we observed these two types of switching in the different systems. For the hysteresis loops, we chose frequencies from 0.006 mHz to 2 mHz and maximum amplitudes from 150 mV up to 325 mV and compared the amplitudes of the resistance change.

[1] Chua et al. 'memristive devices and systems', Proceedings of the IEEE, 64, 209-223, 1976

[2] Yuriy V Pershin and Massimiliano Di Ventra 'Memory effects in complex materials and nanoscale systems', Advances in Physics, 60, 145-227, 2011

DS 12.49 Mon 17:00 Poster A

Molecular Dynamics Approach to Resistive Switching in Thin Film Systems — •Tobias Gergs, Sven Dirkmann, Frederik Schmidt, and Thomas Mussenbrock — Ruhr University Bochum, 44780 Bochum

Resistive switching devices have recently experienced a revival, leading to a remarkable enhancement of the scientific interest due to a wide range of potential applications including non-volatile memories and neural networks. Most of these devices rely on ionic conduction mechanisms. Here the change in resistance is due to the formation and dissolution of electrically conducting paths in solid state electrolytes. This phenomenon is also referred to as electrochemical metallization or metallic bridging. It has recently been shown that kinetic Monte Carlo simulations are capable of mimicking the long time scale dynamics of such devices by imposing potential structures as well as activation energies for the chemical processes. This contribution is devoted to study the short time scale dynamics of a generic Cu/a-SiO$_2$/Cu tri-layer thin film system and its fundamental properties by means of molecular dynamics simulations. Particularly, the influence of an externally applied electric field on the interfacial molecular configuration is discussed. (The work is supported by the German Research Foundation in the frame of FOR 2093.)

DS 12.50 Mon 17:00 Poster A

Impact of disorder on properties of phase change materials — •Felix vom Bruch, Strefan Jakobs, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University,52056 Aachen, Germany

Phase change materials (PCM) combine unique physical properties. They develop a high optical and electrical contrast between their amorphous and crystalline phase. Moreover switching between both states occurs on a nanosecond timescale. The pronounced optical contrast is related to a change in bonding mechanism upon crystallization. The amorphous phase is governed by conventional covalent bonds whereas the crystalline phase is characterized by the formation of resonant bonds [1]. Moreover, in many PCM chemical disorder on the cation sublattice strongly affects electrical properties [2]. Annealing of the material leads to a subsequent reduction of this disorder and finally to a phase transformation. Here we explore the impact of structural and stoichiometric disorder on the properties of phase-change thin films. The samples are deposited using sputter deposition and are subsequently characterized by means of X-ray diffraction, van-der-Pauw measurements and Fourier transform infrared spectroscopy.

[1] Shportko, K., *et al.* Resonant bonding in crystalline phase change materials. Nature Materials (2008) 653-658.

[2] Siegrist, T., *et al.* Disorder-induced localization in crystalline phase-change materials. Nature Materials (2011) 202-208.

DS 12.51 Mon 17:00 Poster A

Designing new Phase Change Materials via Stoichiometry — •Stefan Jakobs[1], Alexander von Hoegen[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA - Fundamentals of Future Information Technology, RWTH Aachen University, Germany

Phase change media utilize a remarkable property portfolio including the ability to rapidly switch between the amorphous and crystalline state, which differ significantly in their properties. This material combination makes them very attractive for data storage application in rewriteable optical data storage, where the pronounced difference of optical properties between the amorphous and crystalline state is used [1] . This unconventional class of materials is also the basis of a storage concept to replace flash memory. This poster will discuss the unique material properties, which characterize phase change materials. In particular, it will be shown that only a rather small group of materials utilizes resonant bonding, a particular flavour of covalent bonding, which can explain many of the characteristic features of phase change materials. This insight is employed to predict systematic property trends and to explore the limits in stoichiometry for such memory applications. It will be demonstrated how this concept can be used to tailor the electrical and thermal conductivity of phase change materials.

[1] Wuttig, M. and Yamanda, N. *Nature materials* **6**(11), 824-832 (2007)

DS 12.52 Mon 17:00 Poster A

Ion transport in memristive double barrier devices — •S. Dirkmann[1], J. Trieschmann[1], T. Gergs[1], E. Solan[2], M. Hansen[3], M. Ziegler[3], K. Ochs[2], H. Kohlstedt[3], and T. Mussenbrock[1] — [1]Ruhr-Universität Bochum, Theoretische Elektrotechnik, 44780 Bochum — [2]Ruhr-Universität Bochum, Digitale Kommunikationssysteme, 44780 Bochum — [3]Christian-Albrechts-Universität Kiel, Nanoelektronik, 24143 Kiel

The memristive double barrier device is an ultra-thin four-layer system (Nb/Al/Al$_2$O$_3$/Nb$_x$O$_y$/Au). Here the memristive layer (Nb$_x$O$_y$) is sandwiched between a Schottky and a tunneling barrier. It has been recently shown that this device offers a number of potentially interesting features [1]: An intrinsic current compliance, improved retention, and – most importantly – no need for an initial electric forming procedure. The latter is particularly attractive for applications in highly dense random access memories or neuromorphic mixed signal circuits. So far a deeper physical understanding of the interplay between the current transport mechanism and inner atomistic device structure is missing. In this contribution, we report on results of kinetic Monte-Carlo simulations of the transport phenomena in these devices. We identify the ion drift of charged point defects within the Nb$_x$O$_y$ layer as a key factor for the resistive switching behavior. We discuss the related current-voltage characteristics which are in excellent agreement with experimentally obtained data. (The work is supported by the German Research Foundation in the frame of FOR 2093.)

[1] M. Hansen et al., Scientific Reports **5**, 13753 (2015)

DS 12.53 Mon 17:00 Poster A

Temperature-driven phase transition in V$_{1-x}$Mo$_x$O$_2$ thin films: Interplay of Structural and Electronic Transitions — Sven Esser, Sebastian Merten, Christoph Meyer, and •Vasily Moshnyaga — I. Physikalisches Institut, Georg-August- Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

VO$_2$ with a metal-insulator transition (MIT) at 340 K and resistivity change by 3-4 orders of magnitude [1] is a promising candidate for fast switching devices. In the same temperature regime a structural phase transition (SPT) from monoclinic structure to rutile [2] also occurs. Both phase transitions could be driven quasi optically, which opens the possibility as fast optical switches (FOS)[2].

Due to several doping values different crystal structures (R, M1, M2, T [3]) of VO$_2$ can be stabilized at room temperature. For high quality films of definite composition a precise control of the Mo-content during preparation is necessary.

We report the growth of epitaxial V$_{1-x}$Mo$_x$O$_2$ ($x = 0 - 0.04$) thin films on Al$_2$O$_3$ (0001) substrates by means of low-oxygen MAD technique. Resistivity and Raman measurements probe the position of the MIT and SPT for a better understanding of the correlation between both phase transitions.

This work is supported by the German Science Foundation through SFB 1073, TP B04.

[1] N. Shukla *et al.*, Nat. Commun. **6**, 7812 (2015)

[2] D. Wegkamp, Dissertation, FU Berlin (2015)

[3] E. Strelcov *et al.*, Nano Lett. **12**, 6198 (2012)

DS 12.54 Mon 17:00 Poster A

Phase Change Characteristics of Sn/Pb Chalcogenides — •Zheng Zeng[1], Stefan Jakobs[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA - Fundamentals of Future Information Technology, RWTH Aachen University, Germany

Phase change materials (PCMs) uniquely combine physical properties. They exhibit a large electrical and optical contrast between their amorphous and crystalline phases. Moreover, the switching between these two phases occurs on a nanosecond timescale rendering those materials perfect candidates for data storage applications.[1]

So far, mainly compositions consisting of Ge, such as Ge$_1$Sb$_4$Te$_7$, Ge$_1$Sb$_2$Te$_4$ and Ge$_2$Sb$_2$Te$_5$, have been identified as PCMs, and some of them are frequently applied in commercial products like rewritable DVD. In this work, we focus on Sn and Pb chalcogenides, which are isoelectronic substitutions of Ge, and explore their potential as possible phase change materials.

Our samples are made as thin films via sputter deposition and are subsequently characterized by means of X-ray diffraction, Van-der-

Pauw measurements and Fourier transform infrared spectroscopy.
[1] Wuttig, M. and Yamanda, N. Nature materials 6(11), 824-832 (2007)

DS 12.55 Mon 17:00 Poster A

Ellipsometric characterization of doped SnO_x layers for novel SPR-based gas sensors — •Daniel Fischer[1], Andreas Hertwig[1], Uwe Beck[1], Martin Kormunda[2], and Norbert Esser[3] — [1]BAM Federal Institute for Materials Research and Testing, Division 6.7 — [2]J.E. Purkyne University, Faculty of Science, Department of Physics — [3]Leibniz-Institut für Analytische Wissenschaften ISAS e.V.

In the present research a surface based gas detection technique is investigated using the SPR effect with ellipsometric readout. The sensor consists of a gold layer (∼40 nm) top-coated with a doped metal-oxide ($M:SnO_x$,∼5 nm). The coating was added by magnetron sputtering with doped targets and different doping concentration. In the past, it could be shown that these type of sensors can detect various gases, e.g. CO, H_2, O_2, O_3, He, N_2 with sensitivities down to the ppm range. The goal of the present study is to characterize the doped metal-oxide top-coating material in dependence of the coating conditions. Changing the properties of the plasma coating process and the doping gives access to a variety of different layer properties and enables us to find the best conditions for the determined gas in selectivity and sensitivity. The resulting layers are analyzed mainly by using spectroscopic ellipsometry to extract the optical constants n and k to find a correlation between the doping properties and the sensing ability for specific gas species. Further methods like TEM, XRD and TOF-SIMS are used to identify the structure of the surface and to extract the doping concentration of the coating.

DS 13: Graphene: Fabrication (Joint session of DS, DY, HL, MA, O and TT organized by HL)

Time: Monday 17:45–18:45 Location: H17

DS 13.1 Mon 17:45 H17

Growth and characterization of mono- and bilayer graphene nanoribbons grown on SiC(0001) — •Lauren Aranha Galves, Joseph Wofford, Uwe Jahn, João Marcelo J. Lopes, and Henning Riechert — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

Graphene Nanoribbons (GNRs) are promising for applications in nanoelectronics due to their unique properties. Unlike graphene sheets, GNRs possess a bandgap and the gap is inversely proportional to their width [1]. Additionally, bilayer GNRs offer the possibility to further tune their bandgap via the application of an external electric field [2]. The thermal decomposition of SiC surfaces is a suitable synthesis method for GNRs due to the control it offers over their size [3].

In this report we present the structural characterization of mono- and bilayer GNRs grown on SiC(0001) by surface graphitization. Bilayer GNRs were obtained via a post-growth air-annealing process [4]. The width of the ribbons were determined via atomic force microscopy (AFM) height and phase imaging as well as scanning electron microscopy (SEM), while the number of layers (i.e. mono or bilayer GNRs) were examined by Raman spectroscopy. Based on these measurements it was possible to identify an activation energy for the formation of the nanostructures and a lateral etching effect in the bilayer GNRs due to the air-annealing process.

[1] Barone et al., Nano Lett. 6, 2748 (2006); [2] Li et al., Eur. Phys. J. 64, 73 (2008); [3] Sprinkle et al. Nat. Nanotechnol. 5, 727 (2010); [4] Oliveira Jr. et al., Nat. Comm. 6, 7632 (2015).

DS 13.2 Mon 18:00 H17

Optoelectronic Properties of Graphene Nano-Ribbons Patterned By Helium Ion Beam Lithography — •Akshay Kumar Mahadev Arabhavi[1], Andreas Brenneis[1,2], Simon Drieschner[1,2], Marcus Altzschner[1], Helmut Karl[3], Jose Garrido[1,2], and Alexander Holleitner[1,2] — [1]Walter Schottky Institut and Physics-Department, Technical University Munich, Am Coulombwall 4a, 85748 Garching, Germany. — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 Munich, Germany. — [3]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany.

High electron mobility, excellent thermal conductivity and uniform absorption in the visible range makes graphene an outstanding material for high-frequency optoelectronic applications. However, the lack of a band gap limits graphene in switching applications. A quantization energy can be introduced by confining graphene to one-dimensional ribbons of widths below 20 nm, for instance, using Helium Ion Beam Lithography (HIBL) [1-2]. We have optimized the parameters to pattern graphene nano-ribbons on sapphire substrates using HIBL, such as dose, beam current, spot control and dwell time. Moreover, we apply an ultrafast photocurrent spectroscopy [3] to investigate the optoelectronic properties of the patterned graphene nano-ribbons with respect to their high-frequency properties. References: [1] M. Han et al., Phys. Rev. Lett. 98, 206805, (2007). [2] Bell DC et al., Nanotechnology 20, 455301, (2009). [3] A. Brenneis, et al., Nature Nanotech, 10, 135, (2015).

DS 13.3 Mon 18:15 H17

High quality bilayer graphene from chemical vapor deposition on reusable copper — •Michael Schmitz[1], Stephan Engels[1,2], Luca Banszerus[1], Kenji Watanabe[3], Takashi Taniguchi[3], Bernd Beschoten[1], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

We recently introduced a dry transfer method for single-layer graphene grown by chemical vapor deposition (CVD) yielding ultra high quality graphene comparable to the best exfoliated samples [1]. Here, we demonstrate that this method can be extended to bilayer graphene. In particular, we show the fabrication and characterization of bilayer graphene/hexagonal boron nitride heterostructures using high quality CVD bilayer graphene grown on reusable copper foils. Raman measurements reveal a high structural quality [2]. We achieve carrier mobilities up to 45,000 $cm^2/(Vs)$ at 1.8 K and up to 17,000 $cm^2/(Vs)$ at room temperature outperforming all state-of-the-art CVD bilayer graphene devices. Finally, we show dual-gated transport measurements to investigate band-gap opening in our CVD grown bilayer graphene.

[1] L. Banszerus, M. Schmitz, S. Engels *et al.*, Science Advances **1**, e1500222 (2015)
[2] C. Neumann, S. Reichardt, P. Venezuela *et al.*, Nature Communications **6**, 8429 (2015)

DS 13.4 Mon 18:30 H17

Graphene-based fast hot-electron bolometer with bandwidth from THz to VIS — Martin Mittendorff[1,2], Josef Kamann[3], Jonathan Eroms[3], Dieter Weiss[3], Christoph Drexler[3], Sergey D. Ganichev[3], Jochen Kerbusch[2], Artur Erbe[2], Ryan J. Suess[1], Thomas E. Murphy[1], Jacob C. König-Otto[2,4], Harald Schneider[2], Manfred Helm[2,4], and •Stephan Winnerl[2] — [1]University of Maryland, College Park, USA — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Universität Regensburg, Regensburg, Germany — [4]Technische Universität Dresden, Dresden, Germany

We present a fast detector (rise time 40 ps) operating at room temperature that is capable to detect radiation from the THz to visible spectral range (demonstrated wavelengths 500 μm - 780 nm) [1]. The detector consists of a CVD-grown graphene flake contacted by a broadband logarithmic periodic antenna. SiC acts as a substrate material that does not interfere with the detection mechanism in the desired frequency range, even within the Reststrahlen band of SiC (6 - 12 μm). The detector is ideal for timing purposes. Near infrared (mid- and far infrared) pulse energies of the order of 10 pJ (1 nJ) are sufficient to obtain good signal-to-noise ratios. We suggest that the bandwidth is limited by the antenna dimensions (typically several mm) on the long wavelength side and by the bandgap of SiC (380 nm) on the short wavelength side.

[1] M. Mittendorff et al., Opt. Express 23, 28728 (2015).

DS 14: Annual Meeting of the Thin Films Division

Organizers: Norbert Esser (ISAS Berlin) and Jürgen Faßbender (HZ Dresden-Rossendorf)

Time: Monday 19:00–20:00 Location: H8

Annual Report

DS 15: Thermoelectric Materials

Time: Tuesday 9:30–12:15 Location: H8

Invited Talk DS 15.1 Tue 9:30 H8

Heterostructures with Targeted Nanoarchitecture and Tunable Properties — •David Johnson — University of Oregon, Department of Chemistry and Materials Science Institute, Eugene, OR, USA

By controlling the composition of an amorphous intermediate on the nanoscale we can kinetically control the self-assembly of new nanostructured compounds consisting of two or more compounds with different crystal structures that are precisely interleaved on the nanoscale. We have used this approach to synthesize hundreds of new metastable heterostructures with designed nanostructure, including structural isomers. Many of these materials have unprecedented physical properties, including the lowest thermal conductivities ever reported for a fully dense solid, systematic structural changes dependent on nanostructure, and charge density wave transitions. The designed precursors enable diffusion to be followed and quantified over distances of less than a nanometer, providing insights to the mechanism that gives control of the nanoarchitecture of the final product. We believe the ability to prepare entire families of new nanostructured compounds permits a new "thin film metallurgy" or *nanochemistry* in which nanostructure and composition can both be used to tailor physical properties, interfacial structures can be determined for precisely defined constituent thicknesses, and interfacial phenomena and modulation doping can be systematically exploited.

DS 15.2 Tue 10:00 H8

Symmetrical and non-symmetrical TiNiSn/HfNiSn superlattices — •Paulina Komar[1,2], Emigdio Chávez Angel[1], Christoph Euler[1], Gregor Fiedler[3], Benjamin Balke[4], Peter Kratzer[3], and Gerhard Jakob[1,2] — [1]Institute of Physics, University of Mainz, Mainz, Germany — [2]Graduate School Materials Science in Mainz, Mainz, Germany — [3]Faculty of Physics, University of Duisburg-Essen, Duisburg, Germany — [4]Institute of Inorganic and Analytical Chemistry, University of Mainz, Mainz, Germany

The goal of our work is to reduce the thermal conductivity by phonon scattering at the superlattice (SL) interfaces and enhance $ZT = \frac{S^2\sigma}{\kappa}T$. For symmetrical SLs (TiNiSn:HfNiSn ratio=1 and variable SL period) we observe a very good agreement between the cross-plane thermal conductivity measured by the 3ω method and a calculation based on Boltzmann transport theory down to a SL period of 3 nm. At the SL period of 3 nm a crossover between the particle- and the wave-like transport of phonons takes place and, therefore, κ increases for decreasing periods [1]. An investigation of non-symmetrical SLs (variable TiNiSn:HfNiSn ratio and constant SL period) reveal that not only the SL period and the number of interfaces have an influence on κ, but the ratio of materials with higher and lower κ influences the thermal conductivity as well. Additionally, a systematic improvement of the in-plane Seebeck coefficient is observed.

We gratefully acknowledge financial support by DFG (Ja821/4-2) and (GSC 266).

[1] P. Hołuj *et al.* Phys. Rev. B 92, 125436 (2015).

DS 15.3 Tue 10:15 H8

Full thermoelectric characterization of individual silver-nanowires — •Rüdiger Mitdank[1], Danny Kojda[1], Zhi Wang[2], Johannes Ruhhammer[2], Michael Kroener[2], Peter Woias[2], Martin Albrecht[3], and Saskia F. Fischer[1] — [1]Novel Materials Group, Institut für Physik der Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Laboratory for Design of Microsystems, University of Freiburg - IMTEK, 79110 Freiburg, Germany — [3]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2 , 12489 Berlin, Germany

A full characterization of the thermoelectric properties of nanowires (NWs) requires information about the Seebeck coefficient as well as the electrical and thermal conductivity. The temperature normalized ratio of both conductivities is known as Lorenz number L and is discussed for Ag-NWs in [1]. In order to determine the thermoelectric figure of merit of Ag-NWs, individual Ag-NWs are transferred to a micro machined measurement platform (TNCP) and contacted by electron beam induced deposition (EBID) with platinum. The focus of this talk is directed to the discussion of the temperature-dependent Seebeck coefficient of Ag-NW's. The thermovoltage of Ag-NWs was measured with respect to Pt between 4 K and 300 K. The Seebeck coefficient S changes the sign at T = 150 K and exhibits a minimum at T = 70 K. This zero-crossing and the influence of the phonon drag are discussed. As a result, the figure of merit S*S/L is discussed for the temperature-range between 4 K and 300 K.

[1] D. Kojda et. al. Phys. Rev. B, 91, 024302 (2015)

DS 15.4 Tue 10:30 H8

Surface Effects on Thermoelectric Properties of Single Crystalline Semiconducting Nanowires — •Danny Kojda[1], Rüdiger Mitdank[1], Anna Mogilatenko[2], William Töllner[3], Zhi Wang[4], Michael Kröner[4], Peter Woias[4], Kornelius Nielsch[3], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, D-12489 Berlin — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, D-12489 Berlin — [3]Institut für Angewandte Physik, Universität Hamburg, D-20355 Hamburg — [4]Laboratory for Design of Microsystems, University of Freiburg - IMTEK, D-79110 Freiburg

Bismuth telluride nanowires (Bi_2Te_3 NWs) are proposed to reveal a thermoelectric figure of merit ZT that is influenced by confinement and surface effects. To determine the role of surface effects we consider individual single crystalline NWs as model system of a high surface-to-volume-ratio for which grain boundary scattering is negligible. We demonstrate the state-of-the-art of the combination of the structural, chemical, and temperature-dependent complete thermoelectric characterization for individual single crystalline $Bi_{0.39}Te_{0.61}$ NWs, which only differ in surface morphology. With the 3ω-method a reduction of the thermal conductivity of about 50 % is measured in a diameter varied NW with respect to a NW with a constant diameter [1]. For homogenous, diameter varied and single indented NWs finite element simulations are performed to interpret the measurement results [2].

[1] D. Kojda *et al.*, Semicond. Sci. Technol. **29**, 124006 (2014).

[2] D. Kojda *et al.*, Phys. Status Solidi A, DOI:10.1002/pssa.201532464.

15 min. break.

DS 15.5 Tue 11:00 H8

Full- and half- Heusler phase coexistence in phase separated Z_{2-x}TiSb (Z=Co,Ni) thermoelectrics. — •Joaquin Miranda, Heiko Schoberth, Thomas Gruhn, and Heike Emmerich — Lehrstuhl für Material- und Prozesssimulation, Universität Bayreuth, Universitätsstraße 30, D-95447 Bayreuth, Germany

During the last year, we have successfully employed ab-initio Density Functional calculations and Monte Carlo simulations to show that some thermoelectric half-Heusler alloys show phase separation [1-3]. Recently, we have studied transition metal alloys with the formula Z_{2-x}TiSb (Z=Co, Ni), where x sets the concentration for a half (if x=1) or full (if x=0) Heusler material. We show that the materials undergo a complex phase separation containing half/full Heusler superstructures. This separation is assumed to have beneficial effects on the charge and heat transports mechanism and to lead to higher figures of merit in thermoelectrics. The interplay of kinetics and transport on the bulk as well as the role of the inter-phases are still under investigation. Here we show simulations that clarify the individual contributions.

1.- Nanophase separation in CoSb-based half-Heusler thermoelectrics: A multiscale simulation study. Phys. Status Solidi A (2015).

2.- Miscibility gap in the phase diagrams of thermoelectric half-Heusler materials CoTi_{1-x}Y_xSb (Y = Sc, V, Mn, Fe). Journal of Electronic Materials (2015).

3.- Ab-initio study of domain structures in half-metallic CoTi_{1-x}Mn_xSb and thermoelectric CoTi_{1-x}Sc_xSb Half-Heusler alloys. Journal of Alloys and Compounds, Vol. 650,25,728 (2015).

DS 15.6 Tue 11:15 H8

Electronic topological transition in epitaxially strained delafossite $PtCoO_2$ — •Markus E. Gruner[1,2], Ulrich Eckern[3], and Rossitza Pentcheva[2,1] — [1]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Technical University Munich — [2]Faculty of Physics and Center for Nanointegration, CENIDE, University of Duisburg-Essen — [3]Institute of Physics, University of Augsburg

The hexagonal delafossites $PdCoO_2$ and $PtCoO_2$ exhibit highly anisotropic transport properties including large negative values of the thermopower S_{zz} perpendicular to the hexagonal plane [1], which is of interest for thermoelectric energy conversion or sensor applications. By means of DFT calculations combined with semiempirical Boltzmann transport theory in the single relaxation time approximation we explore the effect of strain on the thermoelectric properties of both systems. We demonstrate that, despite their rather similar structural response, the isoelectronic compounds differ significantly in their transport behavior under tensile and compressive expitaxial strain [2]. This is related to specific changes of the Fermi surface involving an electronic topological transition, which occurs in $PtCoO_2$ at moderate compressive strain. Combining our first-principles results with available experimental data, we estimate a maximum ZT of 0.25 obtained for $PtCoO_2$ under $-4\,\%$ epitaxial strain. Funding by the DFG (TRR80) is gratefully acknowledged.
[1] K.P. Ong, D.J. Singh, P. Wu, Phys. Rev. Lett. 104, 176601 (2014)
[2] M.E. Gruner, U. Eckern, R. Pentcheva, arXiv:1511.09087

DS 15.7 Tue 11:30 H8

Optimized thermoelectric performance of n-type half-Heusler TiNiSn by addition and substitution with Mn — •Enkhtaivan Lkhagvasuren, Siham Ouardi, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Half-Heusler compounds have attracted considerable attention as high temperature thermoelectric materials. The state of the art n-type half-heusler compounds are based on TiNiSn. Key to their thermoelectric high efficiency is an intrinsic phase separation by Hf substitution. In the present study, the carrier concentration of the n-type half-heusler compound TiNiSn is optimized by addition and substitution of the low-cost Mn. The power factor is increased and the lattice thermal conductivity reduced with increasing Mn concentration.

DS 15.8 Tue 11:45 H8

Calculation of thermal conductivity across an interface using beam matching — •Debanjan Basu and Peter Bloechl — Institute for Theoretical Physics, Clausthal University of Technology

Designing efficient thermoelectric materials requires nanostructures with low thermal conductivity. Our goal is to study thermal transmission in multilayered structures on a mode-by-mode basis. This requires us to determine the “complex bandstructure”, which describes propagating as well as evanescent phonon modes inside each layer. We also describe how to extract the matching conditions from Newton’s equations of motion for the atoms at the interface between two layers.

This work is funded by the DFG Schwerpunktprogramme 1386.

DS 15.9 Tue 12:00 H8

Thermoelectric properties of half-Heusler heterostructures from ab initio calculations — •Peter Kratzer and Gregor Fiedler — Faculty of Physics, University Duisburg-Essen, 47048 Duisburg, Germany

Semiconducting half-Heusler alloys have recently emerged as a class of thermoelectric materials with outstanding performance in the medium-to-high-temperature range. Heterostructures promise further reduction of the thermal conductivity due to phonon scattering at interfaces. Here, both the electronic and phononic spectra of half-Heusler compounds based on Ti, Zr, and Hf are calculated using density functional theory (DFT). With this input, thermoelectric properties are obtained. We demonstrate how the thermal conductivity of a superlattice can be estimated in dependence on its period, by using the mean free path of phonons in bulk materials plus an extension of the diffuse mismatch model. The results are compared to experiment (PRB 92 (2015), 125436). Moreover, we demonstrate that, in a short-period superlattice, a high power factor may be retained, while the thermal conductivity is reduced compared to single-phase half-Heusler crystals.

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

Time: Tuesday 9:30–13:00 Location: H11

DS 16.1 Tue 9:30 H11

About the optical properties of $Li_xV_2O_5$ — •Marina Muñoz-Castro[1], Frank Berkemeier[1], and Guido Schmitz[2] — [1]Institute of Material Physics, University of Münster, Wilhelm-Klemm.Str.10, D-48149, Germany — [2]Institute of Material Science, University of Stuttgart, Heisenbergstr. 3, D-70569, Germany

This work investigates the influence of lithium intercalation on the optical properties of vanadium pentoxide films. V_2O_5 films with a thickness between 700 and 800 nm, were prepared by DC magnetron sputter deposition. Afterwards, cyclic voltammetry and chronopotentiometry were used to set different well defined lithiation states of the $Li_xV_2O_5$ films, between $x = 0$ and $x = 1$. The optical properties of these films were examined in the wavelength range between 500 and 1700 nm by optical reflectometry. From the reflectance data, the refractive index and the extinction coefficient of the films were calculated as a function of wavelength using Cauchy’s dispersion model. The results confirm that the optical behavior of $Li_xV_2O_5$ films varies upon lithium intercalation, and that these changes in the optical properties are completely reversible for low states of lithiation.

DS 16.2 Tue 9:45 H11

Ultrafast dynamics of coherent acoustic phonons in thin gold films investigated by surface plasmon resonance — •Felix Noll, Nico Krauss, and Thomas Dekorsy — Universität Konstanz, Fachbereich Physik, Konstanz, Germany

Coherent acoustic phonons are studied in pump-probe experiments with femtosecond temporal resolution and shot-noise limited detection sensitivity [1]. The measured photo-induced differential reflectivity change is expected to increase by several orders of magnitude when probing under surface plasmon resonance (SPR) condition [2].

In this work, high-speed asynchronous optical sampling is combined with SPR in Kretschmann geometry for highly sensitive pump-probe experiments on gold films with thicknesses ranging from 30 nm to 50 nm. Angular resolved transients yield parameters for optimum enhancement of the coherent acoustic phonons. The fundamental thickness oscillations and their higher harmonics are discussed with regard to frequency and damping time.

[1] Bartels, A. et al., Rev. Sci. Instrum. **78**, 035107 (2007)
[2] Wang, J. et al., Opt. Lett. **32**, 719-721 (2007)

DS 16.3 Tue 10:00 H11

The Effect of Layer Thickness on the Magnetic and Magneto-optical Properties of Sputtered and Annealed $La_{1-x}Sr_xMnO_3$ Thin Films on Silicon — •Manuel Monecke, Oana-Tereza Ciubotariu, Peter Richter, Patrick Thoma, Georgeta Salvan, and Dietrich R.T. Zahn — Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

$La_{1-x}Sr_xMnO_3$ (LSMO) is a conductive oxide with a perovskite crystal structure. Moreover, the high spin polarization makes this material an ideal electrode material for spintronic applications. In particular, the composition $La_{0.67}Sr_{0.33}MnO_3$ was used in spintronic devices due to the nearly 100 % spin polarization at the Fermi level [2]. Here LSMO films with varying film thicknesses between 10 nm and 300 nm were deposited by magnetron sputtering at room temperature on silicon substrates covered with a native oxide. The films were annealed in ambient atmosphere at 775 °C for 20 min, 1 h, 3 h, and

9 h. Afterwards the layers were investigated by spectroscopic ellipsometry, magneto-optical Kerr effect spectroscopy and magnetometry. The main goal of this work is to understand how the magnetic properties, the dielectric function, and the magneto-optical response of post deposition annealed LSMO are influenced by the layer thickness and annealing time. The results show that the magnitude of the off diagonal elements of the dielectric tensor decreases drastically when the layer thickness is smaller than 20 nm. Furthermore, the remanence and coercive field increase with annealing time for films thicker than 20 nm. [1] E. Dagotto *et al.* Physics Reports 344 (2001) [2] J.-H. Park *et al.* Nature Vol 392 (1998)

DS 16.4 Tue 10:15 H11

Resonance X-ray reflectivity — a tool to extract chemical and valence profiles and its application to SmB$_6$. — •Volodymyr Zabolotnyy[1], Katrin Fürsich[1], Robert Green[2], Abdul Tcakaev[1], Ronny Sutarto[3], Feizhou He[3], Maurits Haverkort[4], Dmytro Inosov[5], and Vladimir Hinkov[1] — [1]Universität Würzburg — [2]UBC, Vancouver, Canada — [3]CLS, Saskatoon, Canada — [4]MPI-CPS, Dresden — [5]TU Dresden

SmB$_6$ is a renowned example of a Kondo (mixed valent) insulator. The recently proposed topologically protected surface state upgraded SmB$_6$ to being likely the first topological Kondo insulator, and thus renewed interest in the material, particularly in the Sm^{2+} to Sm^{3+} ratio at the sample surface.

To address this question we combine cluster calculations, providing optical constants for different Sm valences, with x-ray reflectivity measurements — an established method for a non-destructive analysis of heterostructures with high probing depth ($\sim$100 nm) and element/valence sensitivity on a nm-scale. Here we report detailed atomic and valence profiles for *in situ* cleaved single crystals of SmB$_6$, which ensures clean surfaces with negligible traces of air-related contaminants. As the analysis of in-air prepared surfaces is known to be hampered by an uncontrolled built up of a contamination layer that may render reconstruction of chemical profiles very ambiguous, or even modify the surface via unwanted doping, etc., the well controlled surface chemistry proves to be a crucial aspect of the current study.

DS 16.5 Tue 10:30 H11

Surface anchored metal organic framework for direct light emission. — •Nicolò Baroni[1], Ian Howard[1], Andrey Trushtov[1], Redel Engelbert[2], Christof Wöll[2], and Bryce Sydney Richards[1,3] — [1]Institute of Microstructure Technology, Karlsruhe institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Institute of Functional Interfaces, Karlsruhe institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [3]Light Technology Institute, Karlsruhe Institute of Technology, Engesserstrasse 13, 76131 Karlsruhe, Germany

The control of light emission of luminescent molecules is an important goal in the field of luminescent solar concentrators (LSCs) in order to enhance the efficiency of total internal reflection (TIR). Porous metamaterials called surface anchored metal organic frameworks (SURMOFs) provide different kinds of pore sizes and different orientations in the channels that connect all the pores. Our aim is using SURMOFs as host materials for luminescent molecules in order to have loaded molecules aligned in the same direction as the channels.

DS 16.6 Tue 10:45 H11

Plasmonic Gold nanocross array for efficient solar to chemical energy conversion — •Wenxin Wang, Yan Zheng, and Yong Lei — Fachgebiet 3D-Nanostrukturierung, Institut für Physik, Technische Universität, Ilmenau, Germany

Large area plasmonic Au nanocross array with different size and height are fabricated by an novel anodic aluminum oxide (AAO) template in physical vapor deposition (PVD) for efficient solar water splitting. The optical prosperity of Gold nanocross is revealed by systematic experimental and computed extinction spectra. And their performance of solar water splitting is exhibited via photoelectrochemical (PEC) device.

DS 16.7 Tue 11:00 H11

Study of the properties of sputtered ZnO:Al layers on ultra-thin glass — •Jasper Westphalen[1,2], Manuela Junghähnel[1], and Edda Rädlein[2] — [1]Fraunhofer Institute for Organic Electronics, Electron Beam and Plasma Technology FEP — [2]Technische Universität Ilmenau

Ultra-thin glass is a new type of transparent and flexible substrate material. It is a glass with a thickness less than 200 μm. The many advantageous properties, such as the excellent barrier to water and oxygen and the temperature stability up to 700 °C open up new possibilities for transparent electronics, display technology and in photovoltaics. Transparent conductive oxide (TCO) can be used for different functional layers for these topics. As an alternative to the expensive indium doped tin oxide (ITO) aluminum doped zinc oxide ZnO:Al is already used in some devices. In this study, ZnO:Al films were deposited by magnetron sputtering on ultra-thin glass. The influence of the deposition power on the electrical, optical and mechanical properties of the films were investigated. In order to improve the optical and the electrical properties, we used flash lamp annealing (FLA) as a post-deposition annealing method for ultra-short thermal treatment in the millisecond range.

15 min. break.

DS 16.8 Tue 11:30 H11

Epitaxial growth of Fe on Ag(001) and magnetoelastic coupling in Fe — •Kenia Novakoski Fischer and Dirk Sander — Max Planck Institute of Microstructure Physics, Halle, Germany

Epitaxial atomic layers are often in a strain-state, which is determined by the lattice misfit to the substrate. This misfit contributes significantly to the magnetic anisotropy via magnetoelastic coupling. The magnetoelastic coupling coefficients are experimentally accessible from measurements of the stress change of the layers upon a magnetization reorientation [1]. In this work, we present results on the film stress and magnetoelastic stress for 4 to 30 layers of Fe on Ag(001). Our measurements of film stress show a non-monotonic stress change in the first layers, which indicates a deviation from an atomically sharp Ag-Fe interface. We measure an average film stress of 2 GPa, in qualitative agreement with lattice misfit stress. From our Auger measurements, even for 30 ML thick Fe films, we conclude that a few layers of Ag are on top of the Fe film. We measured the magnetoelastic coupling coefficient B2 from an in-plane reorientation of the magnetization along <110> directions of Fe, and we find +4.2, +3.1, +2.7, and +3.7 MJ/m^3 for films of 4, 8, 15, and 30 layers, respectively. These values differ from the respective bulk value of +7.83 MJ/m^3[2], and we discuss the results in view of the segregation of Ag and stress in the Fe films.

[1] Sander D. and Kirschner J., Phys. Status Solidi B 248, 2389, (2011).

[2] Sander D., Rep. Prog. Phys. 62, 809 (1999).

DS 16.9 Tue 11:45 H11

Material parameter determination for ScAlN sputtered layers — •Nicolas Kurz[1,2], Mohammadfazel Parsapourkolour[3], Paul Muralt[3], Yuan Lu[2], Agne Zukauskaite[2], Ulrike Roesler[4], Pascal Nicolay[5], Vadim Lebedev[1,2], and Oliver Ambacher[1,2] — [1]Department of Microsystems Engineering IMTEK, University of Freiburg, Freiburg, Germany — [2]Fraunhofer Institute for Applied Solid State Physics IAF, Freiburg, Germany — [3]Ceramics Laboratory, Ecole Polytechnique Fédérale de Lausanne EPFL, Lausanne, Switzerland — [4]EPCOS AG, Munich, Germany — [5]CTR AG,Villach , Austria

Microelectromechanical systems operating at radio-frequencies (RF) provide excellent properties for RF front end devices like reference oscillators, filters, and duplexer. Today, AlN is commonly used as piezoelectric material for these devices since it provides low acoustic and dielectric losses, and is compatible with CMOS fabrication technology. However, AlN piezoelectric coefficient d33~6 pC/N, and consequently, electromechanical coupling coefficient of ~7 %, limit the available bandwidth for RF components. Akiyama, et al. showed experimentally that the d33 can be increased up to 400 % by alloying AlN with ScN.

In order to determine selected tensor components for AlScN material constants, a set of test resonators have been modeled in this work using finite element method. Based on these results, four different resonator structures operating in different modes were selected for fabrication and characterization by S-parameter analyses and laser Doppler vibrometry. A comparison between model prediction and experimentally obtained results for AlN and AlScN will be presented.

DS 16.10 Tue 12:00 H11

Reactive magnetron sputtering of stress-controlled piezoelectric AlScN thin films — •Yuan Lu[1], Markus Reusch[1,2], Tim Christoph[1], Vadim Lebedev[1], Nicolas Kurz[1,2], Lutz Kirste[1], Oliver Ambacher[1,2], and Agne Zukauskaite[1] — [1]Fraunhofer Institute for Applied Solid State Physics IAF, Tullastr. 72, 79108 Freiburg, Germany — [2]IMTEK, University of Freiburg, Georges-Köhler-Allee 103, 79110 Freiburg, Germany

AlN is a dominant choice for radio frequency microelectromechanical systems (RF-MEMS) used in mobile telecommunications. However, AlN's relatively low piezoelectric response ($d_{33}\approx 6$ pC/N) and electromechanical coupling ($k_t^2\approx 7\%$) limit the bandwidth of the frequency filters. It was recently shown that AlScN has 400% higher $d_{33}=27.6$ pC/N (for $Al_{0.43}Sc_{0.57}N$) and $k_t^2\approx 10$-15%, making this material a very promising alternative to AlN. In addition to piezoelectric properties, parameters such as film stress need to be controlled to fabricate high performance AlScN-based piezoelectric devices. The aim of this work is to synthesize stress-controlled AlScN thin films suitable for RF-MEMS applications. Reactive RF magnetron sputtering with an $Al_{0.83}Sc_{0.17}N$ alloy target is used to produce 250-1000 nm thick AlScN films on Si(100) substrates. Film stress is investigated by wafer geometry measurements, the clamped d_{33} is measured by Berlincourt method, and the film quality is evaluated by using X-ray diffraction. Piezoresponse force microscopy is used to confirm the piezoelectric phase uniformity. The growth process optimization leading to the AlScN films with moderate stress values (<500 MPa) will be discussed.

DS 16.11 Tue 12:15 H11

Vibrational modes of ultrathin carbon nanomembrane mechanical resonators — •Xianghui Zhang[1], Reimar Waitz[2], Fan Yang[2], Carolin Lutz[2], Polina Angelova[1], Armin Gölzhäuser[1], and Elke Scheer[2] — [1]Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany — [2]Fachbereich für Physik, Universität Konstanz, 78457 Konstanz, Germany

We report measurements of vibrational mode shapes of mechanical resonators made from ultrathin carbon nanomembranes (CNMs) with a thickness of approximately 1 nm. CNMs are prepared from electron irradiation induced cross-linking of aromatic self-assembled monolayers (SAMs) and the variation of membrane thickness and/or density can be achieved by varying the precursor molecule. The vibration of the membrane was actuated by applying a sinusoidal voltage to a piezoelectric disk on which the sample was glued. The vibrational mode shapes were visualized with an imaging Mirau interferometer using a stroboscopic light source. Several degenerate normal modes of a square membrane can be readily identified and their dynamic behavior can be well described by linear response theory of a membrane with negligible bending rigidity. Applying Fourier transformations to the time-dependent surface profiles, the dispersion relation of the transverse membrane waves can be obtained and its linear behavior confirms the membrane model. Comparing the dispersion relation to an analytical model, the static stress of the membranes was determined and found to be caused by the fabrication process.

DS 16.12 Tue 12:30 H11

High-temperature micro-mechanical testing of a thin-film CrN tooling system — •James P Best[1], Johannes Zechner[2], Jeffrey M Wheeler[3], Juri Wehrs[1], Marcus Morstein[4], and Johann Michler[1] — [1]EMPA, Thun, Switzerland — [2]KAI GmbH, Villach, Austria — [3]ETH, Zürich, Switzerland — [4]PLATIT AG, Selzach, Switzerland

Forging and cutting tools for high-temperature applications are often protected using hard nanostructured ceramic coatings. While a moderate amount of knowledge exists for material properties at room temperatures, significantly less is known about the system constituents at the elevated temperatures generated during service.

In this work, we present results on both the hard ceramic coating and the nitrided steel substrate using in situ micro-mechanical measurements at temperatures to 500 °C. FIB milled micro-pillars of plasma-nitrided tool steel were first investigated using in situ compression experiments. It was found that elevated temperature led to significant and reversible softening of the nitrided steel and transition from slip-based to more ductile plastic flow.

The fracture toughness behavior was then investigated using various micro-geometries and notching parameters. Toughness measurements at high temperatures highlighted the profound effect of the notching ion during small-scale fracture measurements. It was found that gallium ion implantation led to significant toughening of CrN, based on gallium dosage experiments and alternative notching using both xenon and helium sources.

DS 16.13 Tue 12:45 H11

Structural and optical properties of TiO2-films with thicknesses from 2 to 200 nm deposited with RF-diode sputtering — Jingyi Shi, •Sebastian Schippreit, Klaus Pärschke, and Dieter Mergel — Thin Film Technology Group, Faculty of Physics, University of Duisburg-Essen

TiO2-films with thicknesses from 2 nm to 200 nm have been produced by rf-diode sputtering at various temperatures and their structural and optical properties have been studied. The optical properties of the films were obtained by simulation of their (NIR/UV/VIS) optical spectra with the computer program SCOUT. The films already show optical effects (absorptive and ellipsometric) at a thickness of 2 nm and the simulated film thicknesses suite well to the mechanically obtained values. Structural analysis was performed using X-ray diffraction, Raman spectroscopy and scanning electron microscopy. A phase change occurred in the TiO2-films from mainly rutile to a mixed rutile-anatase phase with increasing substrate temperature as well as with increasing film thickness.

DS 17: 2D Materials: Structure and Electronic Properties (Joint session of DS and O, organized by O)

Time: Tuesday 10:30–13:00 Location: H24

DS 17.1 Tue 10:30 H24

Structural and electronic properties of epitaxial multilayer *h*-BN on Ni(111) — Alexander Tonkikh[1], Elena Voloshina[2], Peter Werner[1], Horst Blumtritt[1], Boris Senkovskiy[3], Gernot Güntherodt[1,4], Stuart Parkin[1], and •Yuriy Dedkov[5,6] — [1]MPI Halle (Saale), Germany — [2]HU Belin, Germany — [3]TU Dresden, Germany — [4]RWTH Aachen, Germany — [5]SPECS GmbH, Germany — [6]IHP Frankfurt (Oder), Germany

Hexagonal boron nitride (*h*-BN) is a promising material for implementation in spintronics due to a large band gap, low spin-orbit coupling, and a small lattice mismatch to graphene and to close-packed surfaces of fcc-Ni(111) and hcp-Co(0001). Epitaxial deposition of *h*-BN on ferromagnetic metals is aimed at small interface scattering of charge and spin carriers. We report on the controlled growth of *h*-BN/Ni(111) by means of molecular beam epitaxy (MBE). Structural and electronic properties of this system are investigated using cross-section transmission electron microscopy (TEM) and electron spectroscopies which confirm good agreement with the properties of bulk *h*-BN. The latter are also corroborated by density functional theory (DFT) calculations, revealing that the first *h*-BN layer at the interface to Ni is metallic. Our investigations demonstrate that MBE is a promising, versatile alternative to both the exfoliation approach and chemical vapour deposition of *h*-BN.

DS 17.2 Tue 10:45 H24

Structural, thermodynamic and electronic properties of two-dimensional SiC, SiGe, and GeC alloys — Ivan Guilhon[1], Friedhelm Bechstedt[2], •Ronaldo Rodrigues Pela[1,3], Marcelo Marques[1], and Lara Kuhl Teles[1] — [1]Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Jena, Germany — [3]Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

We investigate structural, thermodynamic, electronic properties of 2D binary alloys made from graphene, silicene and germanene by means of density functional theory calculations and a statistical method that accounts for disorder and compositional effects. The GGA-1/2 method [1] is used in electronic properties calculations to approximately include quasiparticle corrections. $Si_{1-x}Ge_x$ is the only stable alloy at usual growth temperatures. In $Ge_{1-x}C_x$, strong distortions of the

lattice lead to a pronounced tendency for phase separation. $\mathrm{Si}_{1-x}\mathrm{C}_x$ presents an ordered structure with composition $x = 0.5$ stable up to $T \approx 1000$ K. While $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ and $\mathrm{Ge}_{1-x}\mathrm{C}_x$ are found to have vanishing band gaps, $\mathrm{Si}_{1-x}\mathrm{C}_x$ has, around $x = 0.5$, an appreciable band gap, which decreases exponentially with the growth temperature from ~ 2.2 eV at 300 K to ~ 1.2 eV at 900 K [2].
[1]: Phys. Rev. B 78, 125116 (2008); [2]: Phys. Rev. B 92, 075435 (2015).
Acknowledgments: “Conselho Nacional de Desenvolvimento Científico e Tecnológico” (CNPq), “Coordenação de Aperfeiçoamento de Pessoal de Nível Superior” (CAPES) and “Alexander von Humboldt Stiftung”.

DS 17.3 Tue 11:00 H24

Unoccupied states in silicene nanoribbons on Ag(110) — •Nils Fabian Kleimeier, Luca Bignardi, and Helmut Zacharias — Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Unoccupied electronic states of silicene nanoribbons grown on Ag(110) were measured by inverse photoemission (IPE) in ultra-high vacuum conditions. The IPE setup consisted of a modified Erdmann-Zipf electron gun and an acetone filled Geiger-Müller tube with a CaF2 window acting as a bandpass filter. Three individual unoccupied states can be distinguished at 0.3, 0.9 and 1.4 eV above the Fermi level. To investigate occupied states of the nanoribbons, two-photon photoemission at a photon energy of $h\nu = 3.15\,\mathrm{eV}$ was employed. Occupied states associated with the nanoribbons were only visible in spectra excited with p-polarized light. Electron dynamics of the lowest unoccupied state of the nanoribbons at $E - E_F = 0.3\,\mathrm{eV}$ were measured by time-resolved three-photon photoemission at the same photon energy. The lifetime of the state was determined to $\tau = 20\,\mathrm{fs}$.

DS 17.4 Tue 11:15 H24

Absence of Dirac cones in monolayer silicene and multilayer Si films on Ag(111) — •Paolo Moras[1], Sanjoy K. Mahatha[1], Polina M. Sheverdyaeva[1], Valerio Bellini[1,2], Claudia Struzzi[3], Luca Petaccia[3], Tevfik O. Mentes[3], Andrea Locatelli[3], Roberto Flammini[4], Karsten Horn[5], and Carlo Carbone[1] — [1]Istituto di Struttura della Materia - CNR, Trieste, Italy — [2]Istituto di Nanoscienze - CNR, Modena, Italy — [3]Elettra Sincrotrone Trieste, Trieste, Italy — [4]Istituto di Struttura della Materia - CNR, Roma, Italy — [5]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Monolayer silicene and multilayer silicon films on Ag(111) have been subject of many investigations within the last few years. For both systems, photoemission data have been interpreted in terms of linearly dispersing bands giving rise to the characteristic *Dirac cone* feature in the valence band. Here we show, on the basis of angle-resolved photoemission data and ab-initio calculations [1,2] that this assignment is not correct. In monolayer silicene the *Dirac cone* feature is caused by an Ag-derived interface state, while multilayer Si films exhibit a clear diamond-like structure and bulk-like Si bands. These results question the validity of the claim that graphene-like 2-D silicon and silicene multilayers are in fact formed on Ag(111).

[1] P. Moras et al., J. Phys.: Condens. Matter 26, 185001 (2014).
[2] S. K. Mahatha et al., Phys. Rev. B 89, 201416(R) (2014).

DS 17.5 Tue 11:30 H24

Low energy electron diffraction and angle resolved photoemission studies of Sn/Au(111) reconstructed surfaces — •Mahalingam Maniraj[1], Sebastian Emmerich[1], Dominik Jungkenn[1], Sebastian Jakobs[1], Benjamin Stadtmüller[1], Mirko Cinchetti[1], Stefan Mathias[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Recent experimental realization of Stanene, a two dimensional allotrope of Sn in a graphene-like structure, has motivated intense research on related Sn based ultrathin materials. We have investigated the growth of Sn on Au(111). Using low energy electron diffraction (LEED) and angle-resolved photoemission spectroscopy, we found five surface reconstructions, each with a distinct band structure. Starting from a coverage of 0.3 monolayers, Sn forms a $(\sqrt{3} \times \sqrt{3})\mathrm{R}30^\circ$ surface alloy which transforms into a complex superstructure for higher Sn coverages. An angle-resolved photoemission study shows inverted V-shaped bands which are symmetrically centered at the Gamma-point. Additionally, we observed states with parabolic dispersion showing a Rashba-type spin splitting. A direct comparison between our experimental results and band structure calculations will allow us to discuss the formation of Stanene-like band dispersions for these Sn/Au reconstructed surfaces.

DS 17.6 Tue 11:45 H24

Molecular interactions to control characteristics of transition metal dichalcogenide based atomically thin field effect devices — •Antony George[1], Sina Najmaei[2], Andreas Winter[1], Zian Tang[1], David Kaiser[1], Uwe Hübner[3], Pulickel Ajayan[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, 07743 Jena — [2]Department of Materials Science and Nano Engineering, Rice University, Houston — [3]Leibniz Institute of Photonic Technology, 07702 Jena

Atomically thin field effect transistors (FET) based on monolayer transition metal dichalcogenides have been attracted an immense research interest recently due to their application potential in ultrathin, lightweight transparent device technology. Here we discuss the possibility to tailor the characteristics of monolayer molybdenum disulphide (MoS2) based FET devices using molecular interactions. We have used self-assembled monolayers (SAMs) to control the surface chemistry of the interface between the semiconducting channel and the gate oxide [1]. Therewith such device parameters like mobility, threshold voltage, carrier density can be tuned. We further extend this concept to the development of FETs, which can be tuned by optically switchable molecules. To this end, we fabricated van der Waals heterostructures using MoS2 and carbon nanomembrane (CNM) [2] functionalized with optically switchable molecules. These devices can have different operational modes depending on the type of molecular switching which is triggered by external optical stimulation. [1] Nano Letters 14, 1354 (2014) [2] Prog. Surf. Sci. 87, 108 (2012)

DS 17.7 Tue 12:00 H24

Spatial conductivity mapping of unprotected and capped black phosphorus using microwave microscopy — Pieter J. de Visser[1,2], Rebekah Chua[1,3], Joshua O. Island[1], Matvey Finkel[1,4], Allard J. Katan[1], •Holger Thierschmann[1], Herre S.J. van der Zant[1], and Teun M. Klapwijk[1,4] — [1]Kavli Insitute of Nanoscience, Faculty of Applied Sciences, Delft University of Technology, The Netherlands — [2]Department of Quantum Matter Physics, University of Geneva, Switzerland — [3]Department of Physics, National University of Singapore, Singapore — [4]Physics Department, Moscow State Pedagogical University, Russia

Within the family of 2D materials thin flakes of black Phosphorus (bP) play a special role due to their tuneable direct bandgap and high carrier mobilities. Under ambient conditions, however, degradation changes the electronic properties of bP dramatically within hours [1]. Hence, applying protection measures is essential. We compare different protecting layers by measuring the local conductivity of bP flakes over time with scanning microwave impedance microscopy (sMIM). This novel AFM-based technique [2] probes the local sheet resistance with high spatial resolution and even for buried layers. For a bare bP flake we observe drastic changes in conductivity within 24 h. Coverage with 10 nm of HfOx delays degradation. The bP flake is stable for more than a week. Boron Nitride flakes appear to be less effective as a protection. sMIM reveals that here degradation starts at the edges and evolves over days, indicating a diffusive process. [1] Island J O, et al. 2DMat 2, 011002 (2015). [2] K. Lai, et al. Rev Sci Inst 79, 063703 (2008).

DS 17.8 Tue 12:15 H24

Coulomb interaction in transition metal dichalcogenides: effects on many-body instabilities — •Gunnar Schönhoff[1,2], Malte Rösner[1,2], Stephan Haas[3], and Tim Oliver Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany — [3]Department of Physics and Astronomy, University of Southern California, Los Angeles, CA 90089-0484, USA

We develop a material realistic, microscopic model to describe the Coulomb interaction in a TMDC monolayer, focussing on molybdenum disulfide under electron doping. Starting from ab initio Coulomb interaction for the undoped system, we calculate values for the screened matrix elements in real space and see how the interaction becomes more localized with doping. Additionally, we obtain the doping dependend electron-phonon matrix elements and observe a Charge Density Wave instability at high doping.

To quantify the influence of the Coulomb interaction on the superconducting phase, we calculate the Morel-Anderson coefficient μ^*. In contrast to the frequent use of μ^* as a fit parameter or a constant, this leads to a decrease of μ^* with electron doping from 0.25 to 0.1. The influence of the Coulomb interaction turns out to be most important at the boundary between the metallic and the superconducting phase where it delays the phase transition. We argue that the character of the superconducting phase in MoS_2 is phononic.

DS 17.9 Tue 12:30 H24

The electronic structure of a 2D MoS_2-WSe_2 heterojunction investigated with photoemission spectroscopy — •Mathias Gehlmann[1], Markus Eschbach[1], Pika Gospodaric[1], Ewa Mlynczak[1], Sven Döring[1], Philipp Nagler[2], Tobias Korn[2], Christian Schüller[2], Slavomír Nemšák[1], Lukasz Plucinski[1], and Claus M. Schneider[1] — [1]Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Department of Physics, University of Regensburg, D-93040 Regensburg, Germany

Heterostructures built from van der Waals materials are considered excellent candidates for next generation electronic devices that could overcome the restrictions of classical, Si-based electronics. The weak interlayer interaction in such heterostructures leaves the electronic properties of their building blocks largely intact. Nevertheless, by combining the two different transition metal dichalcogenides (TMDCs) MoS_2 and WSe_2, we produced a two-dimensional p-n junction, with drastically different optical and transport properties compared to the isolated TMDC monolayers and studied the influence of the interlayer coupling on the electronic structure in this novel, two-dimensional heterojunction.

By using photoemission spectroscopy we investigated the band alignment in the two materials. In order to directly observe the electronic band dispersion from micrometer-size flakes we performed k-space microscopy employing a photoemission microscope in angular resolved mode.

DS 17.10 Tue 12:45 H24

Superconductivity in the ferecrystals $(PbSe)_{1.14}(NbSe_2)_n$ — •Corinna Grosse[1], Matti B. Alemayehu[2], Matthias Falmbigl[2], Olivio Chiatti[1], David C. Johnson[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Department of Chemistry, University of Oregon, Eugene, OR, 97401, USA

The ferecrystals $(PbSe)_{1.14}(NbSe_2)_n$ are artificially layered materials consisting of n $NbSe_2$ single-layers stacked alternately with atomic double layers of PbSe. $NbSe_2$ is a transition metal dichalcogenide with interesting electrical properties such as superconductivity and charge density waves. The influence of turbostratic disorder, a random rotation between the $NbSe_2$ and PbSe layers, on the superconducting transition temperature has been unknown so far.

We investigate the structural and temperature-dependent electrical properties of the ferecrystals $(PbSe)_{1.14}(NbSe_2)_n$ by means of scanning transmission electron microscopy, X-ray diffraction, in-plane resistivity and Hall measurements and compare them to those of analogous non-disordered misfit layer compound (MLC) polymorphs. We observe a superconducting transition in the resistivity of the ferecrystals. The transition temperatures are reduced by up to 55 % with respect to the analogous MLC polymorphs. This indicates that turbostratic disorder substantially weakens the electron-phonon coupling in $(PbSe)_{1.14}(NbSe_2)_n$. We discuss the results of the structural and electrical properties of the ferecrystals with respect to their MLC analogues and also with respect to ultra-thin $NbSe_2$ layers.

DS 18: 1D Metal Wires on Semiconductors I (Joint session of DS and O, organized by O)

Time: Tuesday 10:30–13:15 Location: S052

DS 18.1 Tue 10:30 S052

One dimensional plasmons in Si(hhk)-Au — •Timo Lichtenstein[1], Marvin Detert[1], Julian Aulbach[2], Jörg Schäfer[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Physikalisches Institut and RCCM, Universität Würzburg

For future plasmonic devices the understanding of low dimensional collective excitations is indispensable. For quasi one dimensional (1d) structures Au induced wires on regularly stepped Si(hhk) offer the perfect playground. Therefore, Si(553) and Si(775) were prepared at coverages where both surfaces host a double atomic gold chain per terrace. The wire quality was checked with spot profile analysis in low energy electron diffraction (SPA-LEED). A combination of an electron energy loss spectrometer and SPA-LEED providing both high energy and momentum resolution gave access to the plasmon dispersion.

Although 1d metallicity is observed, the plasmon dispersion strongly depends on a two-dimensional crossover: on the lateral distribution of the 1d electron density of states (DOS) within one terrace (intrawire correlation), as well as on the spacing of the wires (interwire correlation). This can quantitatively be described by a modified plasmon model for a wire array. We obtained effective widths of 7.5 Å for Si(553)-Au and 10.2 Å for Si(775)-Au, which are considerably smaller than the terrace widths. A modulated DOS of comparable width can also be seen by tunneling spectroscopy. These effective widths seem to be influenced both by the structural motif, i.e. single or double chain, as well as by the terrace size.

DS 18.2 Tue 10:45 S052

Impurity-mediated early charge density wave condensation in the oxygen-adsorbed In/Si(111)-(4x1)/(8x2) nanowire array — •Stefan Wippermann[1], Andreas Lücke[2], Wolf Gero Schmidt[2], Deok Mahn Oh[3], and Han Woong Yeom[3] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf — [2]Universität Paderborn, Germany — [3]Pohang University, South Korea

The self-assembled In/Si(111)-(4x1) nanowire array is an extremely popular model system for one-dimensional electronic systems and features a reversible temperature-induced phase transition into a charge density wave (CDW) ordered ground state. While impurities have been widely known to affect this phase transition, the atomistic mechanisms have rarely been elucidated. Here we present a joint experimental and first principles study, demonstrating oxygen impurity atoms to condense the In/Si(111) nanowire array locally into its CDW ground state, even above the transition temperature. Interestingly, CDW ordering is induced only by a concerted effect of multiple impurities. The mechanism is explained as a subtle interplay between coherent superposition of local impurity-induced lattice strain, a strong coupling between electronic and lattice degrees of freedom, and phononic effects on the free energy. Funding from DFG FOR1700 is gratefully acknowledged.

Invited Talk DS 18.3 Tue 11:00 S052

Taking Nanoscience to the Edge – The Different Appearances of One-Dimensional Physics — •Jörg Schäfer — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, 97074 Würzburg, Germany

The technologies to fabricate nanostructures on surfaces with atomic precision have become very elaborate, making it possible to play with low-dimensional physical phenomena: among these, approaches to the one-dimensional (1D) world offer a particularly rich arena. What can we expect here? With the lack of effective screening, and in the presence of quasi-1D electron states that promote particular scattering vectors, these systems become susceptible to symmetry-breaking ground states. Idealized examples include, e.g., Peierls instabilities or magnetic ordering – while in real-word systems these phenomena may be far more complex.

The study of such quasi-1D systems on semiconductor surfaces, i.e., atomic wires, has made tremendous progress in the last years. In my talk I will review some of the most interesting realizations. Specifically, I will address the scenarios encountered for multi-band metallic chains with strong spin-orbit coupling, and their tunability. Moreover, as a recent development, we will turn to the step edges of terraced substrates with honeycomb chains, that show strong indications for spin polarization and long-range magnetic ordering. Such setup has intriguing connections to honeycomb topological insulators, predicted to have 1D edge states. The talk will look at this developing field from an overview perspective.

DS 18.4 Tue 11:30 S052

Surface vibrational Raman modes of In/Si(111)-(4x1) and (8x2) nanowires — •Stefan Wippermann[1], Wolf Gero Schmidt[2], Eugen Speiser[3], and Norbert Esser[3] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf — [2]Universität Paderborn, Germany — [3]ISAS Berlin, Germany

The ordered array of atomic-scale In nanowires that self-assembles on the Si(111) surface is a prototypical model system for one-dimensional (1D) electronic systems. It exhibits a Peierls-like instability, inducing a reversible phase transition from the metallic (4x1) phase into the insulating (8x2) ground state at $T_C = 120$ K. The detailed nature and mechanism of this metal-insulator (MI) transition is still discussed controversially. We performed a joint *first principles* and surface vibrational Raman spectroscopy study of the In/Si(111)-(4x1)/(8x2) surfaces' vibrational properties. The measured phonons are assigned to characteristic modes of the quasi-1D In nanowires, employing density functional theory calculations and symmetry considerations. Both the (4x1) and (8x2) phases exhibit a distinct set of phonon modes. The observed strong modifications in the Raman spectra of the (8x2) phase are consistent with a symmetric quadrupling of the surface elementary cell and confirm characteristic structural changes at the surface. Funding from DFG FOR1700 is gratefully acknowledged.

DS 18.5 Tue 11:45 S052

Spin correlations in the Si(553)-Au nanowire system — •B. Hafke[1], T. Frigge[1], B. Krenzer[1], J. Aulbach[2], R. Claessen[2], J. Schaeffer[2], and M. Horn-von Hoegen[1] — [1]Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — [2]Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), 97074 Würzburg

To study the microscopic mechanism of formation, stabilization, and interaction in low dimensional systems we used Si(553) as vicinal surface to enforce the nucleation of Au into one dimensional wires. Deposition of 0.5 ML Au results in the formation of one pair of 1D Au atomic chains per Si terrace exhibiting a twofold periodicity. These metallic wires are structurally terminated by Si step edge atoms, which show a threefold periodicity of the Si atoms along the rows. Theory predicts an antiferromagnetic spin ordering of every third Si step edge atom [1]. The long-range interaction of the twofold and threefold periodicity is investigated by spot-profile analysis in SPA-LEED at a sample temperature of 80 K. The strict twofold periodicity of the Au atoms is not correlated between adjacent wires. In contrast the threefold ordering of the Si spins exhibit a clear short range order perpendicular to the Au wires. Both results support the structure model where the interrow correlation is mediated by the spin-spin interaction of adjacent Si step edge atoms.

[1] S. C. Erwin and F. J. Himpsel, Nature Commun. 1, 58 (2010).

DS 18.6 Tue 12:00 S052

Interwire coupling of In(4×1) reconstruction probed by transport measurements — •Ilio Miccoli[1], Frederik Edler[1], Stephanie Demuth[1], Herbert Pfnür[1], Stephan Wippermann[2], Andreas Lücke[3], Wolf G. Schmidt[3], and Christoph Tegenkamp[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Grenzflächenchemie und Oberflächenphysik, Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [3]Lehrstuhl für Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany

The In(4×1)/Si(111) reconstruction is used as a prototype for the understanding of 1D systems of atomic chains. It shows strong anisotropic transport properties and a temperature driven metal-insulator transition. Although being intensively studied for more than one decade the effect of defects induced by adsorption (e.g. O_2, H_2) are still under current debate. A better understanding of the influence of defects and a correlation with transport measurements can be achieved by a spatial constriction of the electron path. This restriction was realized by optical ex-situ lithography with reactive ion etching. We report a systematic investigation of the confinement effects using a 4-tip STM/SEM system. Moreover, O_2 adsorption dependent transport studies show not only a reduction of conductivity along the direction of atomic chains but also a decrease in the perpendicular. This was not reported before and reveals an effective interwire coupling between the chains, which is in agreement with recent DFT calculations.

DS 18.7 Tue 12:15 S052

Phase transition of In-Si(111) (4x1)- (8x2) nanowires in a new light — •Eugen Speiser[1], Stefan Wippermann[2], Simone Sanna[3], Wolf Gero Schmidt[3], Sandhya Chandola[1], and Norbert Esser[1] — [1]ISAS e.V., Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [3]Lehrstuhl für Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany

Although recognized as a model case for atomic metallic nanowires, the (4x1)-(8x2) phase transition continues to hide behind the complexity of the structure and electronical properties. In cooperation with continuously developing theoretical methods a variety of conventional and newly developed experimental surface investigation methods are actively applied to elucidate the underlying mechanism of the phase transition. Our approach to this problem is the joint work of calculations and measurements of the low energy surface vibrations localized in the top layer. Successful assignment of calculated vibrational patterns and frequencies to measurements of both the insulating (8x2) and metallic (4x1) phases, is a necessary requirement to understand the dynamics of each phase. Based on this knowledge an interpretation of temperature dependency of phonon frequencies near the phase transition will be given in terms of participation of the electron phonon coupling to the phase transition mechanism. Coupling parameters between phonons and electrons can be estimated from an empirical model based on Landau-Ginsberg theory, as already verified in 1D like bulk materials, eg. blue bronze.

DS 18.8 Tue 12:30 S052

Dynamic Ginzburg-Landau theory for the Peierls transition in In/Si(111) — •Yasemin Ergün and Eric Jeckelmann — Leibniz Universität Hannover, Germany

We investigate thermal fluctuations and collective excitations in quasi-one-dimensional charge-density-wave systems using the Ginzburg-Landau (GL) theory. Starting from a microscopic Su-Schrieffer-Heeger-like model for In/Si(111), we generalized the GL theory for grand canonical Peierls transitions. The equilibrium properties and the non-equilibrium dynamics are simulated using the Langevin approach. We discuss our theoretical results in relation to doping and spectroscopy experiments for In/Si(111). Support from the DFG through the Research Unit FOR 1700 is gratefully acknowledged.

DS 18.9 Tue 12:45 S052

Beyond thermal equilibrium: ultrafast non-thermal melting of a surface CDW in the In/Si(111) atomic-wire system — •Tim Frigge, Bernd Hafke, Tobias Witte, Boris Krenzer, and Michael Horn-von Hoegen — Department of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

The wire-type arrangement of Indium atoms on a Silicon(111) surface serves as a famous prototype for the formation of a quasi one-dimensional charge density wave groundstate. We used time-resolved electron diffraction in surface-sensitive geometry to investigate the transient non-equilibrium dynamics of the impulsively driven (8x2)→(4x1) phase transition. Optical excitation of the (8x2) groundstate with fs-laser pulses revealed the existence of a metastable, supercooled (4x1) excited state at 30 K. This phase survives for hundreds of picoseconds because the recovery of the (8x2) phase is hindered due to an energy barrier of 40 meV. At fluences of 3-7 mJ/cm^2 the CDW groundstate is lifted and the structure changes within 350 fs. This photoinduced transition can not be explained by a simple thermal excitation scenario because laser induced heating takes place on timescales 6 times longer. Instead, we explain the observed dynamics through an accelerated displacive excitation scenario upon changes of the potential energy landscape. This also explains the observation of an increase of the excitation time constant towards lower fluences below 3 mJ/cm^2.

DS 18.10 Tue 13:00 S052

Atomistic Mechanism and Dynamics of the Optically Induced In/Si (111) (8x2)-(4x1) Phase Transition — •Andreas Lücke[1], Simone Sanna[1], Uwe Gerstmann[1], Stefan Wippermann[2], and Wolf Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany — [2]Interface Chemistry and Surface Engineering Department Max-Planck-Institute for Iron Research GmbH, 40237 Düsseldorf, Germany

The In-Si(111)(8x2)/(4x1) nanowire array features a Peierls instability-driven phase transition, the mechanism of which has been controversial since its discovery, cf. Ref. [1-3]. Experimentally it has been shown that the insulating (8x2) phase undergoes a phase transition towards the metallic (4x1) phase upon optical excitation far below the critical temperature [4]. Here we rationalize this finding by means of ab-initio total-energy and electronic-structure calculations and provide atomistic insight into the driving force and the dynamics of the optically driven phase transition by performing molecular dynamics simulations on excited-state potential energy surfaces. In particular we relate the phase transition to the population/depopulation of specific surface bonds that excite soft phonon modes. Our results rationalize recent findings from ultra-fast time-resolved electron diffraction.

1. H. W. Yeom, et al. Phys. Rev. Lett. 82, 4898 (1999).
2. J. R. Ahn, et al. Phys. Rev. Lett. 93, 106401 (2004).
3. S. Wippermann, et al., Phys. Rev. Lett. 105, 126102 (2010).
4. S. Wall et al., Phys. Rev. Lett. 109, 186101 (2012).

DS 19: Hybrid and Perovskite Photovoltaics II (Joint session of CPP, DS and HL, organized by CPP)

Time: Tuesday 10:45–13:00 Location: H37

DS 19.1 Tue 10:45 H37

Charge Carrier Recombination Dynamics in Perovskite and Polymer Solar Cells probed by Time-Delayed Collection Field (TDCF) Experiments — •Andreas Paulke[1], Samuel D. Stranks[2], Juliane Kniepert[1], Jona Kupiers[1], Christian M. Wolff[1], Natalie Schön[1], Henry J. Snaith[2], Thomas J.K. Brenner[1], and Dieter Neher[1] — [1]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str.24-25, 14476 Potsdam — [2]Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, United Kingdom

Time-Delayed Collection Field (TDCF) experiments are applied to organometal halide perovskite ($CH_3NH_3PbI_3$) based solar cells to investigate charge carrier recombination in a working solar cell at the nanosecond to microsecond timescale. Planar perovskite solar cells ($ITO/PEDOT : PSS/Perovskite/PCBM/C_{60}/BCP/Al$) display a second-order recombination process with a slow-down of the apparent recombination coefficient over several tens of nanoseconds. In contrast, recombination in the $ITO/TiO_2/mesoporous - TiO_2/Perovskite/Spiro-OMeTAD/Au$ device is governed by a slow first order process, but again with an apparent time-dependence of the recombination coefficient. We also conclude that organometal halide perovskite solar cells differ significantly from prototypical organic bulk heterojunction devices with regard to the mechanism and time-scale of free carrier recombination.

DS 19.2 Tue 11:00 H37

Recombination of photogenerated charge carriers in planar methylammonium lead halide perovskite solar cells — •David Kiermasch[1], Stefan Väth[1], Kristofer Tvingstedt[1], Andreas Baumann[2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern) Bayern, 97074 Würzburg

In the last years, solar cells based on organo-metal halide perovskites gained a lot of attention. The efficiency of solar cells with a perovskite absorber nowadays reaches more than 20%. With charge carrier mobilities up to tens of $cm^2V^{-1}s^{-1}$ and diffusion lengths exceeding 1 μm transport doesn't seem to be a limiting issue in this new kind of photovoltaic technology. However, recombination of the photgenerated charge carriers is an important factor defining e.g. the open circuit voltage of the solar cell. We prepared different methylammonium lead halide perovskite solar cells in planar configuration. Adressing the recombination dynamics, lifetime and concentration of photogenerated charge carriers are studied by transient photovoltage, charge extraction experiments as well as by the technique of open circuit voltage decay. We measured charge carrier lifetimes in the sub-μs-range for high illumination intensities ($\geq$ 1 sun), which is lower than in state of the art bulk heterojunction cells like P3HT:PCBM. Furthermore we discuss our results for different device morphologies and light-absorbing materials.

DS 19.3 Tue 11:15 H37

Correlating charge carrier mobility, morphology and efficiency in hybrid halide perovskite photovoltaic devices — •Irene Grill[1,2], Michiel Petrus[1,2], Nadja Giesbrecht[1,2], Thomas Bein[1,2], Pablo Docampo[1,2], Matthias Handloser[1,2], and Achim Hartschuh[1,2] — [1]Department of Chemistry and CeNS, LMU Munich — [2]Nanosystems Initiative Munich (NIM)

Hybrid perovskites currently represent one of the most promising material systems for incorporation in future solar cell devices since their efficiencies increased enormously in the last few years [1,2]. To date, fundamental physical properties including charge carrier dynamics and transport in these materials are not completely understood and are therefore at the focus of intense research. Here we extract the mobility of charge carriers in working thin film solar cells based on perovskite absorber layers and correlate it to the efficiency of the respective devices. To this end we performed Time-of-flight (ToF) studies on different perovskite thin films serving as photoactive layers. Further, in order to analyze the influence of contacts and other interfaces on charge transport and to identify possible optimization steps in the stacked architecture we carried out additional ToF measurements on each of the individual layers. Our results are discussed in terms of respective device efficiencies, morphologies and optical properties, allowing for a detailed investigation and identification of the limiting factors for the mobility and the efficiency in perovskite based thin film devices.

[1] M.A. Green and T. Bein, Nature Mater. 2015, 14, 559-561.
[2] N. Jeon et al., Nature 2015, 517, 476-480.

DS 19.4 Tue 11:30 H37

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

Organolead halide perovskite solar cells have emerged as one of the most promising technologies in thin-film photovoltaics due to their extraordinary increase in performance in only six years. Yet, the working principles of this material class still lack fundamental understanding. To address the possible influence of electronic traps on device performance, we probed solution processed methylammonium lead halide perovskite solar cells via thermally stimulated current (TSC) analysis.[1] Thereby, the sample is heated from 10 K to 300 K, while monitoring the current flow. This current is attributed to charge carriers being released from previously filled trap states in the semiconductor, allowing drawing conclusions about their distribution and energetic depth. Signals detected at low as well as at high temperatures can be attributed to shallow and deep traps, accordingly. Furthermore, a peak at around T=162 K can be assigned to the reported structural phase transition of the perovskite crystal from orthorhombic to tetragonal crystal lattice structure.

[1] A. Baumann et al., *J. Phys. Chem. Lett.* ***6**, 2350 (2015)*

15 min. break

DS 19.5 Tue 12:00 H37

Tunable ferroelectric polarization and its interplay with spin-orbit coupling in tin iodide perovskite — Alessandro Stroppa[1], •Domenico Di Sante[2], Paolo Barone[1], Menno Bokdam[3], Georg Kresse[3], Cesare Franchini[3], Myung-Hwan Whangbo[4], and Silvia Picozzi[1] — [1]CNR-SPIN L'aquila, Italy — [2]CNR-SPIN L'aquila, Italy and Wuerzburg University — [3]Faculty of Physics, Center for Computational Materials Science, University of Vienna, Wien, Austria — [4]Department of Chemistry, North Carolina State University, USA

Ferroelectricity is a potentially crucial issue in halide perovskites, breakthrough materials in photovoltaic research. Using density functional theory simulations and symmetry analysis, we show that the lead-free perovskite iodide (FA)SnI_3, containing the planar formamidinium cation FA, $(NH2CHNH2)^+$, is ferroelectric. In fact, the perpendicular arrangment of FA planes, leading to a weak polarization, is energetically more stable than parallel arrangements of FA planes, being either antiferroelectric or strong ferroelectric. Moreover, we show that the weak and strong ferroelectric states with the polar axis along different crystallographic directions are energetically competing. Intriguingly, the relatively strong spin-orbit couling in noncentrosymmetric (FA)SnI_3 gives rise to a co-existence of Rashba and Dresselhaus effects and to a spin texture that can be induced, tuned and switched by an electric field controlling the ferroelectric state.

A. Stroppa, D. Di Sante et al., Nature Commun. 5, 5900 (2014)

DS 19.6 Tue 12:15 H37

Mixed Pb:Sn methyl-ammonium halide perovskites: Thermodynamic stability and optoelectronic properties — •Lars Winterfeld, Ksenia Korshunova, Wichard J.D. Beenken, and Erich Runge — Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Using density functional theory, we investigate systematically mixed $MA(Pb:Sn)X_3$ perovskites, where MA is $CH_3NH_3^+$, and X is Cl, Br or I. Our results cover optoelectronic properties, structural and thermodynamic stability. Ab initio calculations of the orthorhombic, tetragonal and cubic perovskite phases show that the substitution of lead by tin has a much weaker influence on both structure and cohesive energies than the substitution of the halogen. The thermodynamic stability of the $MA(Pb:Sn)X_3$ mixtures at finite, non-zero temperatures is studied within the Regular Solution Model. We predict that it will be possible to create iodide mixtures at any temperature. Mixing is unlikely for the low-temperature phase of bromide and chloride compounds, where instead local clusters are more likely to form. We further predict that in the high-temperature cubic phase, Pb and Sn compounds will mix for both $MA(Pb:Sn)Br_3$ and $MA(Pb:Sn)Cl_3$ due to the entropy contribution to the Helmholtz free energy. We calculated optoelectronic properties using both DFT and post-DFT methods (including self-consistent GW) with and without spin orbit coupling. Interestingly, the optoelectronic properties are not just a linear combination of the non-mixed parent structures and are not limited by the non-mixed values, which allows band gap engineering.

DS 19.7 Tue 12:30 H37

A model Hamiltonian for perovskite solar cells — •Martin Schlipf, Marina R. Filip, Miguel A. Pérez-Osorio, and Feliciano Giustino — Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

Hybrid organic-inorganic halide perovskites emerge as one of most promising materials for new solar cells based on their high energy-conversion efficiency. The most commonly investigated materials include a large spin-orbit coupling, which may give rise to Rashba and Dresselhaus effects and makes them suitable for spintronic applications. In this contribution, we develop a simple model Hamiltonian that allows to study the impact of the spin-orbit coupling on the band structure. In particular, we focus on the physics near the bottom of the conduction band. Using group-theoretical considerations, we can reduce the number of parameters that the model exhibits. We apply this model to the prototype material $MAPbI_3$ (MA = CH_3NH_3) and show how different parameters of the model can be obtained from first-principles density functional theory (DFT) calculations. We discuss how the model can assist in designing improved perovskite solar cells.

DS 19.8 Tue 12:45 H37

Stability and electronic properties of novel perovskites for photovoltaics from high-throughput ab initio calculations — •Sabine Körbel[1,2], Miguel A L Marques[2,3], and Silvana Botti[1,2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, F-69622 Villeurbanne Cedex, France — [3]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Using a high-throughput approach based on density functional theory, we perform an extensive search for stable ABX_3 perovskites, where X is a non-metallic anion and A and B are cations spanning the largest portion of the periodic table. Our search is motivated by the necessity to improve the thermodynamic stability of hybrid organo-metal halide perovskite absorbers. We calculate the ternary phase diagram for each composition and we discuss the thermodynamic stability of the perovskite phases. We find a large number of ABX_3 perovskites which are still absent from databases, and which are stable with respect to decomposition into known ternary, binary or elementary phases. For these structures, we then calculate electronic band gaps, hole effective masses, and the spontaneous ferroelectric polarization as relevant material properties for an application as photovoltaic absorbers. We find several novel perovskites which exhibit promising properties for photovoltaic applications. Based on our findings, we discuss possible strategies to improve the thermodynamic stability of perovskite absorbers.

DS 20: Topological Insulators: Status Quo and Future Directions (Joint session of DS, O and TT, organized by DS)

Time: Tuesday 12:30–13:00 Location: H8

DS 20.1 Tue 12:30 H8

Topological invariants in the embedding-potential — Hiroshi Ishida[2] and •Daniel Wortmann[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]College of Humanities and Sciences, Nihon University, Tokyo, Japan

The embedding potential[1] defined at the boundary of a semi-infinite crystal defines the boundary condition for the wavefunction and can be interpreted as its logarithmic derivative. We demonstrate how this embedding potential can be utilized to determine the Z_2 topological invariant in time-reversal invariant insulators and how the formation of the surface states can be understood in terms of properties of the embedding potential.

Besides the general ideas and the theory, numerical examples for simple topological insulators and trivial materials will be shown and compared.

[1] J.E.Inglesfield, J. Phys. C **14**, 3795 (1981)

DS 20.2 Tue 12:45 H8

Quantum-well stabilized two-dimensional topological crystalline insulators — Chengwang Niu, Patrick Buhl, •Gustav Bihlmayer, Daniel Wortmann, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

By means of density functional theory calculations, we find that monolayers of SnTe and PbTe can be characterized as two-dimensional topological crystalline insulators (2D-TCIs) with band gaps of 50 meV and 90 meV, respectively [1]. Embedded in NaCl or NaBr films, these 2D-TCIs are not only structurally stabilized, but also the band gaps can be enhanced up to 470 meV. Moreover, in these quantum-well structures the Madelung potential of the strongly ionic rocksalt lattice acting on the SnTe or PbTe layers enhances the band-inversion. Even in thicker, topologically trivial telluride films band-inversions can be induced that trigger a transition to a TCI state [2]. We further analyse the effect of an external magnetic (exchange) field on the SnTe and PbTe monolayers and find that the quantum anomalous Hall regime can be reached with fields exceeding 0.2 eV. This happens even for an in-plane oriented field where the mirror symmetry, protecting the TCI phase, is broken. We investigate the properties of the edge states for ribbons of different orientations using maximally localized Wannier functions.

Financial support of the DFG (SPP 1666) is gratefully acknowledged.

[1] C. Niu et al., Phys. Rev. B. **91**, 201401(R) (2015).

[2] C. Niu et al., submitted (2015).

DS 21: Gaede Prize Symposium (Joint session of DS and O, organized by DS)

The prestigious Gaede prize of the German Vacuum Society (DVG e.V.) founded by Dr. Manfred Dunkel, head of the Leybold company for many years, is supported by Oerlikon Leybold Vacuum GmbH and regularly presented at the DPG Spring Meeting by the Surface Science and Thin Films Divisions. The Gaede prize is yearly awarded to young scientists (prior to their first professorship) for outstanding basic and applied research in the fields of vacuum physics and technology, thin films, surface science, materials and methods in solid state electronics, or nanotechnology. This symposium celebrates 30 years of Gaede prize, the first one being awarded to J. Kirschner in 1986. It comprises talks by the prize winner of this year, Dr. Julia Stähler (FHI Berlin), and previous winners, Prof. Jürgen Fassbender and Prof. Eberhard Umbach, complemented by the history of Gaede (Dr. Gerhard Voss, DVG and Head of the Vacuum Science and Technology Division of DPG). The list of previous prize winners (http://www.gaedepreis.org/preistraeger.html) comprises a large number of nowadays renowned colleagues for whom the Gaede prize was very supportive for their career.

Organizers: Dietrich R.T. Zahn (TU Chemnitz), Martin Wolf (FHI Berlin) and Norbert Esser (ISAS Berlin)

Time: Tuesday 13:30–15:30 Location: H11

Special Talk DS 21.1 Tue 13:30 H11
Wolfgang Gaede - Wegbereiter der modernen Vakuum-Technik — •Gerhard Voss — Oerlikon Leybold Vacuum, Köln

In diesem Vortrag geht es nicht nur um den Lebenslauf von Wolfgang Gaede, sondern auch um einige seiner wichtigsten Erfindungen, wie die Verbesserung der rotierenden Kapsel-pumpe (= Drehschieber-Pumpe), die Molekular(luft)pumpe, die Diffusionspumpe und die Drehschieber-Pumpe mit Gas-Ballast-Einrichtung.

Die bedeutenden Erfindungen von Wolfgang Gaede haben den enormen Aufschwung der Vakuum-Technik nach dem zweiten Weltkrieg erst möglich gemacht und stehen auch heute noch im Einsatz.

Prize Talk DS 21.2 Tue 14:00 H11
Ultrafast dynamics of many-body effects in solids and at interfaces: Polarons, excitons and correlated electrons — •Julia Stähler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Optical excitation of solids can lead to various interesting non-equilibrium phenomena that occur on electronic time and energy scales. These, for instance, involve the interaction of excited charge carriers among each other as well as with the lattice degrees of freedom. Key ingredient for such many-body effects is the Coulomb interaction and, importantly, its *screening*. Modification of the latter on ultrafast timescales disturbs the balance of competing forces in a system and can, thus, give rise to interesting transient properties. Exemplary for the diversity of such many-body effects and their impact also on the *equilibrium* qualities of materials, I will discuss the following three phenomena:

(i) Ultrafast dynamics of charge injection, trapping and polaronic stabilization during the birth of a solvated electron [1]

(ii) Femtosecond electron relaxation and ultrafast formation of excitons at polar and non-polar ZnO surfaces [2]

(iii) Instantaneous insulator-to-metal transition in photoexcited monoclinic VO_2 [3]

[1] J. Stähler *et al. J. Am. Chem. Soc.* **137**, 3520 (2015)
[2] J.-C. Deinert *et al. Phys. Rev. Lett.* **113**, 057602 (2014)
[3] D. Wegkamp *et al. Phys. Rev. Lett.* **113**, 216401 (2014)

Special Talk DS 21.3 Tue 14:30 H11
Ion beam modification of magnetic materials - revisited — •Jürgen Fassbender — Helmholtz-Zentrum Dresden-Rossendorf

In 2009 the Gaede prize was awarded for the ion induced modification and patterning of thin magnetic films. At that time most of the investigations were dealing with the local modification of magnetic anisotropies and exchange bias phenomena. In recent years we could show that also other magnetic properties, e.g. magnetic relaxation processes [1], can be tailored, but also the ferromagnetic state itself can be created [2] or destroyed depending on the material system under investigation. In particular the latter modifications open a route to the creation of nanomagnets [3] and magnonic crystals [4] by local ion irradiation. A current review will be given.

[1] M. Körner et al., Phys. Rev. B 88, 054405 (2013).
[2] R. Bali et al., Nano Lett. 14, 435 (2014).
[3] F. Röder et al., Sci. Rep. 5, 16786 (2015).
[4] B. Obry et al., Appl. Phys. Lett. 102, 202403 (2013).

Special Talk DS 21.4 Tue 15:00 H11
Large-scale reconstruction of metal-organic interfaces induced by chemisorption and surface stress change — •Eberhard Umbach[1,2], Florian Pollinger[1,3], Stefan Schmitt[1,4], Thomas Schmidt[2], Helder Marchetto[2], and Achim Schöll[1] — [1]Exp. Physik VII, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]Fritz-Haber-Institut der MPG, Abt. CP, 14195 Berlin — [3]Physikalisch-Technische Bundesanstalt, D-38116 Braunschweig — [4]SPECS GmbH, D-13355 Berlin

The adsorption of large organic molecules on metal substrates can have enormous influence on the topography, geometric structure, and electronic properties of this interface provided that the interaction is chemisorptive. Thus, under certain preparation conditions large scale reconstructions may occur which originate from a significant change of surface stress and may involve large mass transport. These reconstructions can lead to regular nano-patterns which are useable as templates in a bottom-up approach in nanotechnology. More important could be that such reconstructions may have considerable influence on the electric and optical properties of metal-organic devices, and can even lead to failure, if, e.g., the interface between metallic electrode and adjacent organic layer changes under operating conditions.

The talk will address this topic using the archetype system PTCDA on various Ag surfaces some of which are highly-indexed (vicinal). Results from various surface methods including STM, spectro-microscopy and a cantilever bending method will be presented to analyze and interpret the results.

DS 22: Transport: Topological Insulators - 3D (Joint session of DS, HL, MA, O and TT, organized by TT)

Time: Tuesday 14:00–15:45 Location: H18

Invited Talk DS 22.1 Tue 14:00 H18
Coupled-wire constructions: New insights into the physics of interacting topological systems in two and three dimension (and beyond) — •Tobias Meng[1], Eran Sela[2], Titus Neupert[3], Martin Greiter[4], Ronny Thomale[4], Adolfo G. Grushin[5], Jens H. Bardarson[5], and Kirill Stengel[6] — [1]Institut für Theoretische

Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Tel Aviv 69978, Israel — [3]Princeton Center for Theoretical Science, Princeton University, Princeton, New Jersey 08544, USA — [4]Institute for Theoretical Physics, University of Würzburg, 97074 Würzburg, Germany — [5]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany. — [6]Department of Physics & Astronomy, University of California, Riverside, California 92521, USA

Recently, it has been shown that coupled-wire constructions (CWCs) reproduce well-known fractional quantum Hall phases, and allow to derive new insights into, and setups for, interacting topological systems. I will review the basic concepts of 2D CWCs, discuss how they can teach us about spontaneous time-reversal symmetry breaking in topological insulators, and how they can be used to engineer chiral spin liquids in arrays of Mott-gapped quantum wires. I will show that 3D CWCs can for instance describe Weyl semimetals, and finally present new results on 4D fractional quantum Hall states built from coupled wires, whose 3D edges support a fractional chiral metal with a fractional chiral anomaly, thus generalizing the Weyl semimetal.

DS 22.2 Tue 14:30 H18

Revealing puddles of electrons and holes in compensated topological insulators — •Nick Borgwardt[1], Jonathan Lux[2], Zhiwei Wang[1,3], Ignacio Vergara[1], Malte Langenbach[1], Achim Rosch[2], Yoichi Ando[1,3], Paul van Loosdrecht[1], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für theoretische Physik, Universität zu Köln — [3]Institute of Scientific and Industrial Research, Osaka University

Three-dimensional topological insulators harbour metallic surface states with exotic properties. In transport or optics, these properties are typically masked by defect-induced bulk carriers. Compensation of donors and acceptors reduces the carrier density, but the bulk resistivity remains disappointingly small. We show that measurements of the optical conductivity in $BiSbTeSe_2$ pinpoint the presence of electron-hole puddles in the bulk at low temperatures, which is essential for understanding DC bulk transport. The puddles arise from large fluctuations of the Coulomb potential of donors and acceptors, even in the case of full compensation. Surprisingly, the number of carriers appearing within puddles drops rapidly with increasing temperature and almost vanishes around 40 K. Monte Carlo simulations show that a highly non-linear screening effect arising from thermally activated carriers destroys the puddles at a temperature scale set by the Coulomb interaction between neighbouring dopants, explaining the experimental observation semi-quantitatively [1].

[1] N. Borgwardt et al., arXiv:1508.03212

DS 22.3 Tue 14:45 H18

Interaction Correction to the Magneto-Electric Polarizability of Z_2 Topological Insulators — •Karin Everschor-Sitte[1], Matthias Sitte[1], and Allan MacDonald[2] — [1]Institut für Physik - Johannes Gutenberg-Universität Mainz, Deutschland — [2]Department of Physics - University of Texas at Austin, USA

When time-reversal symmetry is weakly broken and interactions are neglected, the surface of a Z_2 topological insulator supports a half-quantized Hall conductivity $\sigma_S = e^2/(2h)$. A surface Hall conductivity in an insulator is equivalent to a bulk magneto-electric polarizability, *i.e.* to a magnetic field dependent charge polarization. By performing an explicit calculation for the case in which the surface is approximated by a two-dimensional massive Dirac model and time-reversal symmetry is broken by weak ferromagnetism in the bulk, we demonstrate that there is a non-universal interaction correction to σ_S. Our prediction can be tested by measuring the capacitance of magnetized thin films in which the anomalous quantum Hall effect is absent.

DS 22.4 Tue 15:00 H18

Electron-Phonon Interaction in Surface States of Topological Insulators from First Principles — •Rolf Heid[1], Irina Yu. Sklyadneva[2], and Eugine V. Chulkov[2] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie — [2]Donostia International Physics Center (DICP), San Sebastian/Donostia, Spain

Transport through the metallic 2D surface states of 3D topological insulators with a Dirac-like dispersion is controlled by many-body interactions. In particular, a large electron-phonon interaction could be a limiting factor for applications at elevated temperatures [1]. Previous experimental investigations of the coupling constant remained inconclusive as they found large variations ranging from <0.1 to 3 [2].

Here we present a first principles investigation of the electron-phonon interaction in surface states of topological insulators within density-functional perturbation theory including spin-orbit interaction [3], using Bi_2Se_3, Bi_2Te_3, and Sb_2Te_2S as prominent examples. We discuss the various challenges faced by this approach, such as the rather deep penetration of the surface state and the small momentum range of both electronic and phonon states relevant for the coupling. We find that the coupling strength exhibits a significant dependence on the binding energy, following essentially the available electronic phase space. We further investigate the variation of the coupling with doping to mimic typical experimental conditions.

[1] D. Kim et al., PRL **109**, 166801 (2012)
[2] X. Zhu et al., arXiv: 1307.4559
[3] R. Heid et al., PRB **81**, 174527 (2010)

DS 22.5 Tue 15:15 H18

Detection of current-induced spin polarization in $BiSbTeSe_2$ toplogical insulator — •Fan Yang[1], Subhamoy Ghatak[1], Alexey Taskin[1], Yuichiro Ando[2], and Yoichi Ando[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]Department of Electronic Science and Engineering, Kyoto University, Japan

Topological insulators (TIs) are a class of quantum matter which possess spin-momentum-locked Dirac Fermions on the surfaces. Due to the spin-momentum locking, spin polarization will be induced when a charge current flows through the surface of a TI. Such spin polarization can be detected by using a ferromagnetic tunneling contact as a detector. In this talk, we present our results measured in devices fabricated from $BiSbTeSe_2$ flakes. Spin signals were observed in both n-type and p-type $BiSbTeSe_2$ samples.

DS 22.6 Tue 15:30 H18

Transport measurements on epitaxial $Bi_{1-x}Sb_x$ thin films grown on Si(111) — •Julian Koch, Philipp Kröger, Herbert Pfnür, and Christoph Tegenkamp — Leibniz Universität Hannover, Inst. für Festkörperphysik, Appelstr. 2, 30167 Hannover

The alloy $Bi_{1-x}Sb_x$ can be tuned to be either topologically trivial or non-trivial by changing the relative concentrations of Bismuth and Antimony [1]. In this study we present surface transport measurements performed on non-trivial $Bi_{1-x}Sb_x$ films. Thin films grown by in-situ co-deposition on Si(111) substrates are used, in order to reduce bulk contributions and to provide the possibility of nanostructuring. The morphology was controlled by low energy electron diffraction. Temperature dependent transport measurements for temperatures from 12 to 300 K were performed for films of different stoichiometry ranging from $x = 0.14 - 0.22$ and thicknesses of 4, 8, 16 and 24 nm. We find strong evidence for metallic surface transport in addition to activated bulk transport, which is, to the best of our knowledge, the first observation of metallic surface transport in $Bi_{1-x}Sb_x$ films. In previous studies the transport findings were discussed solely in terms of impurity and bulk bands (see e.g. [2]). For films thinner than 6 nm the surface transport is strongly suppressed, in accordance with measurements on Bi_2Se_3 [3]. The temperature dependent transport behaviour of these films is similar to that of thicker films with substracted surface contribution as well as to films examined in previous studies, further supporting the observation of metallic surface transport in thicker films.

[1] H. Guo, K. Sugawara, A. Takayama, S. Souma, T. Sato, N. Satoh, A. Ohnishi, M. Kitaura, M. Sasaki, Q.-K. Xue, and T. Takahashi, PRB **83**, 201104(R)
[2] S. Cho, A. DiVenere, G. K. Wong, J. B. Ketterson, and J. R. Meyer, PRB **59** 10691
[3] A. A. Taskin, S. Sasaki, K. Segawa, and Y. Ando, PRL **109**, 066803

DS 23: Frontiers of Electronic Structure Theory: Focus on Topology and Transport I (Joint session of DS and O, organized by O)

Time: Tuesday 14:00–16:00 Location: H24

Topical Talk DS 23.1 Tue 14:00 H24

Topological semimetals and chiral transport in inversion asymmetric systems — •Shuichi Murakami — Department of Physics and TIES, Tokyo Institute of Technology, Tokyo, Japan

Weyl semimetals (WS) are semimetals with nondegenerate 3D Dirac cones in the bulk. We showed that in a transition between different Z2 topological phases, the Weyl semimetal phase necessarily appears when inversion symmetry is broken. In the presentation we show that this scenario holds for materials with any space groups without inversion symmetry. Namely, if the gap of an inversion-asymmetric system is closed by a change of an external parameter, the system runs either into (i) a Weyl semimetal phase or (ii) a nodal-line semimetal, but no insulator-to-insulator transition happens. This transition is realized for example in tellurium (Te). Tellurium has a unique lattice structure, consisting of helical chains, and therefore lacks inversion and mirror symmetries. At high pressure the band gap of Te decreases and finally it runs into a Weyl semimetal phase, as confirmed by our ab initio calculation. We also theoretically propose chiral transport in systems with such helical structures.

DS 23.2 Tue 14:30 H24

Topological orbital magnetic moments — •Manuel dos Santos Dias, Juba Bouaziz, Mohammed Bouhassoune, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Orbital magnetic moments are usually associated with the spin-orbit interaction (SOI). We explore from first-principles how topological orbital magnetic moments (TOMs) can emerge in non-trivial magnetic spin textures, even without SOI, justifying the ‘topological’ label. Firstly, the case of magnetic trimers on the Cu(111) surface illustrates the basic symmetry properties of the TOMs, and how to separate their contribution from the usual SOI-driven orbital moments. We then focus on the implications of TOMs for single magnetic skyrmions formed in Pd/Fe/Ir(111) [1], considering their possible use in detecting and distinguishing skyrmions from anti-skyrmions by optical means.

Work funded by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] D.M. Crum et al., Nat. Comms. **6**, 8541 (2015)

DS 23.3 Tue 14:45 H24

The orbital Rashba effect — •Dongwook Go[1,2], Patrick Buhl[1], Gustav Bihlmayer[1], Yuriy Mokrousov[1], Hyun-Woo Lee[2], and Stefan Blügel[1] — [1]Institute for Advanced Simulation and Peter Grünberg Institut, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Department of Physics, Pohang University of Science and Technology, 37673 Pohang, Korea

We present a new surface phenomenon called the *orbital* Rashba effect, analogous to the spin Rashba effect. The effect is described by the orbital Rashba Hamiltonian, $H_{\text{orb-R}}(\mathbf{k}) = \alpha_{\text{orb-R}}\mathbf{L}\cdot(\hat{\mathbf{z}}\times\mathbf{k})$, where $\mathbf{L}$ is the orbital moment derived from atomic orbitals and $\alpha_{\text{orb-R}}$ is the orbital Rashba constant. This leads to orbital-dependent energy splittings and orbital texture in the $\mathbf{k}$-space. The mechanism behind the emergence of the $H_{\text{orb-R}}(\mathbf{k})$ can be understood as the $\mathbf{k}$-dependent magnetoelectric coupling due to atomic orbital hybridization. In the presence of intra-atomic spin-orbit coupling, the spin moment is aligned parallel or antiparallel to the orbital moment, thus the spin Rashba effect is recovered. As an example, we present a tight-binding and an *ab initio* study of the Bi/Ag(111) surface alloy, where the hybridization between a Ag *s*-orbital and a Bi *p*-orbital leads to the orbital Rasbha effect that is dominant over the spin one. The orbital Rashba effect is a key to new physics and to understanding spin-orbit driven physics at surfaces and interfaces, such as Dzyaloshinskii-Moriya interaction, non-collinear magnetism, etc.

DS 23.4 Tue 15:00 H24

Spin and orbital magnetism of Rashba electrons induced by magnetic nanostructures — •Juba Bouaziz, Manuel dos Santos Dias, Phivos Mavropoulos, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We explore theoretically the spin and orbital magnetism of Rashba electrons in the presence of noncollinear impurity-induced magnetic states. The Rashba electron gas mediates the Dzyaloshinksii-Moriya interaction between magnetic impurities favoring chiral states [1]. Here we investigate the back-action of such noncollinear magnetic states on the Rashba electron gas. The presence and distribution of ground state spin and orbital currents is analyzed. Surprisingly, when switching off the spin-orbit coupling, chiral magnetic textures generate bound currents, which implies the existence of orbital magnetic moments originating solely from the peculiar topology of the impurities magnetic moments. In the particular case of a single adatom with an out of plane magnetic moment, we found circular currents flowing around the magnetic impurity in agreement with the continuity equation for the electric charge. Similar results were predicted for magnetic adatoms on superconductor surfaces with a finite spin-orbit coupling [2].

[1] J. Bouaziz *et al.* in preparation.

[2] S. S. Pershoguba *et al.* Phys. Rev. Lett. **115**, 116602 (2015).

This work is supported by the HGF-YIG Programme VH-NG-717 (Functional Nanoscale Structure and Probe Simulation Laboratory).

DS 23.5 Tue 15:15 H24

First-principles investigation of the impact of single atomic defects on magnetic skyrmions — •Imara L. Fernandes, Benedikt Schweflinghaus, Juba Bouaziz, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Chiral magnetic skyrmions are topological spin-swirling textures with rich physics and technological potential in the field of information storage. In a device, skyrmions certainly interact with defects and imperfections resulting into pinning phenomena. We explore from first-principles the non-trivial impact of 3d and 4d impurities on the energetics, electronic and magnetic properties of single magnetic skyrmions. Utilizing the newly developed Jülich full-potential relativistic Korringa-Kohn-Rostoker Green function method [1], we focus on topological magnetic objects of sub-5nm diameters stabilized in a single ferromagnetic layer of Fe sandwiched between the Ir(111) surface and one or two Pd layers, where the tunneling spin-mixing magnetoresistance (TXMR) was demonstrated theoretically [2] and experimentally [3]. – Funding provided by the HGF-YIG Program VH-NG-717 and the CNPq (BRAZIL).

[1] D. S. G. Bauer, Schriften des Forschungszentrum, Key Tech. **79** (2014).

[2] D.M. Crum *et al.*, Nat. Comms. **6**, 8541 (2015).

[3] C. Hanneken *et al.*, Nat. Nanotech. Doi:10.1038/nano.2015.218 (2015).

DS 23.6 Tue 15:30 H24

Topological magnons: Any chance to find them? — •Alexander Mook[1], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — [2]Institut für Physik, Martin-Luther-Universität, D-06120 Halle

Topological magnon insulators (TMIs) have a nontrivial topology due to the Dzyaloshinskii-Moriya interaction which results in spatially confined edge states and, thus, energy and spin currents along their edges [1,2]. Several systems have been identified as TMIs, for example, Cu(1,3-benzenedicarboxylate) consisting of kagome planes [3], or the family of ferromagnetic pyrochlore oxides, e. g., $Lu_2V_2O_7$, showing the magnon Hall effect [4]. However, to date, no direct experimental evidence of a topological magnon band has been provided, what comes down to the small total width of the magnon dispersion relation and the energy resolution of surface sensitive measurements.

We propose Fe_3Sn_2 as promising candidate for a TMI. The total width of its magnon dispersion relation is large, and we determine its nontrivial topology by constructing an effective spin Hamiltonian. On this basis, we discuss signatures of topological magnon states that should be looked for in experiments.

[1] L. Zhang et al., PRB **87**, 144101 (2013); [2] A. Mook et al., Phys. Rev. B **89**, 134409 (2014); *eidem*, Phys. Rev. B **90**, 024412 (2014); *eidem*, Phys. Rev. B **91**, 224411 (2015); *eidem*, Phys. Rev. B **91**, 174409 (2015); [3] R. Chisnell et al., Phys. Rev. Lett. **115**, 147201 (2015); [4] Y. Onose et al., Science **329**, 297 (2010).

DS 23.7 Tue 15:45 H24

Acoustic magnons in the long-wavelength limit: resolving the Goldstone violation in many-body perturbation theory — •Mathias C.T.D. Müller, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Ferromagnetic materials exhibit a spontaneously broken global rotation symmetry in spin space leading to the appearance of massless quasiparticles (zero gap) in the long-wavelength limit. These magnons are formed by the correlated motion of electron-hole pairs with opposite spins, which we describe from first principles employing the T-matrix formalism in the ladder approximation within the FLAPW method [1]. Due to approximations used in the numerical scheme, the acoustic magnon dispersion exhibits a small but finite gap at Γ. We analyze this violation of the Goldstone mode and present an approach that implements the magnetic susceptibility using a renormalized Green function instead of the Kohn-Sham (KS) one. This much more expensive approach shows substantial improvement of the Goldstone-mode condition. In addition, we discuss a possible correction scheme, that involves an adjustment of the KS exchange splitting, which is motivated by the spin-wave solution of the one-band Hubbard model. The new exchange splittings turn out to be closer to experiment. We present corrected magnon spectra for the elementary ferromagnets Fe, Co, and Ni.

[1] E. Şaşıoğlu *et al.*, Phys. Rev. B **81**, 054434 (2010); C. Friedrich *et al.* Top. Curr. Chem. **347**, 259 (2014).

DS 24: 1D Metal Wires on Semiconductors II (Joint session of DS and O, organized by O)

Time: Tuesday 14:00–16:00 Location: S052

DS 24.1 Tue 14:00 S052

Infrared Plasmonic Investigation of Band Filling-Induced Metal-to-Insulator Transition in Au Chains on Si(111)-5x2-Au — •Fabian Hötzel[1], Kaori Seino[2], Friedhelm Bechstedt[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Deutschland — [2]Institut für Festkörpertheorie und -optik, Universität Jena, Jena, Deutschland

The investigation of infrared plasmon polaritons on the Si(111)-5x2-Au surface underlines the metallic character of the system [1] and its Kwon-Kang atomic structure model [2] with seven Au atoms per 5x2 surface unit cell. However, upon evaporating an additional 0.1 monolayer Au amount, the system undergoes a metal-to-insulator transition [3] but the 5x2 symmetry remains unchanged as proven by reflection high energy electron diffraction. This phase transition was in situ observed by means of the infrared plasmonic signal attenuation with coverage. Band-structure calculations reveal that the transition is induced by band filling of the one-dimensional half-filled band at the Fermi energy. The insulating phase represents an indirect semiconductor with a band gap of 0.29 eV. Moreover, a new surface structure model with eight Au atoms per unit cell, including the additional Au atoms, is developed for the 5x2 symmetry. By annealing the system, the plasmonic signal is recovered which shows that the phase transition is reversible. This contribution is part of the DFG Research Unit FOR 1700.

[1] Hötzel, F. et al. Nano Lett. **2015**, 15, 4155-4160.
[2] Kwon, S. G. et al. Phys. Rev. Lett. **2014**, 113, 086101.
[3] Hötzel, F. et al. J. Phys. Chem. Lett. **2015**, 6, 3615-3620.

DS 24.2 Tue 14:15 S052

Optical monitoring of Ag nanostructures on Si(557) — •Sandhya Chandola[1], Eugen Speiser[1], Jochen Räthel[1], Ulrich Krieg[2], Christoph Tegenkamp[2], Herbert Pfnür[2], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167, Hannover, Germany

The optical response of the Si(557)-Ag surface has been studied with reflectance anisotropy spectroscopy (RAS) from 0.5 to 5 eV. Using the Si(557) surface as a template, various quasi-one dimensional (1D) Ag structures were grown and substantial differences between the structures were observed with RAS. At ~ 0.3 ML of Ag, 1D chain structures were observed with STM and a large anisotropic response developed at 2.5 eV, related to the formation of Ag nanowires which are semiconducting. Further deposition up to 1.2 ML of Ag resulted in the formation of the $(\sqrt{3}\times\sqrt{3})$ phase. The anisotropy at 2.5 eV disappeared and the overall optical response showed substantial modification. Small amounts of Ag, from 0.03 ML to 0.1 ML of Ag, were then deposited on the $(\sqrt{3}\times\sqrt{3})$ surface to monitor the effects of doping on these structures. The RAS response showed a significant anisotropy towards the infrared for small amounts of doping. As RAS is only sensitive to the anisotropic optical response, which arises from stepped and facetted regions of the surface, it can be a sensitive tool to monitor the effects of excess Ag atoms concentrated at the step sites of the Si(557) surface which are supposed to be responsible for the doping mechanism.

DS 24.3 Tue 14:30 S052

Fabrication of one-dimensional arrays of magic clusters using a vicinal Si surface as a template — •Martin Franz, Julia Schmermbeck, and Mario Dähne — Technische Universität Berlin, Institut für Festkörperphysik, 10623 Berlin, Germany

Self-assembled magic clusters on surfaces are fascinating not only from a fundamental scientific point of view, they are also promising candidates to employ such zero-dimensional nano objects in future applications such as high-density memory devices or in catalysis. In the present work, magic In clusters that form on the Si(111)7×7 surface are used as a model system to study how the array formation affects the electronic properties and to explore the possibility to produce one-dimensional (1D) arrays of magic clusters. For this purpose, scanning tunneling microscopy and spectroscopy are empoyed. The basic properties of these clusters, such as the atomic structure and the preparation procedure, are well known. In addition, it is possible to produce perfectly ordered two-dimensional (2D) arrays of these clusters on planar Si(111)7×7 samples. In the present work, different electronic properties and in particular different energy gaps are observed for clusters forming in the faulted and unfaulted half unit cell of the 7×7 reconstruction as well as for clusters neighboring other clusters. Furthermore, the Si(557) surface, which is a vicinal surface with narrow Si(111) terraces, is used as a template resulting in the formation of two different types of 1D arrays, similar to the two types of 2D arrays that are found on the planar Si(111) surface. This work was supported by the DFG through FOR 1282 project D.

DS 24.4 Tue 14:45 S052

Selective One-Dimensional Growth of an Alkyl-Sugar Functionalized Ferrocene of Graphite — •Thiruvancheril Gopakumar, Prithwidip Saha, Khushboo Yadav, Shibin Chako, and Ramesh Ramapanicker — Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208016, India

Ferrocene molecules are interesting class of semi-conducting organometallic molecules because of their excellent redox efficiency. In addition the redox potentials may be manipulated substantially by altering functional groups attached directly to Ferrocene. Here we show, using AFM, selective one-dimensional growth of an alkyl-sugar functionalized Ferrocene molecule on graphite basal plane. The assembly is driven by formation of Ferrocene dimers. The one-dimensional growth selectivity is further enhanced by adding a keto (-C=O) group in the alkyl part of alkyl-sugar group. The growth of elongated molecular islands is only limited by terrace edges or other molecular islands and is controlled by additional inter-dimer hydrogen bonding between keto group and alkyl -C-H groups.

DS 24.5 Tue 15:00 S052

Growth and electronic structure of Tb disilicide nanowires

on vicinal Si(111) surfaces — •Stephan Appelfeller, Martin Franz, Christian Hassenstein, Lars Freter, Hans-Ferdinand Jirschik, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

One-dimensional metals may be useful for future applications, but they are especially interesting due to their unique physical phenomena, e.g. Luttinger liquid behavior or the Peierls transition. Vicinal substrates can enable the formation of such nanowires, when thin metallic films grow exclusively on well separated, narrow terraces. $TbSi_2$ forms well ordered metallic monolayer films on planar Si(111) [1]. Here, the nanowire formation of $TbSi_2$ on various vicinal Si(111) samples was investigated. Structural information, e.g. dimensions and edge characteristics, were obtained by scanning tunneling microscopy and confirm, together with the electronic properties obtained by core-level photoemission spectroscopy, the growth of $TbSi_2$. Furthermore, the electronic dimensionality of the nanowires, which is illustrated by their Fermi surfaces, was determined using angle resolved photoemission spectroscopy.

This work was supported by the DFG (FOR1700, project E2). We kindly acknowledge the support of K. Horn and coworkers and of BESSY, where the photoemission experiments were carried out at the beamlines UE56/2 PGM-1 and PGM-2.

[1] M. Franz, J. Große, R. Kohlhaas, and M. Dähne, Surface Science **637**, 149 (2015).

DS 24.6 Tue 15:15 S052

Strain induced quasi one-dimensional rare earth silicides structures on Si(111) — •Frederic Timmer[1], Robert Oelke[1], Martin Franz[2], Stephan Appelfeller[2], Mario Dähne[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Rare earth elements (REE) covered silicon surfaces have been in the focus of research for more than 30 years due to their unique properties. For instance, thin REE-silicide films on n-type Si(111) possess very low Schottky-barriers in conjunction with an abrupt surface making them interesting as ohmic contacts. Furthermore REE-nanowires might be applicable as interconnects in future nanodevices or as plasmonic waveguides due to their quasi one-dimensional structure.

Here, we report on a $\left(2\sqrt{3}\times\sqrt{3}\right)$ R30° reconstruction for REE coverages exceeding 1 ML which is therefore related to the well-known $\left(\sqrt{3}\times\sqrt{3}\right)$ R30° reconstruction. We characterize the structure of the silicide films by means of Low Energy Electron Diffraction (LEED) including Spot Profile Analysis (SPA-LEED) and Scanning Tunneling Microscopy (STM). The stoichiometry of the films and their growth mode is studied by Auger Electron Spectroscopy (AES). Combining experimental results, we develop a complex model for the reconstructed surface including formation of quasi one-dimensional structures, due to striped domains.

DS 24.7 Tue 15:30 S052

Local transport measurements on terbium-silicide nanowires — •Frederik Edler[1], Ilio Miccoli[1], Herbert Pfnür[1], Stephan Appelfeller[2], Mario Dähne[2], Simone Sanna[3], Wolf G. Schmidt[3], and Christoph Tegenkamp[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover — [2]Institut für Festkörperphysik, TU Berlin, 10623 Berlin — [3]Lehrstuhl für Theoretische Physik, Universität Paderborn, 33098 Paderborn

Metal silicide wires play an important role in electronics as ohmic contacts and gate electrodes due to their very low resistivity. Rare-earth (RE) metals (eg. Tb, Dy, Er, Y) can be used to grow long, extremely thin nanowires because of uniaxial lattice matching with Si which could be used for additional downscaling of Si based technology.

The transport properties of Tb silicide wires have been studied via 4-tip STM/SEM system. The SEM allows a fast characterization of sample quality and precise positioning of feedback controlled STM tips, enabling gentle contacts and transport measurements on a nm-scale. Moreover, the STM was used to correlate the surface morphology of nanowires with transport findings.

Our measurements reveal three types of metallic wires mainly depending on the growth parameters. Further analysis shows that the resistivity is strongly depending on the height of wires, which is increased for small heights. The data can be perfectly described by a theoretical model taking into account the surface roughness and lateral surface correlation. STS reveals that the wires are electronically decoupled from the Si substrate in agreement with recent DFT calculations.

DS 24.8 Tue 15:45 S052

Capping of rare earth silicide nanowires on Si(001) — •Stephan Appelfeller[1], Martin Franz[1], Milan Kubicki[1], Paul Reiss[2], Tore Niermann[2], Markus Andreas Schubert[3], Michael Lehmann[2], and Mario Dähne[1] — [1]Institut für Festkörperphysik, TU Berlin, 10623 Berlin — [2]Institut für Optik und Atomare Physik, TU Berlin, 10623 Berlin — [3]IHP - Leibniz-Institut für innovative Mikroelektronik, 15236 Frankfurt (Oder)

Rare earth silicide nanowires are promising candidates for the use of one-dimensional metals in future applications, but they are not stable under ambient conditions. Thus, a protective layer is needed. Here, the capping of Tb and Dy silicide nanowires grown on Si(001) by Si overlayers was studied using scanning tunneling microscopy and cross-sectional high-resolution transmission electron microscopy, also with energy dispersive X-ray analysis. Amorphous Si films deposited at room temperature allow an even capping, while the nanowires maintain their original structural properties. Subsequent recrystallization by thermal annealing leads to more compact nanowire structures and to troughs in the Si layer above the nanowires, which may even reach down to the nanowires in the case of thin Si films, as well as to V-shaped stacking faults forming along {111} lattice planes. This behavior is most probably related to strain due to the lattice mismatch between the Si overlayer and the nanowires.

This work was supported by the DFG (FOR1700, project E2).

DS 25: Organic Electronics and Photovoltaics I (Joint session of CPP, DS, HL and O, organized by CPP)

Time: Tuesday 14:00–15:30 Location: H37

DS 25.1 Tue 14:00 H37

Elucidating the Morphology of Organic Bulk Heterojunction Solar Cells Using Nanoanalytical Transmission Electron Microscopy — •Stefanie Fladischer[1], Tayebeh Ameri[2], Christoph Brabec[2], and Erdmann Spiecker[1] — [1]FAU, CENEM, Erlangen, Deutschland — [2]FAU, i-MEET, Erlangen, Deutschland

Organic photovoltaics is one of the most promising technologies for low cost energy production with the advantages of semi-transparency, flexibility and solution processing. Significant improvement of the power conversion efficiency could be achieved in the last years using novel materials and adapted device engineering. To further improve the efficiency of solar cells the knowledge of the morphology is essential, as it decisively influences the device performance. The morphology of organic bulk heterojunction (BHJ) active layers depends not only on the involved materials but also on their molecular weight and their treatment like thermal annealing and solvent vapor annealing. Analytical Transmission Electron Microscopy (TEM) is a versatile tool to characterize the morphology of organic solar cells concerning on the one hand the interfaces of the various layers and on the other hand the material distribution in BHJ active layers. Combining high-resolution imaging with analytical techniques like electron energy-loss spectroscopy (EELS) and energy filtered TEM (EFTEM) as well as energy-dispersive X-ray spectroscopy (EDXS) the morphology can be determined and thus the device performance can be understood and further improved.

DS 25.2 Tue 14:15 H37

Links between organic solar cell performance and morphological properties — •Daniel Moseguí González[1], Christoph J. Schaffer[1], Stephan Pröller[2], Johannes Schlipf[1], Lin Song[1], Sigrid Bernstorff[3], Eva M. Herzig[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748, Garching, Germany — [2]TU München, Munich

School of Engineering, Herzig Group, 85748 Garching, Germany — [3]Elettra Sincrotrone Trieste S.C.p.A., Basovizza, 34149 Trieste, Italy

Many attempts have been made to establish solid links between morphology and performance of organic solar cells (OSCs) as well as the potential suitability of some materials for solar devices. Eventually, many of these attempts have yielded deeper insight into the physics governing excitonic solar cells. In this regard, one of the most innovative approaches consists in the in-operando observation of solar devices under working conditions in time-resolved grazing incidence X-ray scattering experiments. This configuration allows for simultaneous tracking of morphological and electronic properties as a function of time, making the appearing co-dependences among studied parameters more remarkable. The presented work focuses on the first in-operando observations that showed strong correlations between the crystalline state of P3HT:PCBM OSCs' active layers and the open-circuit voltage delivered by the devices. Up to now, this link was only addressed in a multi-step fashion with works featuring interdependences between properties like crystallinity, recombination, energy disorder, open-circuit voltage, or exciton/charge carrier transport.

DS 25.3 Tue 14:30 H37

Strong influence of morphology on charge transport and recombination in solution processed small molecule based solar cells — •Alexey Gavrik[1], Andreas Baumann[2], Yuriy Luponosov[3], Sergey Ponomarenko[3,4], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg — [3]Enikolopov Inst Synthet Polymer Mat, 117393 Moscow, Russia — [4]Lomonosov Moscow State University, 119991 Moscow, Russia

Solution processed small molecules (SSM) are promising materials for solar cell (SC) applications due to their well defined structure and high chemical reproducibility. Donor-acceptor-donor layout of SSM provides enhanced exciton splitting, as well as good possibility for effective charge transfer. The blend morphology in a bulk-heterojunction (BHJ) SC is assumed to play a crucial role in the cell performance. Therefore, we set to find optimal BHJ fabrication method keeping track of corresponding transport properties. In this work we studied DTS(EtHex)$_2$-(2T-DCV-Me)$_2$:PC$_{60}$BM BHJ SC using the photogenerated charge carrier extraction technique OTRACE in order to analyze non-geminate recombination and determine charge carrier mobility in context of varying blend morphology. We show that different preparation conditions have a strong impact on the blend morphology and thus on the charge carrier transport (i.e. mobility and recombination rate). Furthermore, introduced modifications allowed to achieve a 4-fold enhancement of SC efficiency up to 4.3%.

DS 25.4 Tue 14:45 H37

Direct visualization of charge-extraction in metal-mesh based OPV cells by light-biased LBIC — •Mathias Gruber[1,2], Arne Hendel[1], Vladislav Jovanov[1], Manfred J. Walter[2], and Veit Wagner[1] — [1]Department of Physics and Earth Sciences, Jacobs University Bremen, 28759 Bremen, Germany — [2]PolyIC GmbH & Co. KG, 90763 Fürth, Germany

Metal-mesh based electrode systems are a highly conductive, versatile and unexpensive alternative to ITO-electrodes for organic photovoltaic (OPV) cells. However, as a metal-mesh does not offer full surface conductivity it is usually combined with a less conductive PEDOT:PSS layer, which enables lateral charge-transport in the area in between the metal tracks. The sheet conductivity of this additional lateral conductive layer (LCL) needs to be carefully tuned with respect to the distance of the metal tracks to reduce short circuit current (J_{sc}) losses and additional series resistance due to resistive losses in the LCL material. Usually this is done via electrical simulation or via analysis of IV-measurements of a large number of devices with different LCL sheet conductivities. Here we present a direct way to measure the current collection losses due to PEDOT:PSS sheet resistance by integrating a white light-bias into a LBIC measurement (Light-bias LBIC). We show that we are not only able to directly measure and visualize charge extraction under real device operation conditions but are also able to determine the intrinsic PEDOT:PSS sheet resistance in the operating OPV device.

DS 25.5 Tue 15:00 H37

Morphological Degradation of Polymer-Fullerene Bulk-Heterojunction Solar Cells — •Christoph J. Schaffer[1], Claudia M. Palumbiny[1], Martin A. Niedermeier[1], Christian Burger[1], Gonzalo Santoro[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]DESY, Notkestr. 85, 22607 Hamburg

Organic solar cells offer a wide range of advantages based on their mechanical flexibility, their optical tunability and their ease of production in comparison to conventional photovoltaics. However, elongating their lifetime remains the main challenge after efficiencies exceeding the 10% marker have been recently reported [1]. We focus on the stability of the active bulk-heterojunction layer of polymer-fullerene solar cells. Using in-situ GISAXS and simultaneous current-voltage tracking we have previously shown that the active layer is morphologically unstable during operation of a P3HT:PCBM based solar cell, causing device degradation [2]. In our recent work we observe different degradation mechanisms occurring in other polymer-fullerene blends. This knowledge shows that tailored stabilization methods must be found for each specific material system.

[1] S.-H. Liao et al., Scientific Reports 2014, 4, 6813.

[2] C. J. Schaffer et al., Adv. Mater. 2013, 25, 6760.

DS 25.6 Tue 15:15 H37

Illumination dependent parasitic resistances in organic bulk hetero junction solar cells. — •Arne Hendel and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

During outdoor operation, the solar cell is exposed to AM1.5G during noon only. For other daytimes and for indoor applications the performance of the solar cell at lower light intensities is important. In this study, bulk hetero junction solar cells were exposed to light irradiation from 10^{-5} to several suns intensity. We find a strong illumination dependence of the parasitic resistances. For the different light intensities I-V characteristics were performed. In addition the Jsc-Voc analysis was done to obtain series resistance free I-V measurement. It was found that the series and shunt resistance, which are critical for the solar cell performance, strongly depend on illumination intensity. The light intensity induced conductivity change of the solar cell shows different dependencies for forward and reverse operation. For low light intensities, the shunt resistance can be directly measured via the open circuit voltage assuming the Shockley model for the diode. From these measurements a strong light dependence is obtained. Based on the experimental data a model for the light dependent shunt resistance and series resistance is presented.

DS 26: Plenary Talk XI

Time: Wednesday 8:30–9:15 Location: H1

Plenary Talk DS 26.1 Wed 8:30 H1

Topological Physics in HgTe-based Quantum Devices — •Laurens W. Molenkamp — Physikalisches Institut (EP3), Universität Würzburg

Suitably structured HgTe is a topological insulator in both 2- (a quantum well wider than some 6.3 nm) and 3 (an epilayer grown under tensile strain) dimensions. The material has favorable properties for quantum transport studies, i.e. a good mobility and a complete absence of bulk carriers, which allowed us to demonstrate variety of novel transport effects.

One aspect of these studies is topological superconductivity, which can be achieved by inducing superconductivity in the topological surface states of these materials. Special emphasis will be given to recent results on the ac Josephson effect. I will present data on Shapiro step behavior that is a very strong indication for the presence of a gapless Andreev mode in our Josephson junctions.

Growing HgTe under compressive strain opens up yet another line a research - the material is readily turned into a topological (Weyl) semimetal, exhibiting clear signs of the Adler-Bell-Jackiw anomaly in its magnetoresistance.

DS 27: Symposium Topological Insulators: Status Quo and Future Directions (Joint symposium of DS, HL, MA, O and TT, organized by TT)

Time: Wednesday 9:30–13:00 Location: H1

Invited Talk DS 27.1 Wed 9:30 H1
Topological insulators and topological superconductors — •Shoucheng Zhang — Dept of Physics, Stanford University

In this talk, I will first give a brief overview on topological insulators and superconductors. I will then discuss the recent theoretical prediction and the experimental observation of the quantum anomalous Hall effect in magnetic topological insulators. I shall present a newly predicted material called stanene, and discuss its potential applications.

Invited Talk DS 27.2 Wed 10:10 H1
Three-dimensional topological insulators and superconductors — •Yoichi Ando — II. Physikalisches Institut, Universität zu Köln

A topological quantum state of matter is characterized by a nontrivial topological structure of its Hilbert space. 3D topological insulators are characterized by non-trivial Z_2 topology, which is due to band inversion caused by strong spin-orbit coupling [1]. Intriguingly, when superconductivity shows up upon doping charge carriers into 3D topological insulators, the resulting superconducting state can also be topological [2], because the strong spin-orbit coupling could lead to an unconventional gap function characterized by a new Z_2 topological invariant [3]. In this talk, I will present experimental realizations of these materials and report recent efforts to address their exotic properties.
[1] Y. Ando, J. Phys. Soc. Jpn. **81**, 102001 (2013)
[2] Y. Ando and L. Fu, Ann. Rev. Cond. Mat Phys. **6**, 361 (2015)
[3] S. Sasaki, M. Kriener, K. Segawa, K. Yada, Y. Tanaka, M. Sato, and Y. Ando, PRL **107**, 217001 (2011)

Invited Talk DS 27.3 Wed 10:50 H1
Interplay of magnetic and electronic states in pyrochlore iridates — •Leon Balents — University of California, Santa Barbara, CA, USA

The pyrochlore iridates are a series of compounds undergoing antiferromagnetic ordering and metal-insulator transitions. They are of interest because they combine electron correlation effects and the potential for non-trivial band topology. We will discuss the theoretical picture of these materials, from electronic structure to magnetism and phase transitions, and how they may be controlled through applied fields and temperature. Comparison will be made between theory and recent experiments.

10 min. break

Invited Talk DS 27.4 Wed 11:40 H1
Magnetic imaging of edge states — •Kathryn Moler — Stanford University

Beautiful theoretical proposals launched the field of topological materials, followed rapidly by great initial successes in synthesizing and demonstrating several topological insulators. The challenges now are to understand and control edge and surface scattering, to find materials with no bulk states and large gaps for high-temperature operation, and most importantly, to fabricate integrated devices that include gates, superconductors, and ferromagnets. Scanning SQUID microscopy can aid this effort by imaging magnetism, superconductivity, and current flow. Images of current flow in two quantum spin hall insulators verify that currents really do flow on the edges, provide images of the developing edge states with voltage and temperature, and also help reveal the conditions for achieving topological vs. trivial edge states. Sensitive magnetic measurements characterize superconductor * topological insulator structures, and help to determine the conditions for achieving exotic Josephson junctions.

Invited Talk DS 27.5 Wed 12:20 H1
Sub-nm wide edge states at the dark side of a weak topological insulator — •Markus Morgenstern — II. Institute of Physics B and JARA-FIT, RWTH Aachen, 52074 Aachen

Three-dimensional insulating crystals, which respect time reversal symmetry, can be classified as trivial insulators, strong topological insulators and weak topological insulators (WTIs). Many examples of trivial or strong topological insulators are known, but WTIs have barely been probed. They offer pairs of topologically protected surface states on most surfaces, but exhibit one dark surface without such surface states. The step edges of this dark surface naturally belong to the bright surfaces such that they contain spin helical edge states with perfect e^2/h conductivity. The first WTI $\mathrm{Bi_{14}Rh_3I_9}$ was synthesized recently [1]. Here, we show by scanning tunneling spectroscopy that the edge states indeed exist and are below 1 nm wide. They can be scratched into the surface using an atomic force microscope providing a simple tool to guide them [2]. Moreover, it is shown that the edge state can be removed by chemically dimerizing adjacent layers of the WTI. Strategies to bring the edge state to the Fermi level are discussed.
[1] B. Rasche, A. Isaeva, M. Ruck, S. Borisenko, V. Zabolotnyy, B. Büchner, K. Koepernik, C. Ortix, M. Richter, and J. van den Brink, Nature Mater. **12**, 422 (2012)
[2] C. Pauly, B. Rasche, K. Koepernik, M. Liebmann, M. Pratzer, M. Richter, J. Kellner, M. Eschbach, B. Kaufmann, L. Plucinski, C. M. Schneider, M. Ruck, J. van den Brink, and M. Morgenstern, Nature Phys. **11**, 338 (2015)

DS 28: Thin Film Applications

Time: Wednesday 9:30–12:00 Location: H8

Invited Talk DS 28.1 Wed 9:30 H8
Surface analytics with electron spectroscopy on coated steel sheets — •David Stifter — Christian Doppler Laboratory for microscopic and spectroscopic material characterisation, Zentrum für Oberflächen- und Nanoanalytik, Johannes Kepler Universität Linz, Altenberger Straße 69, A-4040 Linz, Austria

Modern steel industry faces the challenge to provide new innovative materials and products with properties which fulfill the requirements of the market, especially including aspects related to high strength, light weight, reliable galvanizability, increased corrosion resistance and aesthetics. Phenomena like surface segregation of alloying elements, formation of oxide layers and corrosion products as well as gradient formation within organic top coatings call for advanced analytical studies of the developed materials down to the nanoscale.

In this contribution X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES) and reflection electron energy loss spectroscopy (REELS) will be shown to provide as surface sensitive analytical methods valuable insight for understanding the structure and processes occurring on the surfaces and interfaces of modern coated steel materials. In this context it will be underlined in detail that utmost care has to be taken in the investigation of such uncooperative surfaces, which exhibit a highly complex and heterogeneous nature. Adverse effects - related to differential charging or material degradation of partly unstable compounds formed on the surfaces - have to be carefully taken into account to perform accurate surface analytics.

DS 28.2 Wed 10:00 H8
Screening of Copper-Nickel thin film combinatorial library for electrocatalytic applications — •Isabella Pötzelberger[1], Andrei Ionut Mardare[1,2], and Achim Walter Hassel[1,2] — [1]Institute for Chemical Technology of Inorganic Materials Johannes Kepler University Linz, Altenberger Str. 69, 4040 Linz, Austria — [2]Christian Doppler Laboratory for Combinatorial Oxide Chemistry at the Institute for Chemical Technology of Inorganic Materials, Johannes Kepler University Linz, Altenberger Str. 69, 4040 Linz, Austria

A Cu-Ni thin film combinatorial library was screened for electrocatalytic oxidation of formaldehyde in alkaline solution using a 3D-printed flow type scanning droplet cell microscope. The entire compositional spread (1 to 14 at.% Ni) showed suitability for being used in formaldehyde detection with different efficiencies as evidenced by cyclic voltammetry performed with and without formaldehyde addition to the electrolyte. This difference is directly linked to the electrocatalysis of the oxidation process. Therefore a surface microstructure evolution along the library was investigated by SEM. Kinetic studies performed by varying rates of potential increase revealed a diffusion limited process as evidenced by the observed linearity between the current density and inverse scan rate. Amperometric measurements performed at various applied potentials indicated a sufficiently large increase in the current density plateaus responsible for formaldehyde detection suitable for being implemented in device fabrication showing a good reproducibility and stability in the electrocatalytic oxidation of formaldehyde.

DS 28.3 Wed 10:15 H8

Oxidation behaviour of arc evaporated (Ti,Cr,Al)N coatings studied by SR-XRPD — •Daniel Michael Ostach[1], Norbert Schell[1], Andreas Schreyer[1], Jens Birch[2], Jeremy Schroeder[2], Lina Rogström[3], Chen Yu-Hsiang[3], and Mats Johannson-Joesaar[4] — [1]Helmholtz-Zentrum Geesthacht Zentrum für Material- und Küstenforschung, 21502 Geesthacht, Germany — [2]Thin film physics, IFM, Linköping University, 581 83 Linköping, Sweden — [3]Nanostructured materials, IFM, Linköping University, 581 83 Linköping, Sweden — [4]SECO Tools AB, Fagersta, Sweden

Hard and wear resistant cubic (c)-(Ti,Al)N based coatings have many applications, such as protection of the underlying bulk material and improved wear resistance. In the cutting tool industry, the improved wear resistance increases the lifetime of the coated tools. The mechanical properties of TiAlN deteriorates at high temperatures due to formation of the hexagonal (h) AlN phase, while by alloying of Cr in (Ti,Al)N coatings the detrimental effect of h-AlN on the mechanical properties can be reduced. Further, the oxidation resistance of CrAlN coatings is improved compared to that of TiAlN, thus, a TiCrAlN coating could be expected to have both, high oxidation resistance and high mechanical properties. In this study, in-situ high-energy synchrotron radiation x-ray powder diffraction (SR-XRPD) during annealing in an air atmosphere has been performed to study the oxidation process of TiCrAlN. The results reveal that the oxidation behavior changes with Al-content and Ti-content and TiCrAlN with low Ti-content show a higher oxidation resistance.

DS 28.4 Wed 10:30 H8

Hard X-Ray Microscopy with Multilayer Zone Plates — •Christian Eberl[1], Florian Döring[1], Markus Osterhoff[2], Tim Salditt[2], and Hans-Ulrich Krebs[1] — [1]Institut für Materialphysik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institut für Röntgenphysik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

X-ray microscopy is due to the small wavelength and high penetration depth an auspicious technique for improved investigations of materials on nm-scale. For this, multilayer zone plates (MZP) with well-defined and smooth multilayers of low thickness grown on wires are promising optical elements. The combination of pulsed laser deposition (PLD) and focused ion beam (FIB) has been proven to be extraordinarily suitable for the fabrication of MZPs and we could demonstrate a sub-5nm hard x-ray focus [1,2]. In order to make those MZPs applicable for nanoscopy basically a larger overall multilayer thickness is required. For this, a deep understanding of the underlying processes (such as target changes as well as resputtering and backscattering during film growth) is essential. Hence, detailed investigations have been carried out using complementary methods such as X-ray diffraction (XRD), X-ray reflectivity (XRR), transmission electron microscopy (TEM) in cross section as well as SDTrimSP simulations. Here we present our latest results demonstrating that a compound optics (formed by Kirkpatrick-Baez mirrors and a high quality MZP) is usable for microscopy applications.

[1] Döring et al., Opt. Expr. 21 (2013); [2] Eberl et al., Appl. Surf. Sci. 307 (2014)

15 min. break.

DS 28.5 Wed 11:00 H8

Gradient gold island films for the optimization and quantification of surface enhanced infrared absorption — •Christoph Kratz, Tom Oates, and Karsten Hinrichs — Leibniz-Institut für Analytische Wissenschaften -ISAS- e.V., Berlin, Deutschland

Surface enhanced infrared absorption (SEIRA) has gained large interest for biosensor applications. SEIRA enables to boost sensitivity of the label free and non-destructive technique of IR-spectroscopy for studying ultrathin films by a factor of about 10-100. In conjunction with optical modeling and simulations IR spectroscopy allows for the interpretation of molecule specific vibrational bands to determine chemical and structural changes as well as the adsorbed/desorbed amount of molecules and proteins. Application of enhancement substrates with a thickness gradient allows studying the influence of thickness effects on the enhancement on a single substrate. These effects have been studied with a model system of a self-assembled monolayer of 4-mercaptobenzonitrile. Structural and optical properties of the bare and modified enhancement substrate were determined by various methods. The investigations show that an a priori indication of the enhancement can be obtained by the observation of a band related to the native oxide below the island film.

DS 28.6 Wed 11:15 H8

Minimizing thermal conductivity in laser deposited multilayers — •Florian Döring[1], Christian Eberl[1], Bea Jaquet[1], Christina Klamt[1], Henning Ulrichs[2], Maria Mansurova[2], Markus Münzenberg[3], and Hans-Ulrich Krebs[1] — [1]Institute for Materials Physics, University of Göttingen — [2]1st Institute of Physics, University of Göttingen — [3]Institute for Physics, University of Greifswald

Modern materials featuring a minimized thermal conductivity are desired for a variety of applications such as thermal power storage, thermoelectricity, specialized thermal barrier coatings, or even solid state refrigeration. In fundamental research, a good approach towards such materials lies in the combination of metals and insulators in nanoscale thin films, which can be produced by Pulsed Laser Deposition (PLD). This versatile thin film method allows production of ultra-thin multilayer films, which can consist of metals, semiconductors, oxides and polymers enabling fabrication of material stacks with high a high number of interfaces between different materials with a high acoustic mismatch. This composition leads to our goal of a reduced thermal conductivity due to phonon scattering and reflection. In this work, predominantly multilayers consisting of W and ZrO_2 respectively W and PC are pulsed laser deposited and carefully analyzed by electron microscopy, x-ray reflectometry and x-ray diffraction. Afterwards, the phonon dynamics in those materials are studied using fs-pump-probe reflectivity measurements. For the final investigation in thermal conductivity, a transient thermal reflectometry setup was implemented.

DS 28.7 Wed 11:30 H8

Electric Conductivity of Ultrathin Gallium Layers — •Frank Lawrenz[1], Stephan Block[2], and Christiane A. Helm[1] — [1]Inst. for Physics, University Greifswald, 17487 Greifswald, Germany — [2]Chalmers University of Technology, 41296 Göteborg, Sweden

Fabrication of ultrathin conductive layers is important for many technological applications. We describe a simple method for the formation of 3 nm thin gallium layers that extent up to 1 cm^2. UV-vis, ellipsometry and conductivity measurements show that the Ga layers immediately oxidize at their surface under ambient conditions, followed by slow oxidation that is completed within three weeks. The specific conductivity as determined by Ohm's law is 1 order of magnitude smaller than that of bulk Ga even for fresh layers, motivating application of the Fuchs-Sondheimer law for ultrathin metal layers for accurate quantification. The decrease in conductivity shows the same time dependence as the Ga oxidation and is described by a developed rate model.

DS 28.8 Wed 11:45 H8

Creation of various nanoporous surfaces for physically induced osteogenic stem cell differentiation — •Martin Gottschalk[1], Matthias Schürmann[2], Peter Heimann[2], Barbara Kaltschmidt[2], Christian Kaltschmidt[2], and Andreas Hütten[1] — [1]Department of Physics, Center for Spinelectronic Materials and Devices, University of Bielefeld, D-33615, Germany — [2]2Department of Cell Biology, Faculty of Biology, University of Bielefeld, D-33615, Germany

The engraftment of orthopedic implants into bone tissue is mainly achieved by stem cells, which are differentiated into osteoblasts in the vicinity of the bone-implant-interface. It is known, that various surface topographies on the nanoscale are able to promote the differentiation process [2]. Thus, a physically induced differentiation by the topography of a titanium covered surface presents an interesting and promising alternative for future clinical use. It is known that anisotropically distributed 30 nm pores in a titanium coated polycarbonate membrane lead to cell differentiation [1]. The main approach is to generate a well-defined nanoporous surface in the pore-size-range of 30 nm by other approaches, like e-beam-lithography plus sputtering, to investigate further adjustments in the osteogenic cell differentiation. For a more precise analysis of the cell-pore-interaction in a TEM, a FIB-SEM-system is used to structure the needed pores into coated TEM grids.

References [1] M. Schürmann et al., Stem Cell Research 13, 98-110 (2014) [2] T. Sjöström et al., Nanomedicine 8, 89-104 (2013)

DS 29: Hybrid and Perovskite Photovoltaics III (Joint session of CPP, DS and HL, organized by DS)

Time: Wednesday 9:30–11:45 Location: H11

DS 29.1 Wed 9:30 H11

Impact of Preparation Conditions on the Ionization Energy and Electronic Structure of CH3NH3PbI3 Perovskites — •Jennifer Emara[1], Tobias Schnier[1], Neda Pourdavoud[2], Thomas Riedl[2], Klaus Meerholz[1], and Selina Olthof[1] — [1]University of Cologne, Institute for Physical Chemistry, Luxemburger Straße 116, 50939 Köln, Germany — [2]Institute of Electronic Devices, University of Wuppertal, Rainer-Grunter-Straße 21, 42119 Wuppertal, Germany

Hybrid organic/inorganic halide perovskites have lately been a topic of great interest in the field of solar cell applications, with the potential to achieve device efficiencies exceeding other thin film device technologies. Yet, large variations in device efficiency and basic physical properties are reported. This is due to unintentional variations during film processing, which have not been systematically investigated so far. We therefore conducted an extensive study of the electronic structure of a large number of CH3NH3PbI3 perovskite films produced by different preparation methods and by varying precursor ratios. We show that variations in film stoichiometry lead to vast changes in the density of states (DOS), and changes in ionization energy, which can be intentionally tuned by almost 1 eV. Using x-ray diffraction measurements, we find the variations in film stoichiometry are not due to the formation of separate phases, but that interstitials and vacancies are homogeneously distributed within the material. Implementing the prepared perovskite layer materials in solar cells, we find a clear correlation between the changes in DOS with the overall power conversion efficiency.

DS 29.2 Wed 9:45 H11

Two dimensional organometal halid perovskite nanosheets in light emitting application — •Rui Wang[1], Zhendong Fu[1], Vitaliy Pipich[1], Alexandros Koutsioumpas[1], Stefan Mattauch[1], Peter Müller-Buschbaum[2], and Henrich Frielinghaus[1] — [1]Jülich Center for Neutron Science, outstation at FRM II, Lichtenbergstr. 1, 85747 Garching — [2]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Two dimensional functional materials have created intensive research interest for high efficiency solar cells. Recently low dimensional perovskite nanocrystals, such as 2D perovskite nanosheets have been reported to possess reduced fluorescence decay times, an increased exciton binding energy and low conductivity in certain crystallographic directions. Consequently, these lower dimensional perovskites can be utilized for light emitting applications. In the present work, 2D nanosheet perovskites are formed by using octylamine bromide as capping ligands. GISANS combined with neutron reflectivity (NR) are applied to investigate the structure buried inside the thin films. GISANS had proven to be a powerful technique for thin film morphology investigations. NR guarantees that information about nanometer sized layers can be accessed. We present the determined structures in terms of optical properties, grain size information and stacked layered characteristic.

DS 29.3 Wed 10:00 H11

Morphology and crystal orientation of hybrid perovskite thin films for application in high efficiency solar cells — •Johannes Schlipf[1], Lukas Oesinghaus[1], Nadja Giesbrecht[2], Yinghong Hu[2], Sigrid Bernstorff[3], Thomas Bein[2], Pablo Docampo[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Department of Chemistry and CENS, LMU München, 80539 München, Germany — [3]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, 34149 Trieste, Italy

Organo-metal halide perovskites mark a paradigm shift in photovoltaic research, as they combine high efficiencies challenging conventional inorganic solar cells with easy processing and cheap abundant precursor materials. Recent reports of power conversion efficiencies around 20% are possible due to remarkable material properties and their highly crystalline nature even when processed from solution. However, photovoltaic performance is directly linked to film morphology which in turn depends on the fabrication method. We investigate hybrid perovskite thin films of high efficiency solar cells prepared by various synthesis protocols with X-ray diffraction, GIWAXS and GISAXS. Thereby, we evidence different crystallization mechanisms that lead to certain morphologies and crystal orientations reflecting the chosen synthesis method [1]. We link these findings to the photovoltaic performance and aim at a rational development of new synthesis methods for high efficiency perovskite solar cells.

[1] Schlipf et al: J. Phys. Chem. Lett, 6, 1265-1269, 2015.

DS 29.4 Wed 10:15 H11

Influence of annealing time on crystal structure and composition of CH3NH3PbI3-xClx mixed halide perovskite film — •Maryline Ralaiarisoa[1], Yan Busby[2], Johannes Frisch[1], Ingo Salzmann[1], Jean-Jacques Pireaux[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6, 12489 Berlin, Germany — [2]Research Center in the Physics of Matter and Radiation , Laboratoire Interdisciplinaire de Spectroscopie Electronique (LISE), University of Namur, 5000 Namur, Belgium

Thermal annealing is a crucial step for the formation of crystalline perovskite films from precursor solution. However, the structural evolution during perovskite film formation and particularly its composition during annealing have not been thoroughly characterized yet. Such characterization is essential to understand the mechanisms leading to the complete conversion to perovskite. Using ToF-SIMS, we monitored the changes in composition and structure of CH3NH3PbI3-x Clx perovskite films after two different annealing stages, that is, before and after complete perovskite crystallization. At the early stage of annealing, our results show phase separation throughout the entire film depth into one where perovskite was formed and another where mostly the inorganic precursor PbCl2 was detected. After sufficiently long annealing, we found a single perovskite phase of homogeneous composition on the micrometer scale. By means of UPS, we further observed that perovskite films become more n-type for longer annealing time, which correlates the morphological evolution and the surface electronic structure.

15 min. break.

DS 29.5 Wed 10:45 H11

Ferroelasticity in methylammonium lead halide perovskite? — Ilka Hermes[1], Simon Bretschneider[1], Victor Bergmann[1], Dan Li[1], Alexander Klasen[1,2], Julian Mars[1], Wolfgang Tremel[2], Frédéric Laquai[1], Hans-Jürgen Butt[1], Markus Mezger[1,2], Rüdiger Berger[1], Brian Rodriguez[3], and •Stefan Weber[1,2] — [1]MPI for Polymer Research, Mainz — [2]Johannes Gutenberg University, Mainz — [3]University College Dublin, Ireland

Methylammonium lead halide ($MAPbX_3$) perovskite materials show an outstanding performance in photovoltaic devices. However, some material properties, especially the possible ferroic behavior, remain unclear. We observed distinct nanoscale periodic domains in the piezoresponse of $MAPbI_3$(Cl) grains. The structure and the orientation of these striped domains is indicating ferroelasticity as their origin. By correlating vertical and lateral piezoresponse force microscopy experiments performed at different sample orientations with x-ray diffraction, the preferred domain orientation was assigned to the $a_1 - a_2$-phase. The observation of the twin domains appears to strongly depend on the preparation route and the film texture and is thought be induced by internal strain during the cubic-tetragonal phase transition.

DS 29.6 Wed 11:00 H11

XPS study of the ALD growth of Al_2O_3 on the $CH_3NH_3PbI_3$ — •Małgorzata Sowińska[1], Chittaranjan Das[1], Konrad Wojciechowski[2], Henry Snaith[2], and Dieter Schmeisser[1] — [1]Brandenburgische Technische Universität Cottbus-Senftenberg, Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX13PU, UK

Organic-inorganic lead halide perovskites have emerged as very attractive absorber materials for the fabrication of low cost and high efficiency solar cells, but a delicate nature of these films is one of the main challenges for a successful commercialization. Typically, when exposed to air or moisture, perovskite films degrade within a couple of hours or days. Moreover, the methylammonium lead triiodide ($CH_3NH_3PbI_3$) perovskite cannot sustain a prolonged annealing at temperatures around 85°C. In this work, we are investigating stability (upon air and thermal exposure) of a $CH_3NH_3PbI_3$ perovskite film coated with a thin layer of Al_2O_3 deposited by atomic layer deposition (ALD). In particular, the chemical and electronic changes occurred at the $Al_2O_3/CH_3NH_3PbI_3$ interface during the first 50 ALD cycles were monitored ex-situ by high-resolution and surface-sensitive synchrotron-based X-ray photoelectron spectroscopy (SR-XPS). The advantage of the ALD as a deposition method is that it can produce extremely dense layers with a very precise thickness control at room temperature. Detailed SR-XPS data analysis and a stability test of the perovskite film with alumina will be presented.

DS 29.7 Wed 11:15 H11

Water based hybrid solar cells: spray deposition of the active layer monitored with x-ray scattering methods — •Volker Körstgens[1], Christoph Mayr[1], Stephan V. Roth[2], Hristo Iglev[3], Reinhard Kienberger[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]DESY Photon Science, Notkestr. 85, 22607 Hamburg — [3]TU München, Physik-Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748 Garching

Spray-coating is a technique suitable for the large-scale and cost-effective preparation of hybrid photovoltaics. Unique environmentally friendly processing of hybrid solar cells can be realized with systems based on the solvent water. Using an active layer consisting of laser-ablated titania nanoparticles and water-soluble poly[3-(potassium-6-hexanoate)thiophene-2,5-diyl] (P3P6T) hybrid solar cells were realized. [1] For the performance of these devices the morphology of the active layer is of major importance. We followed the development of the morphology in situ with high spatial and temporal resolution. The mesoscale was probed with GISAXS and the crystallinity of the polymer and the inorganic component was probed with GIWAXS. The changes of the morphology of the active layer with increasing thickness and the dependence on the blocking layer chosen as the initial substrate are discussed and implications for an improved spray protocol will be given.

[1] Körstgens et al., Nanoscale 7, 2900 (2015).

DS 29.8 Wed 11:30 H11

A low temperature route towards hierarchically structured titania films for thin hybrid solar cells — •Lin Song[1], Amr Abdelsamie[1], Christoph J. Schaffer[1], Volker Körstgens[1], Weijia Wang[1], Nicola Hüsing[2], Paolo Lugli[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Materialchemie, FB Chemie und Physik der Materialien, Universität Salzburg, Hellbrunnerstr. 34, 5020 Salzburg, Austria — [3]TU München, Department of Electrical Engineering and Information Technology, Institute for Nanoelectronics, 80333 München, Germany

Fabricating titania based solar cells at low temperature has a high significance regarding energy efficacy , since most of photovoltaic devices with titania require high-temperature calcination. Moreover, a low-temperature process offers the potential for flexible solar cells. However, this kind of solar cells has a low efficiency. In order to improve the device performance, we make superimposed structural order on titania films from nanometer to submicrometer length scales. Hierarchical structural order enhances light harvesting in solar cells, thereby enhancing the photovoltaic performance. Titania nanostructures are obtained via PS-b-PEO template assisted sol-gel processing. Nanoimprint lithography (NIL) provides ordered submicrometer patterns as a superstructure over nanostructured titania films. SEM and AFM measurements map the film surface morphology, and GISAXS measurements yield information about the bulk film morphology. The optoelectronic properties are examined by UV/Vis spectroscopy.

DS 30: Transport: Graphene (Joint session of DS, DY, HL, MA, O and TT, organized by TT)

Time: Wednesday 9:30–13:15 Location: H22

Invited Talk DS 30.1 Wed 9:30 H22

Ultrafast photo-thermoelectric currents in graphene — •Alexander Holleitner — Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, D-85748 Garching, Germany.

We show that photo-thermoelectric currents occur on a picosecond time-scale in graphene [1]. To this end, we apply an on-chip pump/probe photocurrent spectroscopy [2,3] to double-gated junctions of graphene. Our experiments reveal the interplay of photogenerated hot electrons with so-called photovoltaic currents. Moreover, we demonstrate that hot electrons allow to read-out an ultrafast non-radiative energy transfer from fluorescent emitters, namely nitrogen-vacancy centers in nano-diamonds. The non-radiative energy transfer can be exploited as an ultrafast, electronic read-out process of the electron spin in nitrogen vacancy centers in the diamond nanocrystals. The detection gives access to fast energy transfer processes, which have not yet been observed by fluorescence measurements because of quenching of the optical signal for short transfer distances [4].

We thank A. Brenneis, F. Schade, L. Gaudreau, M. Seifert, H. Karl, M.S. Brandt, H. Huebl, J.A. Garrido, F.H.L. Koppens, for a very fruitful collaboration, and the ERC-grant ‘NanoREAL’ for financial support.

[1] A. Brenneis et al., (2016)
[2] L. Prechtel et al., Nature Comm. **3**, 646 (2012)
[3] C. Kastl et al. Nature Comm. **6**, 6617 (2015)
[4] A. Brenneis et al. Nature Nanotech. **10**, 135 (2015)

DS 30.2 Wed 10:00 H22

Double-logarithmic velocity renormalization at the Dirac points of graphene — •Peter Kopietz, Anand Sharma, and Carsten Bauer — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Str. 1, 60438 Frankfurt

Using a functional renormalization group approach with partial bosonization in the forward scattering channel we reconsider the effect of long-range Coulomb interactions on the quasi-particle velocity v_k close to the Dirac points of graphene. In contrast to calculations based on perturbation theory and field theoretical renormalization group methods, we find that v_k is proportional to $\ln[\kappa_k/k]$ where k is the deviation of the quasiparticle momentum from the Dirac points and the cutoff scale κ_k vanishes logarithmically for small k. We show that this double-logarithmic singularity is compatible with experiments and with the known three-loop expansion of v_k which contains terms of order $\ln k$ and $\ln^2 k$.

DS 30.3 Wed 10:15 H22

Dirac fermion wave packets in oscillating potential barriers — Walter Pötz[1], Sergey E. Savel'ev[2], Peter Hänggi[3], and •Wolfgang Häusler[3] — [1]Karl Franzens Univ. Graz, Inst. Phys., A-8010 Graz, Austria — [2]Department of Physics, Loughborough University, Loughborough LE11 3TU, United Kingdom — [3]Institut für Physik, Univ. Augsburg, 86135 Augsburg, Germany

We integrate the time-dependent (2+1)D Dirac equation for massless fermions in graphene or topological insulator surfaces. A recently developed staggered-grid leap-frog scheme is employed [1,2]. We con-

sider an initial Gaussian wave packet which moves in the x-direction towards a potential barrier that is homogeneous along y and oscillates periodically in time. As for the x-dependence, we investigate square-well, sinusoidal, and linear-ramp potential profiles. Small transversal momentum components k_y of the wave packet were analyzed analytically [3] and predicted to generate non-zero current densities j_y, even at normal incidence $k_y = 0$ [4]. These findings are consistent with the present numerical studies of particle-, current-, and spin-density. We also investigate massive fermions: regarding some properties they resemble massless fermions, regarding other properties, however, peculiar intrinsic oscillations, reminiscent of Zitterbewegung, appear.
[1] R. Hammer and W. Pötz, PRB **88**, 235119 (2013)
[2] R. Hammer *et al.*, J. Comp. Phys. **265**, 50 – 70 (2014)
[3] S.E. Savel'ev, W. Häusler, and P. Hänggi, PRL **109**, 226602 (2012)
[4] S.E. Savel'ev, W. Häusler, and P. Hänggi, EPJB **86**, 433 (2013).

DS 30.4 Wed 10:30 H22

Electric and magnetic control of electron guiding in graphene — •Ming-Hao Liu and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg

Electrons in graphene are known to behave like massless Dirac fermions, whose transport properties can be best revealed by experiments using ultra-clean graphene. Reliable quantum transport simulations for ballistic graphene is naturally a powerful tool for understanding and predicting high-quality transport experiments. In this talk we show gate-controlled electron guiding along electrically confined channels in suspended graphene, which is a combined work of our transport simulations and the experiment done by the Schönenberger group [1]. We have recently further applied our simulation (Green's function method within the scalable tight-binding model [2]) to revisit the transverse magnetic focusing experiment [3], where the guiding of the electrons is controlled by an external magnetic field, instead of electrical gates. Besides good agreement with the experiments [1,3], our simulations further allow for probing charge flow through an additional scanning probe tip.
[1] P. Rickhaus *et al.*, Nano Lett. **15**, 5819 (2015).
[2] M.-H. Liu *et al.*, Phys. Rev. Lett. **114**, 036601 (2015).
[3] T. Taychatanapat *et al.*, Nat. Phys. **9**, 225 (2013).

DS 30.5 Wed 10:45 H22

Current flow paths in deformed graphene: from quantum transport to classical trajectories in curved space — •Nikodem Szpak[1] and Thomas Stegmann[1,2] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [2]Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca

We compare two contrasting approaches to the electronic transport in deformed graphene: a) the condensed matter approach in which current flow paths are obtained by applying the non-equilibrium Green's function (NEGF) method to the tight-binding model with local strain, b) the general relativistic approach in which classical trajectories of relativistic point particles moving in a curved surface with a pseudo-magnetic field are calculated. The connection between the two is established in the long-wave limit via an effective Dirac Hamiltonian in curved space. Geometrical optics approximation, applied to focused current beams, allows us to directly compare the wave and the particle pictures. We obtain very good numerical agreement between the quantum and the classical approaches for a fairly wide set of parameters. The presented method offers an enormous reduction of complexity from irregular tight-binding Hamiltonians defined on large lattices to geometric language for curved continuous surfaces. It facilitates a comfortable and efficient tool for predicting electronic transport properties in graphene nanostructures with complicated geometries, paving the way to new interesting transport phenomena such as bending or focusing (lensing) of currents depending on the shape of the deformation. It can be applied in designing ultrasensitive sensors or in nanoelectronics.

DS 30.6 Wed 11:00 H22

Trigonal Warping in Bilayer Graphene: Energy versus Entanglement Spectrum — •Sonja Predin, Paul Wenk, and John Schliemann — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We present a mainly analytical study of the entanglement spectrum of Bernal-stacked graphene bilayers in the presence of trigonal warping in the energy spectrum. Upon tracing out one layer, the entanglement spectrum shows qualitative geometric differences to the energy spectrum of a graphene monolayer. However, topological quantities such as Berry phase type contributions to Chern numbers agree. The latter analysis involves not only the eigenvalues of the entanglement Hamiltonian but also its eigenvectors. We also discuss the entanglement spectra resulting from tracing out other sublattices.

15 min. break

DS 30.7 Wed 11:30 H22

Valley-based Cooper pair splitting via topologically confined channels in bilayer graphene — •Alexander Schroer[1], Peter G. Silvestrov[1], and Patrik Recher[1,2] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology Braunschweig, D-38106 Braunschweig, Germany

Bilayer graphene hosts valley-chiral one-dimensional modes at domain walls between regions of different interlayer potential or stacking order. When such a channel is close to a superconductor, the two electrons of a Cooper pair, which tunnel into it, move in opposite directions because they belong to different valleys related by the time-reversal symmetry. This kinetic variant of Cooper pair splitting requires neither Coulomb repulsion nor energy filtering but is enforced by the robustness of the valley isospin in the absence of atomic-scale defects. We derive an effective normal/superconducting/normal (NSN) model of the channel in proximity to an s-wave superconductor, calculate the conductance of split and spin-entangled pairs, and interpret it as a result of *local* Andreev reflection, in contrast to the widespread identification of Cooper pair splitting with crossed Andreev reflection in an NSN geometry.

DS 30.8 Wed 11:45 H22

The decisive role of stacking faults for understanding transport in bilayer graphene — •Heiko B. Weber[1], Ferdinand Kisslinger[1], Christian Ott[1], and Sam Shallcross[2] — [1]Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg (FAU), Erlangen, Germany — [2]Lehrstuhl für Theoretische Festkörperphysik, FAU Erlangen-Nürnberg (FAU)

Charge transport in bilayer graphene provides rich low-temperature phenomena, often assigned to interaction-driven phase transitions. We will discuss charge transport in bilayer graphene in a single-particle picture, but including stacking faults. Such partial dislocations are unavoidable in bilayer graphene and were recently imaged [1]. Depending on details, partial dislocations can introduce improved conductance, fully insulating behaviour or linear magnetoresistance. The latter is reliably found in transport experiments at elevated temperatures [2].
[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer, E. Spiecker, Nature **505**, 533 (2014)
[2] F. Kisslinger, C. Ott, C. Heide, E. Kampert, B. Butz, E. Spiecker, S. Shallcross, H. B. Weber, Nature Phys. **11**, 650 (2015).

DS 30.9 Wed 12:00 H22

Linear magnetoresistance in two-dimensional disordered conductors — •Ferdinand Kisslinger[1], Christian Ott[1], Erik Kampert[2], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg (FAU), Erlangen, Germany. — [2]Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany.

The recent observation of linear magnetoresistance (MR) in large-area bilayer graphene gives a key to the understanding of this old and barely understood phenomenon [1]. In bilayer graphene, it can be traced back to mosaic-like pattern of a partial dislocation network [2]. In this talk we discuss how linear MR evolves in disordered samples, using a two dimensional resistor network model conceptually introduced by Parish and Littlewood [3]. This model is in the weak disorder regime dominated by boundary effects. We identified a new regime representing the bulk situation in a disordered conductor. We investigated different possible sources of disorder: mobility, charge carrier density and network structure. The slope of the MR turned out to be simply governed by the Hall resistance and therefore by the inverse of the charge carrier density. An equivalent circuit model finally gives a consistent explanation as to why the magnetoresistance is linear in mosaic like samples.
[1] F. Kisslinger et al., Nature Physics **11**, 650 (2015)
[2] B. Butz et al., Nature **505**, 533 (2014).
[3] M. M. Parish & P. B. Littlewood, Nature **426**, 162 (2003)

DS 30.10 Wed 12:15 H22

Mechanically strained graphene nanojunctions — •Seddigheh

Nikipar[1], Dmitry Ryndyk[1], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Germany

It has been demonstrated recently that mechanically strained graphene presents interesting electrical properties, which have great potential for novel applications in electronic devices. In particular, the strain in graphene nanoribbons can lead to substantial changes in its electronic properties. Besides, it provides a possibility to develop atomic point contacts and break junctions. The main purpose of this work is to investigate theoretically the influence of uniaxial mechanical strains on graphene nanojunctions in order to design graphene point contact.

To this aim, we developed the computational model by combining density functional theory and molecular dynamics methods. First, we investigated the change of the junction shape with increasing strain and the breaking with the formation of the nanogap. As expected, our theoretical model predicts the deformation of the break junction bottleneck into carbon chains before the rupture of the structure. we evaluated the electronic transmission function of graphene quantum junction by employing a coupled tight bonding and nonequilibrium green function methods. Interestingly it is found that graphene point contact can present resonance transmission in contrast to the conventional metallic point contacts with quantized conductance. This might be originated from influence of other parameters on transmission.

DS 30.11 Wed 12:30 H22

Graphene nanoribbons as effective spin ladders — •Cornelie Koop, Manuel J. Schmidt, and Stefan Wessel — Institut für Theoretische Festkörperphysik, RWTH Aachen University

Zigzag edges of graphene nanoribbons host particular, localized edge states. Since the density of states is strongly enhanced near the edges in graphene, interaction effects between the spins of these edge states become important. We can significantly simplify the analysis of such systems by means of an effective model that separates the edge and bulk states. Treating the effective interactions to first order proves sufficient in most cases, while second order corrections do not dramatically change the results. In many cases, the edge system can be reduced to a general spin ladder model, where the decay of the spin-spin interaction is determined by the shape of the edges. We examine these effective spin ladders at finite temperatures by means of quantum Monte Carlo simulations, using the stochastic series expansion method. Thereby, correlation functions and spin structure factors can be determined for realistically large graphene nanoribbons.

DS 30.12 Wed 12:45 H22

Edge State Structure of the $\nu = 0$ quantum Hall State in monolayer Graphene — •Angelika Knothe[1,2] and Thierry Jolicoeur[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — [2]Université Paris 11, CNRS, LPTMS, UMR 8626, Orsay 91405 France

Single-layer graphene at neutrality under a magnetic field is a many-body insulator whose phase structure is under intense scrutiny. When tilting the applied magnetic field, there is a phase transition towards a conducting state [1]. A plausible description is to start from a SU(4) spin-valley symmetric quantum Hall ferromagnet and add some lattice-scale anisotropies in valley space [2]. In the manifold of ground states captured by this approach, it has been proposed that graphene undergoes a transition between a canted antiferromagnetic state and a ferromagnetic state. While this picture is clear in the bulk of the system, it remains to understand the effect of this phase change on the current-carrying edge states that are formed a the physical boundaries of a real sample [3]. We use an extended Hartree-Fock approach to describe a finite-size system with a simple model for the edge and extract the one-body spectrum. We then describe the current-carrying edge textures.

[1] A. F. Young et al., Nature (London) 505, 528 (2014) [2] M. Kharitonov, Phys. Rev. B 85, 155439 (2012) [3] M. Kharitonov, Phys. Rev. B 86, 075450 (2012); G. Murthy et al., Phys. Rev. B 90, 241410 (2014) and arXiv:1510.04255; A. Knothe and T. Jolicoeur, Phys. Rev. B 92, 165110 (2015)

DS 30.13 Wed 13:00 H22

Spin lifetimes exceeding 12 ns in graphene non-local spin valves at room temperature — •Christopher Franzen[1], Marc Drögeler[1], Frank Volmer[1], Tobias Pohlmann[1], Maik Wolter[1], Kenji Watanabe[2], Takashi Taniguchi[2], Christoph Stampfer[1], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

We present spin transport measurements on graphene non-local spin transport devices by fabricating the electrodes first and subsequently transfer graphene with hexagonal boron nitride on top [1]. We achieve spin lifetimes of 12.6 ns and a spin diffusion length as high as 30 μm at room temperature.
This improvement exceeds all current models for contact-induced spin dephasing which paves the way towards probing intrinsic spin properties of graphene. Furthermore, we investigate the contact properties of our devices using scanning force microscopy (SFM) and conductive SFM. We discuss the importance of using large area hexagonal boron nitride for the transfer process and for achieving such high spin lifetimes and spin diffusion lengths.

[1] M. Drögeler *et al.* Nano Letters **14**, 6050 (2014).

DS 31: Frontiers of Electronic Structure Theory: Focus on Topology and Transport II (Joint session of DS and O, organized by O)

Time: Wednesday 10:30–13:00 Location: H24

DS 31.1 Wed 10:30 H24

Coupled-Cluster approach for both molecules and solids in the numeric atom-center orbital framework — •Tonghao Shen, Arvid Conrad Ihrig, Igor Ying Zhang, and Matthias Scheffler — *Fritz-Haber-Institut der MPG, Berlin.*

For a quantitative prediction of material properties, an advanced description of electronic correlation is crucial. As the "gold standard" correlation method in quantum chemistry, the coupled-cluster (CC) ansatz with singles, doubles and perturbative triples (CCSD(T)) is starting to gain attention in materials science[1]. At present, the CCSD(T)-quality description of the correlation effects in solids can be achieved by either studying the cluster-size convergence toward the bulk in real space[1] or implementing CCSD(T) for extended systems in reciprocal space[2]. In order to investigate and compare these approaches on an equal footing, it is essential to have a computational platform that enables CCSD(T) simulations to be carried out using both cluster and periodic models in a single computational environment. In this report, we present a CCSD(T) implementation for both molecules and solids in the all-electron full-potential code FHI-aims[3] with numeric atom-center orbital(NAO) basis sets. A special memory-distribution strategy is designed to significantly reduce the inter-CPU communication, which is the main challenge for the parallelization of wave-function methods. The accuracy and efficiency are demonstrated for a group of molecules, 1D-, 2D- and 3D-periodic materials. [1] C. Müller, *et al.*, PCCP. **14**, 7605 (2012); [2] A. Grüneis, *et al.*, JCTC **7**, 2780 (2011); [3] V. Blum, *et al.*, CPC **180**, 2175-2196 (2009).

DS 31.2 Wed 10:45 H24

Surface adsorption energetics at the "gold standard": Small molecule binding to TiO_2(110) — •Daniel Berger[1,2], A. Kubas[3], D. Manganas[3], H. Oberhofer[1], F. Neese[3], and K. Reuter[1] — [1]TU München — [2]University of California, Los Angeles — [3]MPI für chemische Energiekonversion, Mülheim an der Ruhr

Adsorption energies at oxide surfaces are central quantities required for catalysis, energy and a multitude of other application areas. At present, the by far dominant computational method to obtain such energetics is density-functional theory (DFT). Unfortunately, systematic benchmarking of such energetics against accurate reference numbers from correlated wave-function theory as known from molecular systems is scarce, largely owing to the fact that the latter techniques are often not available for standard periodic boundary condition supercell calculations.

We address this situation with a solid-state QM/MM embedded cluster approach, in which the adsorbate and immediate surrounding surface atoms are described quantum mechanically, while the long-range electrostatic interactions are accounted for through a polarizable force field. This yields a numerically highly efficient approach that enables use of the recently developed domain-based local pair natural orbital coupled cluster method with single-, double- and perturbative triple-excitations (DLPNO-CCSD(T)) in the quantum region. We exploit corresponding "gold standard" adsorption energies for a set of prototypical small molecules interacting with the rutile $TiO_2(110)$ surface for a systematic benchmark of DFT numbers.

DS 31.3 Wed 11:00 H24

Water adsorpion on surfaces form many-body perturbation theory — •Theodoros Tsatsoulis and Andreas Grüneis — Max-Planck-Institute for Solid State Research, Stuttgart

The accurate description of the interaction of molecules with surfaces is of crucial importance for a wide range of phenomena. While Kohn-Sham density functional theory is one of the most widely-used methods for describing the electronic structure of surfaces, many local and semi-local functionals are often not able to produce accurate molecular adsorption energies. Quantum chemical wave-function based methods such as Møller-Plesset perturbation theory (MP2) and coupled-cluster methods promise controllable accuracy, however, at much higher computational costs. Large part of the latter is due to the number of virtual states. We consider an approach whereby the occupied orbitals are converged in a plane wave basis, whereas the virtual space is then constructed using pseudized Gaussian orbitals expanded in plane waves, leading to reduced computational cost. In particular we study water adsorption on bulk LiH and h-BN sheets at the level of MP2 theory within the projector-augmented-wave method as implemented in VASP [1]. The results are compared to state-of-the-art methods such as hybrid functionals and diffusion Monte Carlo [2].

[1] Marsman et al., The Journal of Chemical Physics, 130, 184103 (2009)

[2] Al-Hamdani et al., The Journal of Chemical Physics, 142, 181101 (2015)

DS 31.4 Wed 11:15 H24

Photo-isomerization in azobenzene-functionalized self-assembled monolayers: The impact of many-body effects — •Caterina Cocchi and Claudia Draxl — Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Self-assembled monolayers (SAMs) of azobenzene-functionalized alkanethiols on gold suffer from hindered photo-isomerization, as observed experimentally [1]. While this behavior is generally ascribed to strong intermolecular coupling, a clear microscopic understanding of this phenomenon is still missing. In order to address this question, we perform a first-principles study of the excited-state properties of azobenzene-functionalized SAMs. In the framework of many-body perturbation theory (GW approximation and Bethe-Salpeter equation), as implemented in the all-electron full-potential code exciting [2], we investigate the optical absorption spectra of these materials, inspecting the influence of packing density and functionalization of the azobenzene molecules with different end groups. Through a systematic analysis of the character of the excitations, we clarify the role and interplay of screening and local-field effects, which strongly impact light absorption and hence photo-isomerization in these systems.

[1] C. Gahl et al. J. Am. Chem. Soc. 132, 1838 (2010). [2] A. Gulans et al. J. Phys.: Condens. Matter 26, 363202 (2014).

DS 31.5 Wed 11:30 H24

Laplace-transformed MP2 with localized Resolution of Identity -efficient in-memory MP2 for large systems — •Arvid Conrad Ihrig[1], Patrick Rinke[2], Igor Ying Zhang[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Aalto University, Helsinki, Finland

A well-known problem in local and semi-local density functional approximations and to a lesser extend also in hybrid functionals is the one-electron self-interaction error, which can lead to a qualitatively wrong description for applications like charge-transfer systems. One possible remedy is the 2nd order Møller-Plesset perturbation theory (MP2), which does not suffer from this error. However, the time and memory requirements for MP2 prevent it routine-use for large molecular and periodic systems. The Laplace-transformed MP2 (LT-MP2) [1] can significantly reduce the computational time, but requires the usage of intermediate variables stored on disk, resulting in an inefficient usage of computational resources. In this work we combine the LT-MP2 with our localized Resolution of Identity (RI-LVL) [2] approach to eliminate the disk-storage bottleneck and fully exploit massive parallelization strategies. RI-LVL expands the basis function pairs in the electron repulsion integrals in local auxiliary basis sets. For the example of water clusters, we demonstrate the favourable memory scaling (at worst N^2) of our new MP2 implementation, which facilitates the in-memory calculation of large systems at high accuracies.

[1] P. Ayala et al., J. Chem. Phys. 110, 3660 (1999)

[2] Ihrig et al., New J. Phys. 17, 093020 (2015)

DS 31.6 Wed 11:45 H24

***GW* singles contributions for the random phase approximation correlation energies** — •Jiri Klimes[1], Merzuk Kaltak[2], Emanuele Maggio[3], and Georg Kresse[3] — [1]J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic — [2]Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY — [3]University of Vienna, Faculty of Physics, Vienna, Austria

The random phase approximation (RPA) to the correlation energy yields often very accurate results for condensed matter systems. However, a general tendency to underbind has been observed for systems such as molecular solids or for adsorption. One of the ways that have been proposed to improve the accuracy of RPA are the so-called singles corrections of Ren and coworkers [1]. We present our derivation of the singles corrections using the assumption that the electron density changes when going from the reference to the interacting system [2]. This leads to a very compact expression for the corrections. Moreover, the singles formula can be easily modified to account for screening effects, giving the *GW* singles. We assess the effect of both the original and modified singles on covalently and metallically bonded systems as well as on simple weakly bonded systems. Finally, we show that adding the singles corrections leads to considerably improved adsorption energies and lattice energies of molecular solids.

[1] Ren, Tkatchenko, Rinke, Scheffler, Phys. Rev. Lett **106**, 153003 (2010).

[2] Klimeš, Kaltak, Maggio, Kresse, J. Chem. Phys. **143**, 102816 (2015).

DS 31.7 Wed 12:00 H24

Long-range corrected DFT meets *GW*: Vibrationally resolved photoelectron spectra from first principles — •Thomas Körzdörfer — Institut für Chemie, Universität Potsdam, D-14476 Potsdam

We introduce an entirely non-empirical and computationally efficient scheme to calculate highly reliable vibrationally resolved photoelectron spectra for molecules from first principles.[1] To this end, we combine non-empirically tuned long-range corrected hybrid functionals with non-self-consistent many-body perturbation theory in the G_0W_0 approximation and a Franck-Condon multi-mode analysis based on DFT-calculated frequencies. The vibrational analysis allows for a direct comparison of the GW-calculated spectra to gas-phase ultraviolet photoelectron measurements of neutral and anionic molecules, respectively. In addition, vertical IPs and EAs were benchmarked against other *GW* methods and basis-set extrapolated CCSD(T) results for a recently introduced test set of 24 molecules frequently used in organic electronics.[2] G_0W_0@LRC-DFT yields mean absolute errors on the order of 0.1 eV for IPs, EAs, and fundamental gaps, clearly outperforming commonly used G_0W_0 approaches as well as partially and fully self-consistent *GW* methods.

[1] L. Gallandi and T. Körzdörfer, JCTC **11**, 5391 (2015).

[2] L. Gallandi, N. Marom, P. Rinke, and T. Körzdörfer, JCTC *accepted for publication* (2015).

DS 31.8 Wed 12:15 H24

LDA-1/2 as a starting point for G_0W_0 calculations — •Ronaldo Rodrigues Pela[1,2], Ute Werner[1], Dmitrii Nabok[1], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany — [2]Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil

For many semiconductors and insulators, LDA represents a bad starting point for G_0W_0 calculations. Hybrid functionals improve upon LDA, but at the price of increasing computational cost of about 2 orders of magnitude. An alternative starting-point for the single-shot G_0W_0 can be the LDA-1/2 method [1], because it approximately includes the self-energy of quasi-particles within a generalized Kohn-Sham scheme, leading to improved band-gaps over the LDA ones, but without being computationally more involved. In this work, we systematically compare 3 starting-points for G_0W_0 calculations: LDA, PBE0, and the LDA-1/2 method. A selection of semiconductors (C, Si, SiC, AlP, LiF, MgO, Ne, Ar, GaN, GaAs, CdS, ZnS, and ZnO) is chosen for this benchmark. We demonstrate that LDA-1/2 is a good choice in most cases, reducing the root mean square error in band-gap predictions by 50% when compared to G_0W_0 on top of LDA or PBE0. With the exception of large band gap materials, LDA-1/2 predictions are already close to the experimental band gaps, and thus G_0W_0 has minor effects.

Reference [1]: Phys. Rev. B 78, 125116 (2008).

Acknowledgements: "Coordenação de Aperfeiçoamento de Pessoal de Nível Superior" (CAPES) and "Alexander von Humboldt Stiftung".

DS 31.9 Wed 12:30 H24

DFT+U within a numeric atom-centered orbital basis — •Matthias Kick, Harald Oberhofer, and Karsten Reuter — Technische Universität München

Materials like transition metal oxides (TMOs) still challenge a description through first-principles density-functional theory (DFT). Appropriately capturing the electron localization in TMOs generally requires at least hybrid exchange-correlation functionals. Such higher-rung functionals come with appreciable computational cost, which limits their use in large supercell calculations. For such applications effective and numerically less intense approaches are therefore still a much sought alternative.

One such method is the DFT+U approach, where the on-site Coulomb correlation effects are treated using a model Hamiltonian, while remaining interactions are treated on the level of semi-local DFT. Full DFT+U functionality including nuclear gradients (forces) has been implemented in the electronic structure code *FHI-aims*. We account for three common occupation matrix representations, differing in the way how the occupations of the correlated subspaces are determined. We critically discuss their performance and differences in the context of the numeric atomic orbital basis sets employed in *FHI-aims*. The established numerically efficient framework is finally used to address neutral and charged oxygen vacancies at the TiO_2(110) surface within a solid-state embedding approach.

DS 31.10 Wed 12:45 H24

High-throughput Screening and Statistical Learning for Design of Transparent Conducting Oxides — •Christopher Sutton, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft

Transparent conducting oxides (TCOs) represent a class of well-developed and commercialized wide-bandgap semiconductors that are crucial for many electronic devices. Ternary Al, Ga, and In-based sesquioxides are investigated as alternative wide-bandgap semiconductors motivated by very intriguing recent experimental work that has demonstrated bandgap engineering in (GayIn1-y)2O3 from 3.8 eV to ca. 5 eV[1] and ca. 5 eV to 7.5 eV for (Al1-xGax)2O3.[2]

New ternary oxides with the chemical structure of (AlxGayIn1-x-y)2O3 have been identified using cluster expansion (CE) models combined with fast stochastic optimization techniques (e.g., Wang-Landau and diffusive nested sampling) in order to efficiently search potential (ordered and disordered) configurations within a given lattice and for different temperatures. Wang-Landau and diffusive nested sampling has also allowed for a consideration of the effect of entropy on the relative stability of ternary oxides. Statistical learning has also been used to identify a structure-property relationship to efficiently identify new wide-band gap TCOs to improve the fundamental chemical and physical properties (e.g., conductivities, mobilities, and optical transparency) by investigating the parameters that control these properties.

[1] F Zhang, et al., Solid State Communications 2014, 186, 28. [2] H Ito, et al., Japanese Journal of Applied Physics 2012, 51, 100207.

DS 32: 2D Materials: Growth (Joint session of DS and O, organized by O)

Time: Wednesday 10:30–13:00 Location: S053

DS 32.1 Wed 10:30 S053

Growth and electronic structure of epitaxial single-layer WS_2 on Au(111) — •Maciej Dendzik, Matteo Michiardi, Charlotte Sanders, Marco Bianchi, Jill A. Miwa, Signe S. Grønborg, Jeppe V. Lauritsen, Albert Bruix, Bjørk Hammer, and Philip Hofmann — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark

Single-layer WS_2 is a promising alternative to the widely studied MoS_2, because of the larger size of the spin-splitting and the lower effective mass of the valence band maximum. Here we present a detailed study of the electronic structure of the large-area single-layer WS_2 grown epitaxially on Au(111) using evaporation of W atoms in a low pressure H_2S atmosphere. The growth process is characterized by means of scanning tunneling microscopy, low-energy electron diffraction and core-level spectroscopy. The electronic band structure of the single-layer WS_2 is determined by angle-resolved photoemission spectroscopy. The valence band maximum at $\bar{K}$ is found to be significantly higher than at $\bar{\Gamma}$. The observed dispersion around $\bar{K}$ is in good agreement with density functional theory calculations for a free-standing monolayer, whereas the bands at $\bar{\Gamma}$ are found to be hybridized with states originating from the Au substrate. Strong spin-orbit coupling leads to a large spin-splitting of the bands in the neighborhood of the $\bar{K}$ points, with a maximum splitting of 419(11) meV. The valence band dispersion around $\bar{K}$ is found to be highly anisotropic with spin-branch dependent effective hole masses of $0.40(02)m_e$ and $0.57(09)m_e$ for the upper and lower split valence band, respectively.

DS 32.2 Wed 10:45 S053

Synthesis of high quality TaS_2 monolayer using molecular beam epitaxy — •Arlette S. Ngankeu, Charlotte E. Sanders, Marco Bianchi, Maciej Dendzik, and Philip Hofmann — Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark

The transition metal dichalcogenide TaS_2 has been intensively studied in its bulk form due to the rich properties arising from the interplay of electronic instabilities. As in many other materials, the electronic properties of TaS_2 might change in interesting ways in the thickness limit of a single layer. However, finding a good method for the production of high quality single layer TaS_2 is still a big challenge, and the thinnest crystals of TaS_2 obtained so far (by exfoliation of the TaS_2 bulk) actually have thicknesses of a few monolayers. In this talk, we report the first successful preparation of single- and few-layered TaS_2 on the Au(111) substrate by molecular beam epitaxy. Scanning tunneling microscopy, low energy electron diffraction and angle resolved photoemission spectroscopy have been used to probe the surface topography and electronic properties of TaS_2/Au.

DS 32.3 Wed 11:00 S053

2D Heterojunctions from Non-local Manipulations of the Interactions — Malte Rösner[1,2], •Christina Steinke[1,2], Michael Lorke[1], Christopher Gies[1], Frank Jahnke[1], and Tim O. Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany

We propose to create lateral heterojunctions in homogeneous two-dimensional materials based on non-local manipulations of the Coulomb interaction using structured dielectric substrates. By means of ab-initio calculations for MoS_2 as well as generic semiconductor models, we show, that changes in the dielectric environment can induce sizeable band-gap modulations. The Coulomb interaction induced self energy corrections in real space are sufficiently non-local, to be manipulated externally, and are clearly localized within a radius of a few unit cell at the same time. This allows to induce spatially sharp interfaces within a single homogeneous monolayer and thus to form a heterojunction by the external manipulation of the Coulomb interaction via structured dielectric substrates. Hence, new kinds of heterojunctions can be constructed by placing semiconducting 2d materials on appropriately structured substrates: For a laterally structured dielectric environment, we find a type-II heterojunction with a sharp band-gap crossover within less than 5 unit cells. By establishing four perpendicular interfaces a band gap modulation reminiscent of a quantum dot can be realised.

DS 32.4 Wed 11:15 S053

TFT Fabrication Based on Liquid Exfoliated MoS_2 Flakes — •Xiaoling Zeng[1], Sonia Metel[2,3], Valeria Nicolosi[2,3,4], and Veit Wagner[1] — [1]Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany — [2]School of Chemistry, Trinity College Dublin, Ireland — [3]CRANN, Trinity College Dublin, Ireland — [4]School of Physics, Trinity College Dublin, Ireland

There is a large interest in establishing cheap, scalable processes for producing low dimensional semiconducting dichalcogenide films for electronic application. In this work, well exfoliated MoS_2 dispersions were prepared through two step liquid phase exfoliation process with N-methyl-pyrrolidone (NMP) and Isopropanol (IPA). The obtained exfoliated MoS_2 flakes were characterized by microscopy (TEM and SEM), Uv - Vis and Raman spectroscopy.

Bottom gate thin film transistors (TFTs) based on exfoliated MoS_2 film were fabricated by using spray coating techniques. The deposition process was optimized to get uniform and percolated MoS_2 film with different thicknesses. Transistors show only minor conductivity directly after layer deposition. However, depositing additional PMMA layer on top shows large improvement in electrical characteristics, i.e. switching behavior with changing gate voltage. Interpretation is that the PMMA layer brings the initially separated flakes into contact and enables proper percolation. Further investigation found that the thickness of PMMA influences the electrical properties. This low-cost and scalable solution-based fabrication process will promote the application of dichalcogenides in future nanoelectronic devices.

DS 32.5 Wed 11:30 S053

Novel Deposition Approach of Semiconducting MoS2 Thin Films and Their Application for Electronic Devices — •Francis Oliver Vinay Gomes[1,2], Marko Marinkovic[1], Jochen Brendt[1], Torsten Balster[2], and Veit Wagner[2] — [1]Evonik Resource Efficiency GmbH, Paul-Baumann-Strasse 1, 45764 Marl, Germany — [2]Jacobs University Bremen, Department of Physics & Earth Science, Campus Ring 1, 28759 Bremen, Germany

In this work, MoS2 films obtained from precursor solution via spin-coating on various substrates were investigated. Molybdenum(V) chloride dissolved in 1-methoxy-2-propanol was used as precursor solution. The MoS2 films obtained from the Mo-precursor upon sulfurization during annealing were analyzed for surface morphology and roughness, chemical composition and crystallinity. In addition, comparison of silicon and sapphire substrates were studied. Our approach focuses on novel deposition technique compared to the current state-of-the-art chemical vapour deposition.

The thickness of the MoS2 films was controlled in the process, and film thicknesses between 2 and 27 nm were obtained. The thickness of the films linearly scaled with precursor concentration. SEM/EDX measurements indicate that the surface morphology and film composition is strongly dependent on the annealing temperature and processing environment. Electrical measurements demonstrate a film conductivity of 0.27 S/cm while XRD confirms the formation of semiconducting 2H-MoS2 films. The future steps will lead towards applying fabricated films in electronic devices such as thin film transistors.

DS 32.6 Wed 11:45 S053

Growing graphene underneath hBN on Rh(111) — •Uta Schlickum[1], Daniel Rosenblatt[1], Sebastian Koslowski[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The stable hexagonal monolayer of hBN is an insulator with excellent dielectric properties. It can be grown on a large variety of transition metal surfaces like Rh(111) on which it shows a hexagonal Moire super-lattice. We grow a single layer of hBN on Rh(111) by chemical vapor deposition and found beside the well known hexagonal structure a new periodic pattern resembling a lattice of a "spoked wheel" (SW). For small coverages this new phase appears at the intersection of the rims connecting three valleys of the Moire lattice, and forms large islands for higher coverage. Atomic resolution topographic images reveal that the phase boundaries do not disturb the atomic lattice periodicity of the hBN. Depending on the preparation parameters, the relative coverage of the two phases can be tuned at will. The crucial parameter determining the relative coverage is the time, the sample stays at about $600^\circ C$ after the exposure to borazine at $800^\circ C$. It is well known that at $600^\circ C$, C impurities segregate and accumulate at the surface. This together with the fact that the hBN lattice itself remains intact crossing a phase boundary, leads us to conclude that the SW phase consists of an additional graphene layer below the hBN layer. Various experimental details, like high resolution spectroscopy, support this interpretation.

DS 32.7 Wed 12:00 S053

Prediction of metastable two-dimensional compounds in the C/Si system using global optimization techniques, and investigation of their electronic properties — •Johann Christian Schön and Rico Gutzler — MPI for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart

We employ the global energy landscape exploration package G42+[1,2] to predict (meta)stable two-dimensional crystalline polymorphs in the carbon/silicon system for a range of compositions: C:Si = 1:0, 3:1, 2:1, 1:1, 1:2, 1:3, and 0:1.[1] During the global search (energy function: DFT), both atom positions and cell parameters in the xy-plane were allowed to vary freely. The global optimization method used was basin-hopping-simulated annealing, with two consecutive local optimizations - the first keeping the atoms restricted to the z = 0 plane, while the second one also permitted relaxation in the z-direction. For all compositions, the lowest energy 2D-structures exhibited a graphene-like super-structure with 6-membered rings, but many quite stable competing minimum structures containing a variety of rings of size 4 - 12 were also observed. Deviations from planarity occurred most frequently for structures where a high local concentration of the Si-atoms was present. Complementing geometric structure prediction, we performed band-structure calculations to investigate the effect of geometry and C:Si ratio on the electronic properties of these 2D-materials.

[1] J. C. Schön, Proc. Appl. Ceram. 9:157-168 (2015); [2] J. C. Schön, G42+ Manual, www.chemie.uni-bonn.de/ac/schoen/forschung/g42-manual, (2015)

DS 32.8 Wed 12:15 S053

Tuning the physical properties of MoS_2 membranes by organophosphonate interfacial chemistry — •Susanne Schwarzwälder[1], Réka Csiki[1], Eric Parzinger[1], Jeffrey Schwartz[2], Alexander Holleitner[1], Martin Stutzmann[1], Ursula Wurstbauer[1], and Anna Cattani-Scholz[1] — [1]Walter Schottky Institut and Physik Department, Technische Universität München, Germany — [2]Princeton University, New Jersey, USA

One of the most prominent members of the 2D material family is the transition metal dichalcogenide MoS_2, due to its natural occurrence and its promising potential applications in nanoelectronic and optoelectronic devices [1]. Interfacial chemistry strongly influences the interaction of molecularly thin semiconducting membranes with the underlying substrate, hence a suitable silicon surface functionalization can be employed for improving the performance of MoS_2-based devices [2]. Our work focuses on the investigation of surface functionalization using homogeneous organophosphonate self-assembled monolayers (SAMs) covalently bonded to SiO_2. In particular, the interaction of single layer (SL) MoS_2 with SAMs based on four different aromatic phosphonic acids are investigated. Modulation of the intrinsic n-type doping of SL-MoS_2 via charge transfer with aromatic SAMs is suggested by a shift in the Raman-active out-of plane vibrational mode A_{1g}, emphasizing the importance of interfacial interactions in MoS_2-based nanodevices.

[1] R. Ganatra, Q. Zhang, ACS Nano 8, 4074 (2014).

[2] S. Najmaei et al., Nano Lett. 14, 1354 (2014).

DS 32.9 Wed 12:30 S053

Structural analysis of one monolayer of hBN on Cu(111) via NIXSW and SPA-LEED — •Timo Heepenstrick[1], Christine Brülke[1], Ina Krieger[1], Sergey Subach[2], Simon Weiss[2], Niklas Humberg[1], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstraße 12, 53115 Bonn, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52452 Jülich, Germany

We present a detailed structural analysis of hBN on Cu(111) with normal incidence x-ray standing waves (NIXSW) supported by spot profile analysis low energy electron diffraction (SPA-LEED). hBN forms an incommensurate structure on Cu(111) with a lattice mismatch of 2.3% corresponding to the unstrained hBN layer. The NIXSW experiments show that the hBN layer is weakly bonded with a distance of 3.23 Å (for the nitrogen) and 3.26 Å (for the boron) and shows little buckling. We also present an analysis for the topmost Cu(111) layer with and without a monolayer of hBN.

DS 32.10 Wed 12:45 S053

Nanotents - 2 nm void-formation and self-healing in 2D monolayers on metals — •Huanyao Cun[1], Marcella Iannuzzi[2], Adrian Hemmi[1], Silvan Roth[1], Jürg Osterwalder[1], and Thomas Greber[1] — [1]Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland — [2]Chemistry-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

At room temperature, it is quite challenging to immobilize single atoms. However, with the single layers of hexagonal boron nitride (h-BN) or graphene, site-selective immobilization of atoms at surfaces becomes feasible. The h-BN nanomesh is a corrugated structure that consists of two regions, the 'pores' with 2 nm diameter and the surrounding 'wire' regions.

In the present study, we demonstrate that the h-BN nanomesh, which acts as thin "rainfly", can trap atoms at distinct subsurface sites and form so-called "nanotents" structure. Remarkably, annealing to 900 K induces the "can-opener" effect: h-BN flakes at pore sites are cut out from the h-BN monolayer and 2 nm voids form on the h-BN surface. We assign the "can-opener" effect to the vacancy defects generated during the Ar+ penetration. Higher temperature annealing leads to the "self-healing" of the h-BN monolayer. Systematic measurements reveal that the entire process, including nanotent formation, "can-opener" effect and nanomesh "self-healing", is well controlled and repeatable. The reported effects are robust and quite general: they are also observed in graphene on ruthenium, for neon and rubidium atoms.

DS 33: Frontiers of Electronic Structure Theory (Joint session of DS and O, organized by DS)

Time: Wednesday 12:00–12:45 Location: H11

DS 33.1 Wed 12:00 H11

Towards Accurate Energy Level Alignment at Physisorbed Molecule-Metal Interfaces from Density Functional Theory — •David A. Egger[1], Zhenfei Liu[2], Jeffrey B. Neaton[2,3,4], and Leeor Kronik[1] — [1]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel — [2]Molecular Foundry and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States — [3]Department of Physics, University of California, Berkeley, California 94720, United States — [4]Kavli Energy Nanosciences Institute at Berkeley, Berkeley, California 94720, United States

A key physical quantity for electronic transport in nanostructured molecule-metal interfaces is the energy level alignment of the molecular electronic states with respect to the Fermi level of the metal. Here, we introduce an efficient theoretical method that is based on density functional theory, but in contrast to common approximations fulfills physically motivated criteria for exchange-correlation interactions and can therefore yield quantitatively accurate energy level alignment information for physisorbed metal-molecule interfaces.[1] We validate our approach by a detailed comparison with experimental and theoretical reference data for several prototypical interfaces of this kind: benzene on graphite (0001), and 1,4-benzenediamine, Cu-phthalocyanine, and 3,4,9,10-perylene-tetracarboxylic-dianhydride on Au(111). Our results indicate that obtaining quantitatively accurate energy level alignment information from density functional theory is possible.
[1] Nano Lett. 15, 2448 (2015)

DS 33.2 Wed 12:15 H11

Fermi orbital self-interaction corrected electronic structure of molecules beyond local density approximation — •Torsten Hahn[1], Simon Liebing[1], Jens Kortus[1], and Mark Pederson[2] — [1]Institute for Theoretical Physics, TU Freiberg, 09599 Freiberg, Germany — [2]Department of Chemistry, Johns Hopkins University, Baltimore, USA

The correction of the self-interaction error that is inherent to all standard density functional theory (DFT) calculations is an object of increasing interest. We present our results on the application of the recently developed Fermi-orbital based approach [1,2] for the self-interaction correction (FO-SIC) to a set of different molecular systems [3]. Our study covers systems ranging from simple diatomic to large organic molecules. Our focus lies on the direct estimation of the ionization potential from orbital eigenvalues and on the ordering of electronic levels in metal-organic molecules. Further, we show that the Fermi orbital positions in structurally similar molecules appear to be transferable.

[1] M. R. Pederson, A. Ruzsinszky, and J. P. Perdew, J. Chem. Phys. 140, 121103 (2014). [2] M. R. Pederson, J. Chem. Phys. 142, 064112 (2015). [3] T. Hahn et al., J. Chem. Phys. (accepted: AIPID 029546JCP).

DS 33.3 Wed 12:30 H11

Charge and spin transport in two-dimensional systems using the KKR-CPA-Kubo approach — •S. Wimmer, K. Chadova, S. Bornemann, D. Ködderitzsch, and H. Ebert — Department Chemie, Ludwig-Maximilians-Universität München

We have applied the fully relativistic spin-polarized Korringa-Kohn-Rostoker method to investigate charge and spin transport properties of various two-dimensional systems such as mono- and multilayers, surfaces and thin films on surfaces. Our theoretical approach is based on the linear response Kubo formalism that allows introducing a layer-resolved conductivity σ^{IJ} [1] and that has been extended to the fully relativistic case. An implementation of the Coherent Potential Approximation for layered systems allows the treatment of disorder effects including the Vertex Corrections to the conductivity [2]. This can be used to study chemical disorder in alloys but also to include the effect of finite temperatures. For the latter the so-called Alloy-Analogy Model [3] is enployed to treat vibrations and spin fluctuations. Besides convergence tests on simple homogeneous systems the approach has been applied, e.g., to the Fe_n/GaAs(001) metal/semiconductor surface system, the topological insulator surfaces $\mathrm{Bi_2X_3}$(111) (X = Se, Te, and $\mathrm{Se}_{1-x}\mathrm{Te}_x$), and, using a generalization of the Mott formula for thermoelectric transport [4], also to spincaloritronic transport.

[1] W.H. Butler *et al.*, *Phys. Rev. B* **52**, 13399 (1995). [2] W.H. Butler, *Phys. Rev. B* **31**, 3260 (1985); K. Palotás *et al.*, *Phys. Rev. B* **67**, 174404 (2003). [3] H. Ebert *et al.*, *Phys. Rev. B* **91**, 165132 (2015). [4] M. Jonson and G.D. Mahan, *Phys. Rev. B* **21**, 4223 (1980).

DS 34: Atomic Layer Deposition

Time: Wednesday 12:15–12:45 Location: H8

DS 34.1 Wed 12:15 H8

Quartz Crystal Microbalance Studies of the First Few ALD Cycles of Alternated Grown Titania and Alumina Layers — •Robert Zierold[1], René Faust[1], Christoph Wiegand[1], Martin Waleczek[1], Robert H. Blick[1], and Kornelius Nielsch[1,2] — [1]Institute of Nanostructure and Solid State Physics, Universität Hamburg, Hamburg, Germany — [2]Institute for Metallic Materials, Leibniz Institute for Solid State and Materials Research Dresden, Dresden, Germany

Atomic layer deposition (ALD) in a supercyclic fashion is a common approach to synthesize tailor-made ternary materials, to prepare nanolaminates, or to distribute a doping species in a host material. However, assuming the growth rates of the two underlying individual ALD processes to calculate the overall thickness or the composition of the ternary material often results in a deviation to the experimentally observed values.

Herein, we present detailed, ultra precise quartz crystal microbalance (QCM) studies of the first few ALD cycles of $\mathrm{TiO_2}$ deposited on an $\mathrm{Al_2O_3}$ surface grown by ALD , and vice versa. A significantly altered initial growth per cycle (GPC) compared to the equilibrium (literature) value is observed. In detail, the growth of TiO_2 on Al_2O_3 is enhanced whereas the growth of Al_2O_3 on TiO_2 is reduced: In both cases, the initial GPC of the deposited oxide matches the ALD growth rate of the substrate material. Our observation can be explained by an intrinsic growth inhibition caused by the less reactive, sticking isopropyl groups occurring in the TiO_2 deposition process.

DS 34.2 Wed 12:30 H8

Frontiers of Thin-Film Deposition: MAD-ALE growth and optical properties of Ruddlesden-Popper $SrO(SrTiO_3)_n$ phase — •Fryderyk Lyzwa[1], Premysl Marsik[2], Vladimir Roddatis[1], Markus Jungbauer[1], Christian Bernhard[2], and Vasily Moshnyaga[1] — [1]Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Université de Fribourg, Département de Physique Chemin du Musée 3, 1700 Fribourg, Switzerland

As an unconventional method to deposit oxide films, Metalorganic Aerosol Deposition (MAD) shows an immense growth control up to submonolayer basis. The possiblities of MAD are presented by complex Ruddlesden-Popper (RP) n=4 films with the general formula $SrO(SrTiO_3)_n$ in which perovskite layers of $(SrTiO_3)_n$ are separated by single SrO layers. Those dielectrics are promising due to low-loss for microwave frequencies and could replace the well-studied system of $BaSrTiO_3$.

The films were grown in atomic layer epitaxy (ALE) mode by sequential deposition of Sr-O/Ti-O_2 atomic layers, monitored by optical in-situ ellipsometry, on SrTiO3(100) (unstrained), on LSAT(100) and on $DyScO_3$(110). The RP structure was confirmed by x-ray diffraction and transmission electron microscopy. A 10nm-thick buffer enables an additional control nearby the substrate surface; it reduces significally the film roughness. Further we measured the infrared active phonon modes as a function of temperatureto in order to study the structure.

DS 35: Thin Film Characterisation: Structure Analysis and Composition II

Time: Wednesday 15:00–18:15 Location: H8

DS 35.1 Wed 15:00 H8

Transrotational microcrystals: novel solid state order formed in amorphous films — •Vladimir Yu. Kolosov — Ural Federal University, Ekaterinburg, Russia

Exotic thin crystals with unexpected **transrotational** microstructures [1] have been discovered by transmission electron microscopy (TEM) for crystal growth in thin (10-100 nm) amorphous films of different chemical nature (oxides, chalcogenides, metals and alloys) prepared by various methods. Primarily we use TEM bend contour technique for crystallographic orientation analysis [2]. The unusual phenomenon can be observed ***in situ*** in TEM column: dislocation independent regular internal bending of crystal lattice planes in a growing crystal. Such transrotation (unit cell **trans**lation is complicated by small **rotation** realized round an axis lying in the film plane) results in strong regular lattice orientation gradients (up to 300 degrees per micrometer) of different geometries: cylindrical, ellipsoidal, toroidal, saddle, etc. Transrotation is strongly increasing as the film gets thinner. Transrotational crystal resembles ideal single crystal enclosed in a curved space. Transrotational micro crystals have been eventually recognized by other authors for some vital thin film materials, i.e. PCMs (phasechage materials) for memory, silicides, SrTiO3. Atomic model and possible mechanisms of the phenomenon are discussed.

Basing on the above findings we also propose new hypothetic transrotational nanocrystalline model of amorphous state.

[1] V.Yu. Kolosov and A.R.Tholen, Acta Mater., **48** (2000) 1829.
[2] I. E. Bolotov and V. Yu. Kolosov, Phys. Stat. Sol. **69**a (1982) 85.

DS 35.2 Wed 15:15 H8

Electronic properties of $LaPO_4$ nanoparticles studied by thehard X-Ray photoelectron spectroscopy. — •A. Gloskovskii[1], Ya. Chornodolskyy[2], V. Vistovskyy[2], O. Shevchuk[3], O. Myagkota[3], S. Syrotyuk[3], A. Zaichenko[3], A. Voloshinovskii[2], and W. Drube[1] — [1]Photon Science/DESY, Hamburg — [2]Ivan Franko National University of Lviv, Ukraine — [3]Lviv Polytechnic National University, Ukraine

Photoelectron spectroscopy using excitation by hard X-rays in the range of 2 - 15 eV (HAXPES) is rapidly developing at synchrotron light sources worldwide. Its comparatively large probing depth (10-30 nm) makes it a powerful tool for studies of complex materials, buried nanostructures and multilayered structures relevant for device applications. We are presenting a new approach for HAXPES of insulating nanoparticles by covering them with thin metal shell. It makes it feasible to probe density of occupied states (DOS) for insulating nanoparticles. $LaPO_4$-Eu nanoparticles with mean grain size of 50-60 nm were covered by 1 nm Ag resulting in core-shell particles. DOS of conductive silver shell is not overlapping with DOS of wide bandgap $LaPO_4$. We carried out HAXPES measurements with variable linear light polarizations using 5.95 keV photons. The intensity of s-states can be considerably suppressed by rotating the light polarization perpendicularly to the analyzer's axis. In this way the extraction of the s- and p- contributions to $LaPO_4$ valence band becomes feasible. Experimentally measured valence band DOS correlates well with calculations using projector augemented wave method.

DS 35.3 Wed 15:30 H8

Determination of thickness and refractive index of ulta-thin films via ellipsometry — Peter Nestler and •Christiane A. Helm — Institut für Physik, Greifswald University, D-17487 Greifswald, Germany

Ellipsometric measurements of layered media deliver information on film parameters like layer thickness and refractive indices with high precision. In the simplest case the substrate is covered with a single homogenous, transparent layer only. Yet, the simultaneous determination of both parameters, thickness and refractive index of the layer, via ellipsometry is immediately possible only if the layer thickness exceeds 15 nm.

Here we present a technique to cross this limitation: A series expansion of the ellipsometric ratio ρ to the second order of the layer thickness relative to the wavelength reveals the first and second ellipsometric moment. These moments are properties of the layered surface and independent of incident angle. Using both moments and one additional reference measurement of the bare substrate enables to simultaneously determine both thickness and refractive index of ultra-thin layers down to 5 nm thickness.

DS 35.4 Wed 15:45 H8

Depth-resolved image of the LaAlO3/SrTiO3 system from Resonant Soft X-ray Reflectivity — •Martin Zwiebler[1], Fabio Miletto Granozio[2], Emiliano Di Gennaro[2], Jorge Enrique Hamann-Borrero[1], Enrico Schierle[3], Eugen Weschke[3], Jochen Geck[4], Marco Salluzzo[5], and Umberto Scotti di Uccio[5] — [1]Leibniz Institute for Solid State and Materials Research, IFW-Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]CNR-SPIN and Dipartimento di Fisica, Complesso universitario di Monte S.Angelo Via Cinti, 80126, Naples, Italy — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert Einstein-Str. 15, 12489 Berlin, Germany — [4]Universität Salzburg, Hellbrunner Str. 34, 5020 Salzburg, Austria — [5]2CNR-SPIN and Dipartimento di Fisica, Complesso universitario di Monte S.Angelo Via Cinti, 80126, Naples, Italy

When LaAlO3 is grown epitaxially on a 001 Ti-terminated SrTiO3 substrate, a conductive 2D electron system (2DES) emerges, even though both parent compounds are bulk insulators. The conductivity of the 2DES is (i) tunable using the field effect, (ii) very sensitive to photon irradiation and (iii) can even show superconductivity at low temperatures. The reasons for the emergence of the 2DES at the STO/LAO interface remain elusive. Popular and intensively discussed scenarios include the layer polarity change at the interface, chemical doping via oxygen vacancies, interdiffusion, and structural changes. Here we show depth-resolved spectroscopic information, obtained from Resonant Soft X-Ray Reflectivity at the Ti L2,3 edge. Our results provide new insights about chemical interdiffusion, charge accumulation and structural distortions in these systems, which clarify the emergence of the 2DES and its response to photon irradiation.

DS 35.5 Wed 16:00 H8

Analysis of interface properties of multilayer mirrors with sub-nanometer layer thicknesses — •Anton Haase[1],

Saša Bajt[2], Victor Soltwisch[1], Philipp Hönicke[1], Christian Laubis[1], and Frank Scholze[1] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin — [2]Photon Science, DESY, Notkestr. 85, 22607 Hamburg

The spectral range from 2.2 nm to 4.4 nm, also known as the water window, has a high relevance in the investigation of biological samples in a wet environment due to the low absorbance of these particular wavelengths in water. Multilayers composed out of Cr and Sc provide enough optical contrast to serve as mirrors for this wavelength range, while maintaining low absorption. However, a respective choice of layer thicknesses down to the sub-nanometer regime directly related to the desired peak reflectivity at a certain wavelength and angle of incidence are required. Disturbances of interfaces with respect to the ideal multilayer such as interdiffusion and roughness diminish the theoretically achievable maximum reflectivity. Experimental reflectivities show values below 20%, i.e. less than half of the theoretically achievable maximum. We show how the combination of several complementary experiments, such as EUV and X-ray reflectivity, resonant EUV reflectivity at the L-edge and X-ray standing wave analysis are necessary to obtain a consistent model. Based on this results a analysis of the diffuse scattering is performed to asses the interface roughness and determine a effective power spectral density.

DS 35.6 Wed 16:15 H8

Sample thickness in Transmission Kikuchi Diffraction via Monte Carlo Simulations — •Nathanael Jöhrmann and Michael Hietschold — Institut für Physik, TU Chemnitz, Deutschland

Transmission Kikuchi Diffraction in a Scanning Electron Microscope is an interesting modification of Electron Backscatter Diffraction to get information about crystalline structures with high spatial resolution [1]. The achievable lateral resolution and the measurement time depend strongly on several parameters, particularly on sample thickness, sample tilt and acceleration voltage. To better understand measurement results, especially unindexed areas, and to optimize sample preparation and TKD setup, it would be helpful to get information about sample thickness as additional information of a measurement. To achieve this, the background signal of measured diffraction patterns is compared with Monte Carlo simulations.

[1] R. R. Keller und R. H. Geiss, Journal of Microscopy 245 (2011), pp. 245-251

15 min. break.

DS 35.7 Wed 16:45 H8

Chemical Characterization of electrodeposited transition metal chalcogenite layers — Talha Nisar, •Torsten Balster, and Veit Wagner — Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany

Transition metal chalcogenides are promising materials for catalysis as well as semiconducting layers in thin film transistors, e.g. amorphous molybdenum and tungsten sulfide layers are successfully applied for water electrolysis.

In this study, we investigated the electrochemical deposition of ammonium tetrathiomolybdate (ATTM) and the subsequent annealing steps by means of x-ray photoelectron spectroscopy. The electrochemical deposition was carried out with a concentration of 0.5 mmol ATTM at room temperature in the cathodic regime with respect to Ag/Ag-Cl reference electrode. This resulted in homogenous layers with thicknesses of MoS_x (x=2..3) from 1 up to 10 nm. This layer show promising morphology to cover also complex surfaces. The deposition process results in a minor oxygen and carbon contamination, which can be reduced by proper post growth annealing conditions. Further annealing steps in an inert Ar (99.999%) atmosphere to improve crystallinity resulted in a reduction of the S content of the surface, which can be avoided in a S-containing atmosphere.

DS 35.8 Wed 17:00 H8

Surface chemistry of free-base corrole on Ag(111): Complementary insights from X-ray spectroscopy, DFT and STM. — •Mateusz Paszkiewicz[1], Stefano Tebi[2], Hazem Aldahhak[3], Wolfgang Schöfberger[4], Stefan Müllegger[2], Uwe Gerstmann[3], Eva Rauls[3], Wolf Gero Schmidt[3], Reinhold Koch[2], David Duncan[1], Francesco Allegretti[1], Johannes Barth[1], and Florian Klappenberger[1] — [1]Physic department, E20, Technische Universität München, Garching, Germany — [2]JKU, Solid state physics department, Linz, Austria — [3]University of Paderborn, Physik department, Paderborn, Germany — [4]JKU, Institute of organic chemistry, Linz, Austria

The investigated fluorophenyl-free base corrole (3H-C) is famous for its ability to act as a three-fold anionic ligand and for stabilizing metals in high oxidation states. Our multitechnic study combines X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption-fine-structure (NEXAFS) spectroscopy with density functional theory (DFT) simulations and scanning tunneling microscopy (STM). First, we present a spectroscopic reference of all relevant regions and edges (C1s, F1, and N1s regions for XPS and C and N K-edge for NEXAFS) of the 3H-C multilayer and interpret their features on the basis of the theoretic investigations. Then, we unravel the influence of the molecule surface interaction. At room temperature we observe unordered layers of partially deprotonated species (2H-C) exhibiting a near-to-planar macrocycle. After annealing to around 400 K, ordered layers of stacked molecules are present with an intriguing spectroscopic signature.

DS 35.9 Wed 17:15 H8

Dependence of Optoelectronic Properties on Composition in CuInSe2 — •Sergiu Levcenco, Helena Stange, Roland Mainz, and Thomas Unold — Hahn-Meitner-Platz 1 D-14109 Berlin, Germany

Thin film solar cells based on chalcopyrite absorber have demonstrated more than 21% efficiency although the material used is strongly non-stoichiometric, and thus contains large quantities of defects. To investigate the effect of composition on the optoelectronic properties CuInSe2 samples were grown by coevaporation in with an intentional lateral variation of composition, leading to Cu-poor, Cu-rich and stoichiometric regions within the same sample. Photoluminescence, Raman spectroscopy and reflectometry was performed to investigate the optical and structural properties and recombination processes within on sample. The band gap is found to continuously increase when the composition approaches stoichiometry, whereas the recombination physics yields a much more complex behaviour.

DS 35.10 Wed 17:30 H8

Nanostructured surface of multilayer graphene on 3C-SiC (001) — •Victor Aristov[1,2,3], Olga Molodtsova[1,4], Sergey Babenkov[1], Dmitry Marchenko[5], Jaime Sánchez-Barriga[5], Partha Sarathi Mandal[5], Andrei Varykhalov[5], Alexei Zakharov[6], Yuran Niu[6], Alexei Preobrajenski[6], Denis Vyalikh[7], Marc Portail[8], Marcin Zielinski[9], Barry Murphy[10], Sergey Krasnikov[10], Olaf Luebben[10], Igor Shvets[10], and Alexander Chaika[2,10] — [1]DESY, Hamburg, Germany — [2]ISSP RAS, Chernogolovka, Russia — [3]TU Bergakademie, Freiberg, Germany — [4]ITMO, Saint Petersburg, Russia — [5]BESSY, Berlin, Germany — [6]Max-lab, Lund, Sweden — [7]TU Dresden, Germany — [8]CNRS-CRHEA Valbonne, France — [9]NOVASiC Le Bourget du Lac, France — [10]Trinity College, Dublin, Ireland

The results of atomically resolved scanning tunneling microscopy, low energy electron diffraction, low energy electron microscopy, micro-LEED and angle resolved photoelectron spectroscopy studies of graphene synthesized on cubic-SiC(001) will be presented. Uniform few layer graphene was fabricated on SiC(001)/Si(001) wafers using Si-atom sublimation followed by SiC surface layer graphitization during high-temperature annealing in ultrahigh vacuum. This work was supported by the RAS, RFBR grants No 140200949 and 140201234, by the BMBF-Project No. 05K12GU2, PSP-Element No. U4606BMB1211, by a Marie Curie IIF grant No 12/IA/1264, by SPP 1459 of DFG.

DS 35.11 Wed 17:45 H8

Study of amorphous chalcogenide alloys by optical and electrical investigation — •Ju-Young Cho[1] and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA-FIT, RWTH Aachen University, Germany

Amorphous phase change materials (PCMs) show unusual phenomena compared to ordinary covalent glass. Amorphous PCMs usually show significantly different local chemical order as compared with their crystalline phase, while ordinary covalent glass exhibits a similar local chemical order as compared with its crystalline counterpart. Unraveling the local structure and the relevant characteristics is highly rewarding task because this is a key to understand the unique features of the amorphous PCMs, e.g. the extremely rapid crystallization, high fragility as well as temporal drift of the electrical resistance.

When alloying PCMs, constitute elements and compositional variation significantly affect the local chemical order of amorphous PCMs. This dependency becomes more obvious when PCMs and non-PCMs are alloyed. In this study, we have performed FT-IR and Raman spectroscopy, Van der Pauw and X-ray reflectivity measurements of co-sputtered amorphous chalcogenide alloy films with various compositions and elements to exploit the change in the structural properties as well as the crystallization kinetics of PCMs. The resulting insight will reveal the correlation between the local chemical order and the properties varying with composition, possibly enabling the prediction of phase change memory characteristics.

DS 35.12 Wed 18:00 H8

Quantitative AM-FM Mode for Fast, Versatile Imaging of Nanoscale Elastic Modulus — Marta Kocun, Aleksander Labuda, Waiman Meinhold, •Florian Johann, and Roger Proksch — Asylum Research, an Oxford Instruments Company, Wiesbaden, Germany

Tapping mode AFM imaging, also known as amplitude-modulated (AM) atomic force microscopy (AFM), is fast, gentle and provides the high spatial resolution necessary for imaging nanoscale features. However, until recently, mechanical characterization with tapping mode was limited to only qualitative results. In AM-FM mode, a bimodal (dual-frequency) technique, the first resonant mode is operated in AM, whereas a higher resonant mode is frequency modulated (FM). As expected from regular tapping mode, AM-FM mode delivers topographical information. Additionally, it provides quantitative data on contact stiffness, from which elastic modulus can be calculated with appropriate models for the tip-sample contact mechanics. Experimental results on different samples such as metals, alloys and polymers will be presented to demonstrate the applicability of AM-FM mode for materials with a wide range of modulus (MPa-GPa).

DS 36: Focussed Session: Semiconductor Heteroepitaxy on Nanopatterned Substrates (Joint session of DS and HL, organized by DS)

State-of-the-art electronic and optoelectronic devices are widely based on layered heteroepitaxial semiconductor systems. As the crystal quality of planar heteroepitaxial layers is often limited by lattice misfit relieving defects, the selective growth on small areas as well as on non-planar, nanopatterned substrates has attracted increasing interest. In these cases the three-dimensional elastic lattice relaxation largely extends the range of material combinations, for which defect-free heteroepitaxial growth is possible. In tandem with the nanopattern-induced modifications of the surface potential and growth characteristics this sets the fundament for the realization of unique architectures and new classes of self-assembled and site-controlled nanostructures, which are required for high-performance devices. Selective-area grown nanowires for example have been demonstrated to exhibit outstanding luminescence properties, and complex hierarchical heterostructures grown on nanowire templates have paved the way for new types of quantum structures and innovative device architectures. Worldwide, numerous research groups and institutes are involved in exploring the fabrication and properties of such nano-heteroepitaxial systems. Therefore, the proposed symposium focusses on experiments and simulations of the heteroepitaxial growth on nanopatterned substrates, structural and nanomorphological aspects as well as control of optical, electronic and transport properties, and device applications. The symposium aims at bundling the extensive research activitities in this area and at offering a forum for scientists from fields of epitaxial growth, nanopatterning, theory, surface science, characterization, and device fabrication.

Organizers: Thomas Riedl (U Paderborn), Gregor Koblmüller (WSI München), Martin Eickhoff (JLU Gießen)

Time: Wednesday 15:00–18:30 Location: H11

Topical Talk DS 36.1 Wed 15:00 H11

Single site-controlled InGaAs quantum dots grown on patterned GaAs nanoholes — •S. Höfling, S. Maier, S. Unsleber, M. Kamp, and C. Schneider — Technische Physik, Würzburg University

Single semiconductor quantum dots (QDs) are very attractive candidates to control charge and spin carries at the quantum level. They are therefore very promising for applications in fields ranging from nanoelectronics over nanophotonics to spintronics. One of the major challenges regarding the scalable fabrication of single QD based devices is however the precise control of the QD position within device structures. In this presentation, we summarize our results obtained on the site-controlled growth using pre-patterned nanohole templates for the controlled integration of site-controlled QDs into nanoscale devices. By combining this growth technique with a process capable of accurately aligning QDs relatively to subsequently fabricated quantum device structures, several interesting devices like single photon sources and quantum dot memories have been realized.

Topical Talk DS 36.2 Wed 15:30 H11

Nanometer scale correlation of structural and optical properties of individual GaAs/AlGaAs nanorodsby Scanning Transmission Electron Microscope Cathodoluminescence — •Frank Bertram, Marcus Müller, Peter Veit, and Jürgen Christen — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg

We will present a direct correlation of the luminescence with crystallographic realstructure of novel GaAs/AlGaAs coreshell nanowires using cathodoluminescence directly performed in transmission electron microscope at liquid helium temperature. The GaAs/AlGaAs coreshell NWs were produced by a unique twostep process enabling the growth of ultrathin GaAs cores. First, GaAs NWs were obtained by molecular beam epitaxy on a [111]-oriented Si. In a second step the GaAs core diameter was reduced by a reverse-reaction using in-situ thermal decomposition of the {110} side wall surfaces leading typically to a diameter down to 7 nm. Subsequently, the cores were overgrown by an AlGaAs passivation shell and a GaAs cap. TEM investigations reveal wurzite structure in the bottom part of the NW with a high density of extended defects whereas the upper part is dominated by the zincblende phase containing few twindefects. Highly spatially resolved CL measurements exhibit a blue shifted emission up to 1.66 eV as compared to bulk GaAs. In particular, we will present a detailed analysis of the impact of structural properties on the luminescence along the wire. Locally sharp emission lines originating from vicinity of twindefects within the ZB-structure indicate effective localization.

Topical Talk DS 36.3 Wed 16:00 H11

Local Heteroepitaxy for Large-Scale Integration — •Heinz Schmid, Mattias Borg, Davide Cutaia, Kirsten Moselund, Moritz Knoedler, Nicolas Bologna, and Heike Riel — IBM Research - Zurich , 8803 Rueschlikon, Switzerland

The cooperative use of unequal materials like silicon and III-Vs can lead to performance benefits and even enable novel devices and applications. Traditionally this has been achieved by clever joining of the individual Si and III-V components in a common package. Alternatively this could be achieved by building the devices directly from Si wafers with embedded III-V layers. However, such wafers are not readily available yet. Here we review our effort on local epitaxy of III-Vs on Si and introduce the concept of template-assisted selective epitaxy (TASE). Various III-V materials with nanowire or thin-film geometries were successfully grown with high yield on Si using TASE and further processed into field effect transistors (FETs) and tunnel-FETs that exhibited excellent performance.

15 min. break.

Topical Talk DS 36.4 Wed 16:45 H11

Fabrication and study of metal contacts on germanium nanowires using electrical biasing in a transmission electron microscope — •Martien den-Hertog[1], Khalil El-Hajroui[1], Clemens Zeiner[3], Alois Lugstein[3], Eric Robin[2], Miguel Lopez-Haro[2], and Jean-Luc Rouviere[2] — [1]Institut Neel, CNRS/UJF/UGA, Grenoble, France — [2]INAC, CEA-Grenoble/UGA, Grenoble, France — [3]Institute for solid state electronics, Vienna, Autriche

Semiconductor nanowires (NWs) are promising candidates for many device applications ranging from electronics and optoelectronics to energy conversion and spintronics. To allow successful device integration the contact quality between for example a NW and metal is of paramount importance. An interesting approach to create an atomically abrupt contact with low electrical resistance on NWs of group IV (silicon and germanium) is to create a metal-semiconductor phase in the extremities of the NW. To understand and control the metal diffusion into the NW that creates a metallic phase, detailed characterization at atomic length scales is necessary to understand how the metal atoms diffuse and incorporate into the formed phase at the reaction front and how these parameters relate to the electrical properties of the same interface. In this work we study two different kind of semiconducting NW devices fabricated on electron transparent Si3N4 membranes. We show in-situ phase propagation of a metal-semiconductor phase of Cu and Al in Ge NWs in the TEM while measuring the current through the device, and analyze the metal diffusion process.

Topical Talk DS 36.5 Wed 17:15 H11

Cubic GaN on pre-patterned 3C-SiC/Si (001) substrates — •Donat Josef As, Ricarda Maria Kemper, Thomas Riedl, and Jörg K.N. Lindner — Department Physik, Universität Paderborn, Warburgerstrasse 100, 33098 Paderborn, Germany

The influence of growth area reduction towards length scales predicted to be effective for defect reduction by the theory of nano-hetero-epitaxy (NHE) is analyzed. This is studied in detail for the first time in the system of meta-stable cubic GaN (c-GaN) grown by plasma-assisted molecular beam epitaxy on pre-patterned 3C-SiC/Si (001) substrates. It is demonstrated that regardless of the pattern symmetry or size, the cubic phase of GaN nucleates on top of all investigated mesa structures. Electron beam lithography followed by a lift-off and a reactive ion etching process is used for tailoring post-shaped SiC structures. A successful reduction of the {111} stacking fault (SF) density is achieved by reducing the (001) top edge length of the posts from ~500 nm down to ~20 nm. Transmission electron microscopy reveals a nucleation of phase-pure and almost defect free c-GaN on top of the smallest SiC nanostructures as predicted by theoretical calculations.

DS 36.6 Wed 17:45 H11

GaAs-based nanowire integration on silicon via template-assisted selective epitaxy — •Moritz Knoedler, Nicolas Bologna, Mattias Borg, Heinz Schmid, Giorgio Signorello, Davide Cutaia, Kirsten Moselund, Marta Rossell, and Heike Riel — IBM Research Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland

As the scaling-down of conventional Si microelectronics is approaching fundamental physical limits, novel materials are heavily being investigated as alternative channel materials, with III-V semiconductor compounds being particularly promising candidates. Thus far, III-V integration into Si technologies has been limited due to poor epitaxial material quality. Our group has recently demonstrated a novel method to directly integrate III-V nanostructures on silicon called template-assisted selective epitaxy (TASE). Nanowires are grown inside lithographically pre-defined oxide templates, allowing for precise tuning of composition and crystal quality, independent from their shape and substrate orientation.

Here we present a comprehensive investigation of GaAs-based epitaxy directly on Si wafers via TASE, by correlating growth parameters with crystal morphology. To this end, nanowires were grown with metal-organic chemical vapour deposition (MOCVD) under different conditions by varying template width, growth duration, temperature, group III molar flows and V/III precursor ratio. Crystal quality was then analyzed at atomic resolution by state-of-the-art double-aberration-corrected (scanning) transmission electron microscopy (STEM/TEM). Zinc blende/wurtzite polytypism and twin defect formation were investigated in detail.

Low-temperature and temperature-dependent micro photoluminescence (PL) spectroscopy was used to further characterize their optical properties. Significant photoemission of the nanostructures even at room temperature was observed. When the GaAs is surrounded by the oxide template or an AlGaAs shell luminescence is much enhanced, indicating reduced surface recombination velocity.

DS 36.7 Wed 18:00 H11

Theoretical analysis of strain and misfit dislocation stability in axial-heteroepitaxial GaAs/InAs nanopillars — •Thomas Riedl[1,2] and Jörg Lindner[1,2] — [1]University of Paderborn, Department of Physics, Warburger Straße 100, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), Warburger Straße 100, 33098 Paderborn, Germany

Heteroepitaxial nanopillars and -wires represent a promising building block for advanced optoeletronic devices like dot-in-wire LEDs or lasers. Such structures offer a large surface-to-volume ratio and the possibility to accommodate considerable lattice mismatch in a pure elastic manner without formation of misfit relieving defects. As misfit dislocations are reported to occur in heterostructure nanowires in case of larger misfit and diameter, it is important to determine the critical wire dimensions for dislocation stability. In the present contribution we analyze this for the case of [111] orientied axial-heteroepitaxial GaAs/InAs nanopillars with zinc blende structure. Because of its applicability to various dislocation configurations and the availability of suitable parametrizations we use atomistic molecular statics simulation based on the Tersoff potential. We find that the defect-free elastically strained state is stable for small wire diameters ($<$ 10 nm for a single 60° dislocation), whereas the dislocated state becomes favorable for larger diameters. In this presentation the influence of dislocation type, wire morphology and chemical width of the heterointerface on the coherent-semicoherent transition is analyzed and discussed. The results are compared with the literature.

DS 36.8 Wed 18:15 H11

Selective nano-heteroepitaxial growth of GeSn islands on nano-patterned Si(001) — Viktoria Schlykow[1], Noriyuki Taoka[1], Marvin Zöllner[1], Oliver Skibitzki[1], Peter Zaumseil[1], •Giovanni Capellini[1,2], Yuji Yamamoto[1], Thomas Schröder[1,3], and Gang Niu[1] — [1]IHP, Frankfurt (Oder) — [2]Dipartimento di Scienze, Italy — [3]BTU Cottbus-Senftenberg

Ge is a promising candidate for optical devices due to its band gap, resulting in high absorption at the telecommunication wavelength. The introduction of Sn into Ge forming GeSn alloys enables further flexibility to engineer the optical properties like the semiconductor band gap. However, crystalline defects induced by lattice mismatch between GeSn and Si are a crucial challenge to realize high performance optical devices. Recently, we demonstrated fully coherent, dislocation free Ge islands on nano-pillar patterned Si (NPP-Si) substrates using nano heteroepitaxy approach. In this study, we demonstrate the selective MBE growth of GeSn islands on NPP-Si at high temperatures. In order to establish selective MBE growth of GeSn on NPP-Si surrounded by SiO2, the impact of growth temperature (500-750 °C) on the selectivity and the Sn incorporation was investigated. XRD, TEM and micro-PL studies confirmed that the growth at 600 °C results in good selectivity and homogeneous distribution of Sn in Ge nano-islands and good optical properties. Growth below 600 °C results in non-selectivity whereas growth above 600 °C leads to better selectivity but an enhanced Sn migration to {111} facets thus reduced Sn incorporation.

DS 37: Frontiers of Electronic Structure Theory: Focus on Topology and Transport III (Joint session of DS and O, organized by O)

Time: Wednesday 15:00–18:30 Location: H24

Topical Talk DS 37.1 Wed 15:00 H24

Topological semimetal phases in strained HgTe-based alloys — Tomáš Rauch[1], Steven Achilles[1], •Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

Topological insulators (TIs) have matured to a class of materials that is studied worldwide with great effort. Prominent examples are HgTe, the Bi chalcogenides, and SnTe. Recently, the set of "original" TIs has been extended by topological semimetals: the topological Dirac and the Weyl semimetals, both of them showing point-like Fermi surfaces in the bulk. Weyl points appear always in pairs with opposite topological charges of ± 1; their projections onto the surface Brillouin zone are connected by a Fermi arc, i. e. a sizably spin-polarized topological surface state with an open Fermi contour.

In this presentation I report on theoretical investigations of strained $\mathrm{HgTe}_{1-x}\mathrm{S}_x$ alloys [1], with surprising results. *(i)* In the strong TI phase, the spin chirality of the topological nontrivial surface state can be reversed by moderate strain and changing the alloy concentration x. *(ii)* On top of this, we observe a Dirac and a Weyl semimetal phase. These findings call for experimental verification and extend significantly the "topological playground" for spin-dependent transport.

[1] T. Rauch, S. Achilles, JH, I. Mertig, Phys. Rev. Letters **114** (2015) 236805.

Topical Talk DS 37.2 Wed 15:30 H24

Topological surface Fermi arcs and the chiral anomaly in Weyl semimetal materials — •Binghai Yan — Max Planck Institute for Chemical Physics of Solids, Dresden

Topological Weyl semimetals represent a novel state of topological quantum matter, which not only possesses Weyl fermions (massless chiral particles that can be viewed as magnetic monopoles in momentum space) in the bulk and unique Fermi arcs generated by topological surface states, but also exhibits appealing physical properties such as extremely large magnetoresistance and ultra-high carrier mobility. In this talk, I will first present our recent theoretical [1] and ARPES [2,3] study on the topological surface states of transition-metal monopnictides, NbP, NbAs, TaP and TaAs. By visualizing the surface Fermi arcs, we discovered their Fermiology evolution with spin*orbit coupling strength. Further, we found a way to manipulate the Fermi arcs by the Lifshitz transition. I will also introduce our recent progress on the magneto-transport in the search for the chiral anomaly effect[4,5]. References: [1] Y. Sun, S. C. Wu, and B. Yan, Phys. Rev. B 92, 115428 (2015). [2] L. X. Yang, et al. Nature Physics 11, 728 (2015). [3] Z. K. Liu, et al. Nature Materials DOI: 10.1038/NMAT4457 (2015). [4] C. Shekhar, et al. Nature Physics 11, 645 (2015). [5] C. Shekhar, et al. arXiv:1506.06577 (2015).

DS 37.3 Wed 16:00 H24

Type-II Dirac cones as unified topological origin of the exotic electronic properties of WTe$_2$ — •Lukas Muechler[1], Aris Alexandradinata[2], Titus Neupert[3], and Roberto Car[1] — [1]Dept. of Chemistry, Princeton University — [2]Dept. of Physics, Yale University — [3]Princeton Center for Theoretical Science, Princeton University

WTe$_2$ is a recently discovered layered material with remarkable electronic properties. Transport measurements show an extremely large non-saturating magnetoresistance (MR) with mobilities as high as 167 000 cm^2/Vs at 2 K. Furthermore, recent photoemission experiments discovered circular dichroism in the bulk band structure. We propose a unified explanation for these exotic observations by relating key properties of the bulk electronic structure to that of to that of the mono- and bi-layer material. In particular, we demonstrate that the monolayer is a novel type-II Dirac semimetal in absence of spin-orbit coupling, with Dirac cones that are sufficiently anisotropic to simultaneously harbor electron and hole pockets. The band structure can be characterized by a new $\mathbb{Z}_2 \times \mathbb{Z}_2$ topological invariant defined through non-Abelian Wilson loops. We develop a tight-binding model for the mono- and bilayer of WTe$_2$ based on Wannier functions from *ab-inito* calculations and extend our findings to the iso-structural compounds MoTe$_2$ and ZrI$_2$.

DS 37.4 Wed 16:15 H24

Topological surface Fermi arcs and spin-textures of the Weyl semimetals TaAs, TaP, NbAs, and NbP — •Yan Sun[1], Shu-Chun Wu[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany. — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Very recently the topological Weyl semimetal (WSM) was predicted in the noncentrosymmetric compounds NbP, NbAs, TaP, and TaAs and soon led to photoemission experiments to verify the presumed topological Fermi arcs (FAs)[1,2]. In this work we have performed fully ab initio calculations of these four WSMs and revealed the FAs with spin-momentum-locked spin texture[3]. On the (001) surface, the anion (P or As) terminated surfaces are found to fit photoemission measurements well. By tracing the spin polarization of the Fermi surface, one can distinguish FAs from trivial Fermi circles. By comparing their surface states, we reveal the evolution of topological Fermi arcs from the spin-degenerate Fermi circle to spin-split arcs when the SOC increases from zero to a finite value. Our work presents a comprehensive understanding of the topological surface states of WSMs, which will be helpful for spin-revolved photoemission and transport experiments.

References

[1] L. X. Yang, Z. K. Liu, Y. Sun, et. al. Nat.Phys.11,728, (2015).

[2] Z. K. Liu, L. X. Yang, Y. Sun, et.al Nat. Mater., doi:10.1038/nmat4457,(2015).

[3] Y. Sun, S. Wu, and B. Yan, Phy. Rev. B, 92, 115428, (2015).

DS 37.5 Wed 16:30 H24

New electron states at the Bi/InAs(111) interface — •L Nicolaï[1,2,3], K Hricovini[2,3], J-M Mariot[4], M C Richter[2,3], O Heckmann[2,3], U Djukic[2], T Balasubramanian[5], M Leandersson[5], J Sadowski[5], J Denlinger[6], I Vobornik[7], J Braun[7], H Ebert[7], and J Minár[7,8] — [1]LMU, Munich — [2]LPMS, UCP, Cergy, France — [3]DSM-IRAMIS, Spec, Cea-Saclay, France — [4]LCP-MR, UPMC Univ. Paris 06/CNRS, France — [5]MAX-lab, Lund Univ., Sweden — [6]ALS, Berkeley, USA — [7]EST, Trieste, Italy — [8]Univ. of West Bohemia, Plzeň, Czech Republic

The Bi(111) surface is a prototype system that shows Rashba-split surface states. Theoretical studies [1] predicted non-trivial topological surface states appearing on a single bi-layer of Bi(111) and a more complex behavior was suggested for a variable film thickness as a function of the layer thickness [2]. This clearly indicates that the electronic properties of thin films of this material are quite complex and far from being fully understood. Here we present combined theoretical and ARPES studies on the electronic structure of Bi(111) films grown on InAs(111). Bi grows epitaxially on this substrate and a monocrystal of very high quality is obtained after depositing several monolayers. ARPES experiments on the samples prepared show several new electronic states not reported before. The one-step model of photoemission as implemented in the SPR-KKR package [3] allows us to identify pristine Bi bulk states coexisting with InBi surface states.[1] M. Wada et al., Phys. Rev. B 83, 121310 (2011). [2] Z. Liu et al., Phys. Rev. Lett. 107, 136805 (2011). [3] J. Braun, Rep. Prog. Phys. 59, 1267-1338 (1996).

DS 37.6 Wed 16:45 H24

Two-dimensional topological phases and electronic spectra of topological insulator thin films from *GW* calculations — •Tobias Förster, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

We have investigated topological and electronic properties of thin films of the topological insulators Bi$_2$Se$_3$, Bi$_2$Te$_3$, and Sb$_2$Te$_3$ with thicknesses from one to six quintuple layers employing the *GW* method. The quasiparticle band structures show highly improved agreement with experiments compared to DFT. In addition to a correction of the band gaps, the energetic positions and dispersions of the surface states change significantly around $\bar{\Gamma}$ [1]. The common approach of taking the diagonal elements of the self-energy Σ as quasiparticle energies and leaving the wave functions unchanged yields unphysical results which can be overcome by diagonalizing $\mathcal{H}^{\mathrm{QP}}$. The origin of the respective off-diagonal elements in $(\Sigma - V_{xc})$ will be discussed. As the wave functions are updated, the two-dimensional topological phases (quantum spin Hall or trivial) in *GW* differ from DFT for many systems. On the basis of our results, we further argue that one cannot unambiguously conclude the topological phase from fits to ARPES band structures as performed in recent experimental studies.

[1] T. Förster, P. Krüger, and M. Rohlfing, Phys. Rev. B **92**, 201404(R) (2015)

DS 37.7 Wed 17:00 H24

Steady-State Density Functional Theory for Finite Bias Conductances — •Stefan Kurth[1,2] and Gianluca Stefanucci[3,4] — [1]Dept. of Materials Physics, Univ. of the Basque Country UPV/EHU, San Sebastian, Spain — [2]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [3]Dept. of Physics, Univ. of Rome "Tor Vergata", Rome, Italy — [4]INFN, Frascati, Italy

In the framework of density functional theory a formalism to describe electronic transport in the steady state is proposed which uses the density on the junction and the steady current as basic variables. In a finite window around zero bias, a one-to-one map is established between the basic variables and both local potential on as well as bias across the junction. The resulting Kohn-Sham system features two exchange-correlation (xc) potentials, a local xc potential and an xc contribution to the bias. For weakly coupled junctions the xc potentials exhibit steps in the density-current plane which are shown to be crucial to describe the Coulomb blockade diamonds. At small currents these steps emerge as the equilibrium xc discontinuity bifurcates. The formalism is applied to a model benzene junction, finding perfect agreement with the orthodox theory of Coulomb blockade.

DS 37.8 Wed 17:15 H24

Revealing the intra-molecular origin of inelastic electron tunneling signal by means of first-principles calculations — •Giuseppe Foti and Hector Vazquez — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, Prague, Czech Republic

We explore the intra-molecular contributions to the peaks in the Inelastic Electron Tunneling Spectrum (IETS) of a benzene-based molecular junction by means of DFT-NEGF simulations [1,2]. These contributions are calculated from the bracket of the left- and right- transmission channels with the e-ph coupling matrix by grouping the products into one- and two-atom terms. This combines the geometrical information of the vibrational modes with the electronic properties of the scattering states. Our calculations show how the partial contributions of each atom and bond in the molecule combine to give the total inelastic signal. We find that, for most of the high intensity peaks, these terms sum up constructively while dark modes result from cancellations. We also investigate the relation between the symmetry of the vibrational modes and the cancellation pattern of the different contributions. This analysis enables a real space representation of the intra-molecular contributions associated to each vibrational mode and allows a complete mapping and characterization of the origin of the IETS peaks.

[1] J. M. Soler et al. J. Phys.: Condens. Matter 14, 2745 (2002)

[2] T. Frederiksen et al. Phys. Rev. B 75, 205413 (2007)

DS 37.9 Wed 17:30 H24

An efficient real-time time-dependent density functional theory method and its applications — •Zhi Wang[1], Shu-Shen Li[2], and Lin-Wang Wang[3] — [1]Institut für Physikalische Chemie, Uni-Hamburg, Hamburg, Germany — [2]Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China — [3]Lawrence Berkeley National Laboratory, Berkeley, United States

We have developed an efficient real-time time-dependent density functional theory (TDDFT) method that can increase the effective time step from <1 as in traditional methods to ~0.1 fs. With this algorithm, the TDDFT simulation can have comparable speed to the Born-Oppenheimer (BO) ab initio molecular dynamics (MD). The application of the method will be illustrated for several non-equilibrium systems, e.g., energetic particle colliding onto a TMDC monolayer, and ultrafast charge seperations in photovoltaic systems.

DS 37.10 Wed 17:45 H24

Nonadiabatic geometric phase of a pseudorotating triatomic molecule — •Ryan Requist and Eberhard K. U. Gross — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The geometric phase of a real-valued Born-Oppenheimer electronic wavefunction is a topological quantity depending on the winding number of the path around a conical intersection of the adiabatic potential energy surfaces in nuclear coordinate space. We report the calculation of a nonadiabatic molecular geometric phase that takes the full quantum mechanical motion of the nuclei into account through the exact factorization scheme [1]. Nonadiabatic contributions "smear out" the point-like adiabatic Berry curvature, changing the topological invariant into a genuine path-dependent geometric phase [2].

[1] S. K. Min, A. Abedi, K. S. Kim and E. K. U. Gross, Phys. Rev. Lett. 113, 263004 (2014). [2] R. Requist and E. K. U. Gross, arxiv:1506.09193.

DS 37.11 Wed 18:00 H24

Theoretical investigations of magnetically doped topological insulators — •Jan Minar[1,2], Jurgen Braun[1], and Hubert Ebert[1] — [1]LMU München, Germany — [2]University of West Bohemia, Plzen, Czech Rep.

Band gap opening of topological surface states due to magnetic doping are the subject of a long standing discussion. However, in spite of the progress made during the last years in this field there are still phenomena that are poorly understood and many open issues to be addressed. In several cases, like for example Mn doped Bi_2Se_3 band gap opening does not seem to be of magnetic origin. Here we will present several examples detailed theoretical studies on various bulk as well as surface doped topological insulators by means of the SPR-KKR band structure method. Our results will be discussed in a direct comparison with the corresponding ARPES [1] as well as XAS and XMCD [2,3] experimental data.

[1] J. Sanchez-Barriga et al., Nat. Communications, submitted (2015) [2] A. Ney et al., in preparation [3] J. Honolka et al., in preparation

DS 37.12 Wed 18:15 H24

Trions in a carbon nanotube from ab-initio many-body perturbation theory — •Thorsten Deilmann, Matthias Drüppel, and Michael Rohlfing — Institut für Festkörpertheorie, Universität Münster, Germany

Trion states of three correlated particles (e.g. two electrons and one hole) show up in the optical spectra of doped or gated nanostructures, like carbon nanotubes or transition-metal dichalcogenides.

We demonstrate that trions can be described within ab-initio many-body perturbation theory, as a natural extension of the widely used *GW* method and Bethe-Salpeter equation. This allows for a direct comparison with excitons on equal footing.

We investigate trion states in a semiconducting $(8,0)$ carbon nanotube, and discuss their spectra, composition, and wave functions. Luminescence from the trions is red-shifted by $\sim 135\,\mathrm{meV}$ compared to the excitons.

DS 38: Topological Insulators
(Joint session of DS, HL, MA, O and TT, organized by MA)

Time: Wednesday 15:00–17:45 Location: H32

DS 38.1 Wed 15:00 H32

Bulk and surface properties of topological insulators from *GW* calculations. — •Irene Aguilera, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany.

Many-body calculations within the *GW* approximation are attracting much attention in the study of topological insulators (TIs). They have shown to be critical both in the one-shot approach [1] (e.g. for the Bi_2Se_3 family) and in a quasiparticle self-consistent (QS) *GW* method [2] (e.g. for Bi). In both cases, the spin-orbit coupling has to be incorporated directly into the *GW* self-energy [3]. Within the all-electron FLAPW formalism, we have performed DFT, one-shot *GW*, and QS*GW* calculations for well-known TIs. These calculations are very demanding for low-dimensional systems. Therefore, we construct a tight-binding Hamiltonian for the description of topological surface states in a slab geometry. The corresponding parameters are deduced from *GW* calculations of the bulk. With this approach, we discuss the effects of quasiparticle corrections on the surface states of TIs and on the interaction between bulk and surface states. We show that the *GW* bulk and surface band structure agrees better to results from photoemission experiments than the DFT one. [1] Phys. Rev. B 87, 121111(R) (2013). [2] *Ibid* 91, 125129 (2015). [3] *Ibid* 88, 165136 (2013).

We acknowledge the Virtual Institute for Topological Insulators of the Helmholtz Association.

DS 38.2 Wed 15:15 H32

Magnetic Properties of Mn-doped Bi_2Se_3 and Bi_2Te_3: Ab Initio and Atomistic Simulations — •Pavel Baláž[1], Karel Carva[1], Róbert Tarasenko[1], Vladimír Tkáč[1], Jan Honolka[2], and Josef Kudrnovský[2] — [1]DCMP, Charles University, Ke Karlovu 5, CZ-12116 Prague 2, Czech Republic — [2]Institute of Physics, ASCR, Na Slovance 2, CZ-18221 Prague 8, Czech Republic

Ferromagnetic Curie temperature and other magnetic magnetic properties of bulk Mn-doped Bi_2Se_3 and Bi_2Te_3 3D topological insulators are systematically studied by means of atomistic Monte Carlo simulations. Exchange interactions between the Mn magnetic moments have been calculated using ab initio methods. Tight-binding linear muffin-tin orbital method has been employed, together with the coherent potential approximation to describe the high degree of disorder in the system. Spin-orbit interaction is included in the ground state calculation. In the studied materials Mn atoms might either replace a Bi atom (substitutional position) or fill an empty position in van Der Waals gap between the atomic layers (substitutional position). It has been shown that exchange interaction between Mn magnetic moments might lead to a ferromagnetic phase transition. The Curie temperature is shown to be significantly dependent on the concentration of Mn atoms in substitutional and interstitial positions. Theoretical results were compared to recent experimental studies [1].

[1] R. Tarasenko et al., to be published in Physica B: Phys. Cond. Mat., DOI: 10.1016/j.physb.2015.11.022

DS 38.3 Wed 15:30 H32

Transport measurements on ferromagnet / Half Heusler TI bilayer structures — •Benedikt Ernst[1], Robin Klett[2], Jan Haskenhoff[2], James Taylor[3], Yong Pu[3], Günter Reiss[2], Stuard S. P. Parkin[3], and Claudia Felser[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden — [2]Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld — [3]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle

Heusler compounds exhibit a manifold of physical properties and attracted in the recent past a lot of interest in the field of spintronic applications due to their half-metallic properties.

In the present work bilayer systems of ferromagnetic materials and half Heusler topological insulators (TI) are studied. The systems were deposited using DC- and RF magnetron co-sputtering. The samples were characterized by X-ray diffraction and electron microscopy techniques. On fabricated devices, the transport properties and spin properties were studied by different measurement techniques including ST-FMR and spin injection experiments.

Additional measurements of the unidirectional spin Hall magnetoresistance were realized. In this effect, we measure a change in the magnetoresistance depending on the direction of the magnetization, which is proportional to the spin Hall angle. We varied the combination of different ferromagnetic materials with different Tis of the YPtBi, YPdBi, LaPtBi and LaPdBi system, and the thicknesses of the layers, to investigate the effects on the transport properties.

DS 38.4 Wed 15:45 H32

Surface preparation and momentum microscopy of the „topological Kondo insulator“ SmB_6 — •Christian Tusche[1,2], Martin Ellguth[1], Fumitoshi Iga[3], and Shigemasa Suga[2,4] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]College of Science, Ibaraki University, Japan — [4]Institute of Scientific and Industrial Research, Osaka University, Osaka, Japan

The strongly correlated rare-earth compound SmB_6 is believed to be a topological Kondo insulator, where a topologically non-trivial surface state lives in the hybridization gap at low temperatures. While most experimental studies rely on cleaved surfaces, high resolution- and spin resolved photoemission experiments [1] usually suffer from the short live time of the reactive surface at low temperatures.

Here we present the reproducible surface preparation of large high quality SmB_6 single crystals by in-situ Ar-ion sputtering and controlled annealing. In particular, Sm-rich or B-rich surface terminations are obtained by low (≈1080°C) or high (>1200°C) temperature annealing. Using a momentum microscope [2], wide wave vector regions are studied by photoemission with He-I ($h\nu$=21.2 eV) and laser ($h\nu$=6.0 eV) excitations, on the Sm-terminated surface. The results reveal localized f-electron resonances at E_F and strong hybridization, paving the way to measure detailed Fermi surface and valence band spin textures.

[1] Suga et al., J., Phys. Soc. Japan 83, 014705 (2014)

[2] C. Tusche, A. Krasyuk, J. Kirschner, Ultramicroscopy (2015)

DS 38.5 Wed 16:00 H32

Spin control in the topological surface state of SnTe — •Nicolas Klier[1], Sam Shallcross[1], Sangeeta Sharma[2], and Oleg Pankratov[1] — [1]Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7-B2, 91058 Erlangen — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

The interface of SnTe with a vacuum results in a topological Dirac surface state [1,2]. Based on an effective Hamiltonian derived from tight-binding we investigate the properties of this surface state both with and without an in-plane electric current. The RKKY interaction is found to be strongly non-collinear due to the spin texture of the Dirac state. In the presence of an in-plane current we find (i) a polarization of the surface state and (ii) that the RKKY interaction is strongly modified by the presence of a current leading to a possible “topological spin torque effect”.

[1] B.A. Volkov, and O.A. Pankratov, Zh.Eksp. Theor. Fiz. 75, 1362, 1978.

[2] B.A. Volkov, and O.A. Pankratov, JETP Lett.42, 178, 1985.

15 min. break

DS 38.6 Wed 16:30 H32

Adiabatic Pumping of Chern-Simons Axion Coupling — •Maryam Taherinejad[1] and David Vanderbilt[2] — [1]Materials Theory, ETH Zurich, Wolfgang-Pauli-Strasse 27, 8093 Zurich, Switzerland — [2]Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854-0849, USA

The Chern-Simons axion (CSA) coupling θ makes a contribution of topological origin to the magnetoelectric response of insulating materials. Here we study the adiabatic pumping of the CSA coupling along a parametric loop characterized by a non-zero second Chern number $C^{(2)}$ from the viewpoint of the hybrid Wannier representation. The hybrid Wannier charge centers (WCCs), when plotted over the 2D projected Brillouin zone, were previously shown to give an insightful visualization of the topological character of a 3D insulator. By defining Berry connections and curvatures on these WCC sheets, we derive a new formula for θ, emphasizing that it is naturally decomposed into a topological Berry-curvature dipole term and a nontopological correction term. By explicit calculations on a model tight-binding Hamiltonian, we show how the Berry curvature on the WCC sheets is transported by a lattice vector via a series of Dirac sheet-touching events, resulting in the pumping of e^2/h units of CSA coupling during one closed cycle. The new formulation may provide a particularly efficient means of computing the CSA coupling θ in practice, since there is no need to establish a smooth gauge in the 3D Brillouin zone.

DS 38.7 Wed 16:45 H32

Accessing the transport limits of topological states — •Thomas Bathon[1], Paolo Sessi[1], Konstantin Kokh[2], Oleg Tereshchenko[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Novosibirsk State University, 630090 Novosibirsk, Russia

Topological insulators host on their surface spin-momentum locked Dirac states. Beyond their fundamental interest, these materials raised great expectations to create new functionalities in spintronics and magneto-electrics. Their success depends on our understanding of their response to Coulomb perturbations such as electric fields, which can be effectively used to gate their surface. These phenomena have so far been primarily explored by spatially averaging techniques.

Here, by using scanning tunneling microscopy and spectroscopy, we visualize the response of topological states to local charges and electric fields at the nanoscale. We demonstrate that, contrary to the general believe, local electric fields can not be effectively screened by topological states, but penetrate into the bulk indicating a behavior which is far from being metallic. The analysis of our data allows to detect the existence of a finite conductivity which, because of the local character of our measurements, can be safely quantified without being affected by sample inhomogeinities. Finally, we will show how, by taking advantage of this intrinsic limitation, a new approach to tune both charge and spin transport in this fascinating class of materials can be explored.

DS 38.8 Wed 17:00 H32

Interplay between warping and magnetic effects in Fe monolayer on Sb2Te3 — •Farideh Hajiheidari[1], Wei Zhang[1,2], and Riccardo Mazzarello[1,3] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52074 Aachen, Germany — [2]Center for Advancing Materials Performance from the Nanoscale, State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, PR China — [3]JARA-FIT and JARA-HPC, RWTH Aachen University, D-52074 Aachen, Germany

Three-dimensional topological insulators (TIs) realize an unconventional electronic phase originating from time-reversal symmetry and strong spin-orbit interaction (SOI). These materials are bulk insulators but possess conducting surface states in the bulk band gap. The surface states are topologically protected against non-magnetic disorder. However, impurities which break time-reversal symmetry induce a band gap in the system. This is of critical importance for potential device applications involving spin-based transport. In this work, we present a density-functional-theory study of the magnetic properties of a Fe monolayer on the (111) surface of the topological insulator Sb2Te3. We optimize the geometry of the system and determine the band structure and the easy axis of magnetization for the Fe atoms. We show that the easy axis is in-plane. In spite of this, the presence of the monolayer leads due to the opening of a gap of the order of meV, due to the interplay between magnetism and warping effects. Finally, we discuss the relevance of our findings to recent experiments about magnetic adatoms and monolayers deposited on TIs.

DS 38.9 Wed 17:15 H32

Towards topological tunnel devices - A versatile method for processing tunnel junctions from high quality single crystals — •Robin Klett[1,2], Karsten Rott[1,2], Daniel Ebke[3], Chandra Shekhar[3], Joachim Schönle[4], Wolfgang Wernsdorfer[4], Stuart Parkin[5], Claudia Felser[1,2], and Günter Reiss[1,2] — [1]Physics Department, Bielefeld University, Germany — [2]Center for Spinelectronic Materials and Devices, Universitätsstraße 25, 33605 Bielefeld, Germany — [3]Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [4]CNRS, Institut NEEL and Univ. Grenoble Alpes, F-38000 Grenoble, France — [5]Max Planck Institute for Microstructure Physics, 06120 Halle/Saale, Germany

We present a new and versatile concept for devices based on topological materials. To maintain their topological character high quality samples with clean interfaces to adjacent functional device components are mandatory. This requirement forms a bottleneck of current research, because very often the established thin film deposition fails to produce such high quality samples and bare surfaces of single crystals lack the necessary flatness. We demonstrate a novel, all-in-ultrahigh-vacuum process that enables to realize, e.g. tunnel junctions, Andreev contacts or SQUID rings from single crystalline bulk material. The validity of the technique is verified and illustrated with tunnel junctions made from cleaved single crystals of the half-Heusler topological superconductor candidate YPtBi.

DS 38.10 Wed 17:30 H32

Effective geometric phases and topological transitions in SO(3) and SU(2) rotations — •Henri Saarikoski[1], J. Enrique Vázquez-Lozano[2], José Pablo Baltanás[2], Junsaku Nitta[3], and Diego Frustaglia[2] — [1]RIKEN Center for Emergent Matter Science, Japan — [2]Departamento de Física Aplicada II, Universidad de Sevilla, Spain — [3]Department of Materials Science, Tohoku University, Japan

We address the development of geometric phases in classical and quantum magnetic moments (spin-1/2) precessing in an external magnetic field. We show that nonadiabatic dynamics lead to a topological phase transition determined by a change in the driving field topology. The transition is associated with an *effective* geometric phase which is identified from the paths of the magnetic moments in a spherical geometry. The topological transition presents close similarities between SO(3) and SU(2) cases but features differences in e.g. the limiting values of the geometric phases [1]. We discuss possible experiments where the effective geometric phase would be observable [2].

[1] H. Saarikoski, J. E. Vázquez-Lozano, J. P. Baltanás, J. Nitta, and D. Frustaglia, arXiv:1511.08315 (2015). [2] H. Saarikoski, J. E. Vázquez-Lozano, J. P. Baltanás, F. Nagasawa, J. Nitta, and D. Frustaglia, Phys. Rev. B 91, 241406(R) (2015).

DS 39: Resistive Effects I

Time: Thursday 9:30–11:00 Location: H8

DS 39.1 Thu 9:30 H8

Investigation of oxygen vacancy formation and migration in HfO_2 from density functional theory — •Marta Gibertini, Daniel Wortmann, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH and JARA, D-52425 Jülich, Germany

Oxygen vacancies are crucial in the performance of resistive random access memory (ReRAM), one of the most promising device concepts for nonvolatile memory. However, the exact mechanism of switching of a ReRAMs between two states (low and high resistance) is still not clear, especially at the microscopic level. In the formation process of conductive pathways, the vacancy formation and migration play an important role. Therefore, we present a density functional theory (DFT) study of the formation energy and the diffusion barrier of oxygen vacancies in HfO_2. Different structures (cubic, tetragonal, monoclinic), different charge states of the vacancy and different pathways are considered. The role of electronic correlations is investigated in the DFT+U model. The calculations are done for different supercell sizes employing the electronic structure code juRS, a real-space finite-difference implementation of the projector augmented wave (PAW) method.

DS 39.2 Thu 9:45 H8

Impact of Cation-Stoichiometry on Switching Speed and Data Retention in $SrTiO_3$ Thin Film Devices — •Nicolas Raab[1], Christoph Bäumer[1], Karsten Fleck[2], Stephan Menzel[1], and Regina Dittmann[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, 52428 Jülich — [2]Institut für Werkstoffe der Elektrotechnik (IWE-2), RWTH Aachen, 52074 Aachen

$SrTiO_3$ is a model material for resistive switching oxides. Among various proposed switching models, the filamentary switching based on oxygen migration is widely accepted for $SrTiO_3$. It is generally assumed that defects have a strong impact on the resistive switching properties of $SrTiO_3$. However, the correlation between different types of defects present in thin film devices and the resistively switching properties remains elusive.

We fabricated single-crystalline $SrTiO_3$ thin films with different cation ratio to investigate the stoichiometry-related and therefore defect-dependent influence on the resistive switching properties. Beyond a certain degree, non-stoichiometry is accommodated by the formation of extended defects rather than by point defects which are the dominant defect type in the more stoichiometric case. In the devices with either Ti- or Sr-excess a lower current in the pristine state and a higher current in the low resistance state was observed. These non-stoichiometric devices exhibit a larger memory window and a significantly better data retention. We will present a consistent explanation for this modified switching properties in non-stoichiometric thin film devices, supported by an estimation of the filament diameters.

DS 39.3 Thu 10:00 H8

Resistive switching devices with ultrathin graphene top electrodes for in situ spectromicroscopic characterization —

•Richard Valenta, Christoph Bäumer, Christoph Schmitz, David Müller, Nicolas Raab, Slavomir Nemsak, Claus Michael Schneider, Rainer Waser, and Regina Dittmann — Peter Grünberg Institut and JARA-Fit, Forschungszentrum Jülich, 52425 Jülich

Resistively switching transition metal oxides are gaining in importance as a promising alternative for future non-volatile memory. Although the switching mechanism is not fully understood, it has been shown that nanoscale redox reactions are responsible for a localized change of the resistance. Spectromicroscopic measurements present a powerful tool to investigate such localized chemical and structural changes and can give a deeper understanding of the switching mechanism.

Here we will present local changes in the electronic structure of $SrTiO_3$-based memristive devices in two different resistance states, utilizing in-operando photoemission electron microscopy measurements (PEEM). Since PEEM is very surface sensitive, ultrathin graphene top electrodes are used to attain spectroscopic information from the active $SrTiO_3$ layer of a functioning device. Localized changes of the work function as well as changes in the O K-edge spectra indicate that the resistance change coincides with redox reactions within confined switching filaments. This finding substantiates the expected filamentary switching of $SrTiO_3$ and confirms that the resistance change is caused by oxygen migration.

DS 39.4 Thu 10:15 H8

Energy-efficient and fast BiFeO3-based artificial synapses with a time window of 25ms to 125μs — •Nan Du[1], Tiangui You[1], Mahdi Kiani[1], Christian Mayr[2], Danilo Bürger[1], Ilona Skorupa[1,3], Oliver G. Schmidt[1,4], and Heidemarie Schmidt[1] — [1]Faculty of Electrical and Information Engineering, TU Chemnitz — [2]Faculty of Electrical Engineering and Information Technology, TU Dresden — [3]Institute of Ion Beam Physics and Materials Research, HZDR — [4]Institute for Integrative Nanosciences, IFW Dresden

Memristive devices can be used to emulate spike-driven synaptic plasticity (STDP) by applying specific voltage waveforms at their two terminals. In this work, we investigate STDP [1] with a simplified single pairing of one presynaptic voltage spike and one postsynaptic voltage spike in a BiFeO3 (BFO)-based memristive device [2-4]. We show that the analog resistive switching of BFO memristors allows to shorten the learning time constant of the STDP function to 125 μs. As the power consumption is a major constraint in neuromorphic circuits, the energy-efficient setting process has also be demonstrated for BFO-based artificial synapse with short and simplified spike sequences (4.5 pJ). [1] C. Mayr, P. Stärke, J. Partzsch, L. Cederstroem, R. Schüffny, Y. Shuai, N. Du, H. Schmidt, Adv. Neural Inf. Process. Syst. 25, 1700-1708 (2012).[2] Y. Shuai et.al., IEEE Elec. Dev. Lett. 34, 54-56 (2013). [3] N. Du et. al., Front. Neurosci. 9, 227 (2015). [4] T. You, Y. Shuai, W. Luo, N. Du, D. Bürger, I. Skorupa, R. Hübner, S. Henker, C. Mayr, R. Schüffny, T. Mikolajick, O. G. Schmidt, H. Schmidt, Adv. Funct. Mater. 24, 3357-3365(2014)

DS 39.5 Thu 10:30 H8

Influence of Stack Order on the Forming and Switching Behavior of HfO_2/TiO_2 Bilayer Cells for ReRAM Applications — •Alexander Hardtdegen, Hehe Zhang, and Susanne Hoffmann-Eifert — Peter Grünberg Institut (PGI-7) and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany

In this study we investigate the potential of HfO_2/TiO_2 bilayers composed of 3 nm thin ALD films for application in resistive devices. Special focus is on the influence of the stack sequence on the forming and switching behavior of nano crossbar structures of 100 x 100 nm^2 area. The Pt bottom electrode serves as inert layer, while sputtered Ti and Hf are chosen as oxygen exchange layers (OEL), depending on the top layer of the oxide film stack, TiO_2 and HfO_2, respectively.

The stack order and the OEL layer show influences on the forming and switching properties of the cells. Stacks with $Pt/HfO_2/TiO_2/Ti$ exhibit a forming voltage of 2.65 V which is significantly higher as the value of 1.90 V obtained for the stack with $Pt/TiO_2/HfO_2/Hf$, although the thicknesses of the oxide layers are identical. After forming into the ON state and subsequent reset, both cells show stable bipolar resistive switching with SET voltages lower than 1.0 V. A resistance ratio of about 100 is obtained for an operation current of about 300 μA with ON and OFF resistances of 1-5 kΩ and 100-300 kΩ, respectively. For current compliances higher than 500 μA, the devices of both stacks show self-limited switching behavior. Additionally, devices were switched with voltage pulses of about 100 ns. Dependencies of the switching time on the switching voltage and power are discussed.

DS 39.6 Thu 10:45 H8

Hanle magnetoresistance in thin metal films with strong spin-orbit coupling — Saül Vélez[1], •Vitaly Golovach[2,3,4], Amilcar Bedoya-Pinto[1], Miren Isasa[1], Edurne Sagasta[1], Mikel Abadia[2,3], Celia Rogero[2,3], Luis Hueso[1,4], Sebastian Bergeret[2,3], and Fèlix Casanova[1,4] — [1]CIC nanoGUNE, 20018 Donostia-San Sebastián, Basque Country, Spain — [2]Centro de Física de Materiales (CFM-MPC), Centro Mixto CSIC-UPV/EHU, 20018 Donostia-San Sebastián, Basque Country, Spain — [3]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastián, Basque Country, Spain — [4]IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Basque Country, Spain

The theory of Hanle magnetoresistance is worked out and applied to thin metal films with strong spin-orbit interaction, exhibiting the spin Hall effect. A correction to the resistivity tensor is derived and analyzed for the case of a classically weak magnetic field. The spin accumulation created at the surfaces of the film by the spin Hall effect decreases with the magnetic field because of the Hanle effect, resulting in an increase of the electrical resistance. The angular dependence of this magnetoresistance resembles the recently discovered spin Hall magnetoresistance in $Pt/Y_3Fe_5O_{12}$ bilayers, although the presence of a ferromagnetic insulator is not required. We show that this Hanle magnetoresistance is an alternative, simple way to quantitatively study the coupling between charge and spin currents in metals with strong spin-orbit coupling. The theory is compared against experiments carried out for Pt and Ta thin films.

DS 40: Focussed Session: Oxide Semiconductors for Device and Energy Applications I (Joint session of DS and HL, organized by DS)

Semiconducting metal oxides possess a very high potential for electronic devices and energy applications. For example, the n-type semiconductor Ga_2O_3 is currently intensively investigated due to its favorable semiconducor properties for power electronics, whereas the p-type semiconductor NiO can serve as important charge extraction barrier, to increase the efficiency of organic photovoltaics. The scope of this focus session encompasses well defined oxide structures of highest material quality and the understanding of their device-related physical properties as essential prerequisites for the application-relevant technological control of semiconducting metal oxides.

Organizers: Andreas Klein (TU Darmstadt), Oliver Bierwagen (PDI Berlin), Holger von Wenckstern (U Leipzig), and Martin Feneberg (OvGU Magdeburg)

Time: Thursday 9:30–13:15 Location: H11

Topical Talk DS 40.1 Thu 9:30 H11

Oxide semiconductors: materials design and applications — •Hideo Hosono — Tokyo Institute of Technology, Yokohama, Japan,

Oxide semiconductors have a long history comparable to IV group element semiconductors. Although industrial application remains still a few, industrial application of thin film transistors with oxide semiconductor (IGZO) channel has started to drive high resolution, large sized OLED-TVs as well as energy-saving LCDs recently, and Ga2O3 with a band gap of ~5eV is attracting as a semiconductor for power electronic applications.

The chemical bonding of oxides is rather different from that of typical semiconductors, which in turn gives unique band structure and crystal structure. In this talk, I review the progress of oxide semiconductors in last 2 decades focusing on materials design and applications utilizing the unique nature of oxides.

Topical Talk DS 40.2 Thu 10:15 H11

Mixing In and Ga sesquioxides - and their polar phases — •Vincenzo Fiorentini — Dept of Physics, Cagliari University, Italy — CNR-IOM, UOS Cagliari, Italy

This talks will report on recent first-principles theoretical work on the In and Ga sesquioxides and their ternary alloy, an up-and-coming materials system for near to deep-UV large-breakdown and transparent-conducting materials. Firstly, a qualitative phase diagram is proposed over all the full composition range. Three structures –monoclinicβ, layered-hexagonal, and cubic bixbyite– are competing for the ground state, and several regions of miscibility and phase separation interlace as function of composition, more or less independently of temperature. Electronic properties, including absorption anisotropy at low x, and a selection of interface band offsets will also be presented. Secondly, the metastable polar phase ε-Ga_2O_3 is shown to be pyroelectric (i.e. locked in a non-switchable polarized structure) with a large ferroelectric-like polarization 0.23 C/m^2 and a diagonal piezoelectric coefficient (0.77 C/m^2) in line with those of III-V nitrides and II-VI oxides. In view of recent growth successes in that direction, the interface of ε-Ga_2O_3 to GaN is studied, both in terms of geometry, offsets, and polarization difference, suggesting interesting potential for power applications. Work in collaboration with M. B. Maccioni, F. Ricci, R. Fornari.

Topical Talk DS 40.3 Thu 10:45 H11

Exploring and tailoring conductance phenomena in oxide films: An STM study — •Niklas Nilius — Carl von Ossietzky Universität Oldenburg

Electronic properties of classical semiconductors, e.g. Si, are adjustable with high accuracy and form the basis of todays information technology. Also oxides exhibit fascinating electronic features, e.g. a large spread in gap sizes, a correlated electronic behavior, metal-insulator transitions, anomalous temperature and voltage dependencies and superconductivity. Despite this potential, no satisfactory mechanistic understanding of oxide properties has been achieved so far and preparation of phase-clean materials remains challenging.

My talk demonstrates how thin-film oxides of high structural quality can be prepared and explored at atomic length-scales by STM. The approach yields direct correlation between structural parameters and electronic properties of the materials. Moreover, their conductance behavior becomes tunable, e.g. by stoichiometry and defect engineering, doping and interface control. I will present examples for low-gap oxides, e.g. Cu_2O and V_2O_3, and discuss how their electronic response is affected by intrinsic defects and dopants. For wide-gap materials, such as MgO and CeO_2, the interplay between conductance and low-dimensional edge and surface states as well as uncompensated polarity is addressed. Finally, the transition from binary to ternary oxides is introduced as a route to tune electronic properties. My talk aims at providing mechanistic insights into the structure-conductivity relationship rather than presenting materials of direct technological relevance.

15 min. break.

Topical Talk DS 40.4 Thu 11:30 H11

Miscibility and phase separation in $(In_xGa_{1-x})_2O_3$ — •Martin Albrecht[1], Robert Schewski[1], Toni Markurt[1], Tobias Schulz[1], Michele Baldini[1], Günter Wagner[1], Holger von Wenckstern[2], Marius Grundmann[2], Hartwin Peelaers[3], Joel Varley[3], and Chris Van de Walle[3] — [1]Institute for Crystal Growth, Berlin, Germany — [2]Universität Leipzig — [3]Materials Department, University of California, Santa Barbara, California, USA

Group III sesquioxides are distinguished from other wide band gap semiconductors by the fact, that they can be efficiently n-doped despite a wide band gap that ranges from 2.7 eV for In_2O_3 over 4.8 eV for Ga_2O_3 to 8.9 eV for Al_2O_3. Full exploitation of their properties for electronic applications requires band gap engineering formation of solid solutions. The formation of solid solutions in group III sesquioxides is challenging, since, at thermodynamic equilibrium, the binaries exhibit different thermodynamically stable structures (cubic, rhombohedral, and monoclinic) besides a significant lattice mismatch. The oxygen coordination of the metal atoms in the binary alloys is either octahedral, or mixed tetrahedral and octahedral. In this presentation we report on transmission electron microscopy studies on miscibility and phase separation in the system $(In_xGa_{1-x})_2O_3$ grown by PLD. We identify essentially three different phases as dependent on composition, i.e. the monoclinic β-phase in the compositional range up to $x = 0.5$, an ordered hexagonal phase in the range between $x = 0.5$ and 0.75 and the cubic bixbyite phase at higher In contents. In atoms occupy octahedrally coordinated cation sites in the monoclinic phase.

DS 40.5 Thu 12:00 H11

Infrared response of cubic In_2O_3 — •Martin Feneberg[1], Christian Lidig[1], Jakob Nixdorf[1], Oliver Bierwagen[2,3], James S. Speck[3], Zbigniew Galazka[4], and Rüdiger Goldhahn[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke Universität Magdeburg — [2]Paul Drude Institut für Festkörperelektronik, Berlin — [3]Materials Department, University of California, Santa Barbara, USA — [4]Leibniz-Institut für Kristallzüchtung, Berlin

The infrared optical response of cubic bixbyite In_2O_3 samples is investigated in detail. Samples with different concentrations of free electrons from 1.5×10^{17} up to 1.6×10^{21} cm^{-3} are measured by spectroscopic ellipsometry yielding dielectric functions. Besides transerse optical phonon modes a Drude contribution accounting for the free electron gas is observed and analyzed.

The broadening factor in the Drude contribution can be understood as characteristic relaxation time constant. Its frequency dependency is visible in point-by-point fitted dielectric functions, i.e. without assumptions about the line shape. The broadening factor is found to be a constant within errors of measurement.

By comparison with Hall-effect data, the effective electron mass is found to be a function of energy increasing from $m^* = 0.18m_0$ at the Γ-point of the Brillouin zone. This is direct proof of the non-parabolic nature of the conduction band.

DS 40.6 Thu 12:15 H11

Electrical conductivity and gas-response of the In_2O_3 surface electron accumulation layer — •Julius Rombach[1], Oliver Bierwagen[1], Alexandra Papadogianni[1], Markus Mischo[2], Volker Cimalla[2], Oliver Ambacher[3], Theresa Berthold[4], Marcel Himmerlich[4], and Stefan Krischok[4] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin — [2]Fraunhofer Institut für Angewandte Festkörperphysik, Freiburg — [3]Institut für Mikrosystemtechnik, Freiburg — [4]Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany

Indium oxide is a well-known material for conductometric gas sensors, showing a decrease in conductance when exposed to oxidizing gases. In contrast to typically used polycrystalline films, we study MBE-grown single-crystalline In_2O_3 thin films as a model system with reduced complexity. Electrical conductivity of these films essentially consists of two parallel contributions: the bulk of the film and the surface electron accumulation layer (SEAL) of unknown conductance. Both these contributions are varied to understand their effect on the sensor response. Conductivity changes induced by UV illumination in air, forcing desorption of oxygen adatoms on the surface, and gas-response measurements in ozone atmosphere give a measure of the sensor response and show that the sensor effect is only due to the SEAL conductivity. Therefore, a strong sensitivity increase is achieved by reducing the bulk (or intra-grain) conductivity. Hall and Seebeck measurements will give further details helping to estimate the SEAL electron concentration and mobility.

DS 40.7 Thu 12:30 H11

Surface structure of β-Ga_2O_3(100) via classical and quantum mechanical rainbow scattering — •Marco Busch[1], Eric Meyer[1], Helmut Winter[1], Zbigniew Galazka[2], Klaus Irmscher[2], and Konrad Gärtner[3] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstrasse 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Strasse 2, 12489 Berlin, Germany — [3]Institut für Fest- körperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Fast light atoms and molecules with energies from 200 eV up to several tens of keV are grazingly scattered from a clean and well-ordered β-Ga_2O_3(100) surface. The angular distributions of projectiles scattered in the regime of axial surface channeling show intensity maxima, which can be described with the concept of the classical rainbow scattering and offer the determination of the interaction surface potential. However, for decreasing projectile energy one can observe Bragg peaks in the angular distributions, which can be interpreted within the framework of quantum mechanics only. Here, we present investigations of the quantum scattering from the ex-situ cleaved and in-situ annealed (100) surface of β-Ga_2O_3 single crystals, grown by the Czochralski method. The splittings of Bragg peaks and their intensity modulations were so far exploited to deduce information on the arrangement of the atoms and thereby the termination and relaxation of the topmost surface layer [1]. Based on these investigations, the adsorption of atoms and molecules on the β-Ga_2O_3(100) surface can be studied in detail. [1] M. Busch et al., Appl. Phys. Lett. **105**, 051603 (2014).

DS 40.8 Thu 12:45 H11

Vibrational spectra, Raman and IR properties of Copper-Oxide Phases from first principles — •Marcel Giar, Markus Heinemann, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-University, D-35392 Giessen, Germany

Vibrational properties of the three copper oxide phases Cu_2O, Cu_4O_3, and CuO are derived from DFT calculations. Phonon dispersions including non-analytical contributions to the dynamical matrix in the limit $\mathbf{q} \to \mathbf{0}$ are presented as well as derived quantities such as acoustic phonon group velocities and thermodynamics. We further examine Raman and IR properties and their behavior under uniform external pressure. The frequency dependence of the Raman susceptibility and resulting changes in the Raman scattering intensities are also assessed.

DS 40.9 Thu 13:00 H11

Optical properties of single crystalline $SrMoO_3$ thin films — •Aldin Radetinac, Jörg Zimmermann, Karoline Hoyer, Hongbin Zhang, Philipp Komissinskiy, and Lambert Alff — Institute for Materials Science, TU Darmstadt, Germany

The optical properties of pulsed laser deposited highly crystalline $SrMoO_3$ thin films were investigated.[1] Due to their low resistivity below $30\,\mu\Omega$cm, thin films of $SrMoO_3$ are candidates for transparent conductor applications. The transparency of $SrMoO_3$ extends into the ultraviolet range to about 300 nm. In this range, $SrMoO_3$ has a higher transparency at similar sheet resistance as compared to alternative oxide or metallic materials. Density functional theory shows that electron-electron correlation effects are small in $SrMoO_3$ as compared to other low-resistivity transition metal oxides and predicts the optical properties in good agreement with experiment. This work was supported by the DFG project KO 4093/1-1.

[1] A. Radetinac, J. Zimmermann, K. Hoyer, H. Zhang, P. Komissinskiy and L. Alff submitted to J. Appl. Phys. (2015)

DS 41: Transport: Molecular Electronics and Photonics I (Joint session of CPP, DS, HL, MA, O and TT, organized by TT)

Time: Thursday 9:30–13:00 Location: H23

DS 41.1 Thu 9:30 H23

Pulling and Stretching a Molecular Wire to Tune its Conductance — •Gaël Reecht[1,4], Hervé Bulou[1], Fabrice Scheurer[1], Virginie Speisser[1], Fabrice Mathevet[2], César González[3], Yannick J. Dappe[3], and Guillaume Schull[1] — [1]IPCMS, Strasbourg, France — [2]Laboratoire de Chimie des Polymères, Paris, France — [3]CEA IRAMIS, Saclay, France — [4]Freie Universität Berlin, Berlin, Germany

Molecular junctions are perceived as the ultimate step toward the miniaturization of electronic components based on organic materials. Here, a low temperature scanning tunnelling microscope is used to lift a polythiophene wire from a Au(111) surface while measuring the current traversing the molecular junction. Conductance traces recorded during the lifting procedures reveal abrupt increases of the current intensity, which we associate to detachments of the wire subunits from the surface, in apparent contradiction with the expected exponential decrease of the conductance with wire length. With, ab initio simulations we reproduce the experimental data and demonstrate that this unexpected behavior is due to release of mechanical stress in the wire. Therefore, with the high control ability of the STM, by stretching the suspended molecular wire, we are able to tune its conductance properties.

DS 41.2 Thu 9:45 H23

STM-induced luminescence of single molecule junction — •Michael Chong[1], Gael Reecht[1], Hervé Bulou[1], Alex Boeglin[1], Fabrice Mathevet[2], Fabrice Scheurer[1], and Guillaume Schull[1] — [1]Institut de Physique et Chimie des Matériaux de Strasbourg - CNRS - France — [2]Laboratoire de Chimie des Polymères - CNRS - Université Pierre et Marie Curie, Paris, France

Electroluminescence of a single molecule can be induced by means of scanning tunneling microscopy. When a molecule is placed between two metallic electrodes it is necessary to decouple it using thin insulating layers in order to measure its intrinsic luminescence. A direct contact with the electrodes (tip and substrate), necessary if we envision to build single molecule electronic devices, results in quenching or broadening of the fluorescence of the molecule. We use on-surface polymerization to embed a cromphore molecule in a molecular chain. The STM tip is then used to lift the chain in order to decouple the cromophore from the surface yet mantaining a circuit like configuration trough the molecular chain. The current generated by applying a bias to the electrodes excites the cromophore that then exhibits narrow line luminescence and vibronic peaks allowing chemical identification the emitting unit.

Moreover we demonstrate that this configuration allows to control the lifetime of the excited state of the emitting molecule by two orders of magnitude by changing the coupling of the single molecle with the substrate adjusting the tip-sample separation. This system might open the way to electro-plasmonic devices at the single molecule level.

DS 41.3 Thu 10:00 H23

Effects of spin-orbit coupling and many-body correlations in STM transport through copper phthalocyanine — Benjamin Siegert, •Andrea Donarini, and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

The interplay of exchange correlations and spin-orbit interaction (SOI) on the many-body spectrum of a copper phtalocyanine (CuPc) molecule and their signatures in transport are investigated. We first derive a minimal model Hamiltonian in a basis of frontier orbitals which is able to reproduce experimentally observed singlet-triplet splittings; in a second step SOI effects are included perturbatively. Major consequences of the SOI are the splitting of former degenerate levels and a sizable magnetic anisotropy, which can be captured by an effective low-energy spin Hamiltonian. We show that STM-based magnetoconductance measurements can yield clear signatures of both these SOI induced effects.

DS 41.4 Thu 10:15 H23

Conductance trend in linear oligoacenes controlled by quantum size-effects — •Richard Korytar[1], Tamar Yelin[2], Nirit Sukenik[2], Ran Vardimon[2], Bharat Kumar[3], Colin Nuckolls[3], Oren Tal[2], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, Germany — [2]Chemical Physics Department, Weizmann Institute of Science, Rehovot, Israel — [3]Department of Chemistry, Columbia University, New York, United States

In conventional electronics, the conductance of a wire decreases with length according to Ohm's law. In molecular electronics, quantum effects lead to a richer phenomenology. Oligoacenes are organic molecules which consist of (linearly) fused benzene rings. Recently, Yelin et al. [submitted] studied conductance of oligoacenes directly coupled to Ag leads and found increase of conductance with molecular length.

I will show that transport through oligoacenes is governed by a quantum size effect which controls the alignment and width of the lowest unoccupied molecular orbital. These ideas will be supported by first-principles transport calculations using density-functional theory.

Linear oligoacenes are one of the simplest realizations of zig-zag terminated graphene nano-ribbons. In the long-wire limit, I will demonstrate that the conductance as a function of the molecular length shows surprising oscillations with period of approx. 11 rings [1].

[1] R. Korytár, D. Xenioti, P. Schmitteckert, M. Alouani, and F. Evers, Nature Communications **5**, 5000 (2014).

DS 41.5 Thu 10:30 H23

Investigation of charge transfer processes in single crystals based on π-conjugated molecules — •Antonia Morherr[1], Alisa Chernenkaya[2], Sebastian Witt[1], Katerina Medjanik[3], Michael Bolte[1], Martin Baumgarten[4], Harald O. Jeschke[1], Roser Valentí[1], and Cornelius Krellner[1] — [1]Goethe-Universität Frankfurt, 60438 Frankfurt a. M., Germany — [2]Johannes Gutenberg-Universität, 55099 Mainz, Germany — [3]Lund University, MAX-lab, 22100 Lund, Sweden — [4]MPI für Polymerforschung, 55021 Mainz, Germany

Designing new charge transfer (CT) materials for tuning the physical properties ranging from metallicity over superconductivity to Mott insulators and the understanding of mechanisms of CT is of great interest [1]. New CT crystals of π-conjugated molecules as donors can be obtained by physical vapor transport (PVT) [2]. (Fluorinated) tetracyanoquinodimethane (TCNQ-F$_x$, x=0, 2, 4) was used as acceptor material to grow different CT salts. The crystal structure was detected by X-ray diffraction. Further spectroscopic measurements as infrared and NEXAFS measurements were applied on these single crystals to investigate the CT process. The analysis of N1s and F1s K-edge spectra shows changes for different acceptor strengths. Ab initio calculations for all compounds underline these results. This systematic investigation of CT materials helps to understand the CT process in more detail.

[1] N. Toyota, M. Lang, J. Müller, Low-Dimensional Molecular Metals, Springer-Verlag, Berlin, 2007

[2] B. Mahns et al., Cryst. Growth Des. **14**, 1338 (2014)

DS 41.6 Thu 10:45 H23

Single Molecule Junctions with Epitaxial Monolayer Graphene Electrodes — •Konrad Ullmann[1], Pedro B. Coto[2], Susanne Leitherer[2], Michael Thoss[2], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik und Interdisziplinäres Zentrum für Molekulare Materialien, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) — [2]Institut für Theoretische Physik und Interdisziplinäres Zentrum für Molekulare Materialien, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

To study transport through single molecules, a two dimensional, open-access testbed for individual molecules is desirable. Therefore we use epitaxial monolayer graphene to fabricate electrodes for single molecule junctions. With the help of a feedback-controlled electro-burning process nanometer sized gaps can be formed reproducibly. Using these electrodes, we studied transport through molecules with different anchor groups at low temperatures. Strong similarities in results obtained with the MCBJ-technique underline the high quality of our experimental data. For a fullerene-endcapped molecule we are able to assign features from the I-V characteristics to internal molecular degrees of freedom [1].

[1] K. Ullmann et al., Nano Lett. **15**, 3512 (2015)

DS 41.7 Thu 11:00 H23

Simulation of Electron Transport through Graphene-Molecule Junctions — •Susanne Leitherer[1], Uwe Frank[1], Konrad Ullmann[2], Pedro B. Coto[1], Heiko Weber[2], and Michael Thoss[1] — [1]Institute for Theoretical Physics and Interdisciplinary Center for Molecular Materials, University Erlangen-Nürnberg — [2]Chair of Applied Physics and Interdisciplinary Center for Molecular Materials, University Erlangen-Nürnberg

Charge transport in single-molecule junctions with graphene electrodes is investigated using a combination of density functional theory (DFT) electronic structure calculations and Landauer transport theory. In particular, we study covalently bonded molecule-graphene junctions as well as junctions, where the molecule is weakly bonded to graphene by van der Waals interaction [1]. Considering different examples for molecular bridges between graphene electrodes, we analyze the transmission probability and current-voltage characteristics. In junctions with zigzag terminated graphene electrodes, we find edge states, which can induce additional transport channels [2]. Furthermore, local conductance properties are investigated in the nanojunctions.

[1] K. Ullmann et al., Nano Lett. **15**, 3512 (2015)

[2] I. Pshenichnyuk et al., J. Phys. Chem. Lett. **5**, 809 (2013)

15 min. break

DS 41.8 Thu 11:30 H23

Electron transport through C$_{20}$ molecular junction — •Shigeru Tsukamoto and Stefan Blügel — PGI-1/IAS-1, Forschungszentrum Jülich and JARA, Jülich, Germany

We present electron transport properties of C$_{20}$ molecular junctions, which are evaluated within the framework of the density functional theory. The C$_{20}$ molecular junctions employed in this work are composed of a pair of Al bulk electrodes and a single C$_{20}$ molecule, which is known as the smallest fullerene molecule. The scattering wave functions of the molecular junctions are calculated by solving the Kohn-Sham equation by means of the over-bridging boundary matching method, which is based on the real-space finite-difference formalism. The transmission properties are extracted from the scattering wave functions and the electron transmissions are evaluated by the Landauer-Büttiker formula. The electron transmissions and the scattering wave functions are further analyzed by using the eigenchannel decomposition technique. As the result of the eigenchannel analysis, although the total transmission value is $\sim 3.0 G_0$ at around the Fermi level, more than five transmission channels are found to contribute to the electron transport, and none of the eigenchannels are opened to 100%. From the spatial distributions of the eigenchannels, we can see that the HOMO states of C$_{20}$ molecule, which are three-fold degenerated and occupied to one-third, mainly contribute to the transport. In addition, the LUMO state is also found to contribute as one of the eigenchannels at around the Fermi level. In the talk, we will present electron transport calculations with different molecular orientations.

DS 41.9 Thu 11:45 H23

Quantum interference effect transistor via "Kondo Blockade" in single molecule junctions — •Andrew Mitchell[1] and Jens Paaske[2] — [1]Institute for Theoretical Physics, Utrecht University, 3584 CE Utrecht, The Netherlands — [2]Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark

Single molecule junctions are basic building blocks of molecular electronics devices. The full power of these devices will be realized by exploiting inherent quantum mechanical effects. Two of the most striking quantum phenomena, with no classical analogue, are quantum interference (QI) due to competing electron transport pathways, and the Kondo effect (KE) due to entanglement and strong electronic interactions. Both QI and KE are widely observed in experiments. The description of QI accounts for the complexities of molecular structure, but is typically non-interacting. By contrast, the Anderson impurity model is usually used to describe interactions and the Kondo effect, but totally neglects molecular structure. In this talk I discuss the subtle interplay between QI and KE in a unified theory, showing that a novel gate-tunable "Kondo Blockade" regime can be exploited to realize an efficient quantum interference effect transistor.

DS 41.10 Thu 12:00 H23

Quantitative *ab initio* simulations of nanocarbon-metal extended contacts — •Artem Fediai[1,2], Dmitry Ryndyk[1,2], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden — [2]Center for Advancing Electronics Dresden, TU Dresden — [3]Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany

Recently developed approach presented in [1] allows to get quantitative information about the resistance R_c, effective contact length L_c, and contacts resistance scaling $R_c(L_c)$ in different extended side contacts depending on the electrode material. We apply this approach to find a contact resistance of side CNT-metal contacts, transfer length in graphene-metal contacts and electronic properties of the diodes with CNT channel and asymmetric contacts (with the electrodes made of different metals). These kinds of *ab initio* simulations were previously impossible due to numerical intractability of the side contacts longer then several nanometers. Our approach explicitly uses extended contact model concept, enforced by modular approach. This allows us to overcome numerical problems and understand physical processes in extended contacts.

[1] A. Fediai, D.A. Ryndyk, G. Cuniberti, PRB **91**, 165404 (2015)

DS 41.11 Thu 12:15 H23

Molecular switches for dangling bond circuits — •Thomas Lehmann[1,2], Dmitry A. Ryndyk[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann

Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Germany

On the road to atomic-scale electronic circuits, dangling bond wires are promising candidates. Dangling bonds are formed by selectively removing hydrogen from a passivated silicon surface [1,2] and multiple dangling bonds in a row feature extended electronic states. Those quasi 1D surface structures can be used as atomic scale interconnects. In such circuits, molecules, which can controllably passivate or depassivate a dangling bond can provide logical inputs for constructing simple logic elements. In this talk, we present recent studies combining density-functional based approaches with Green function methods of a molecular switch for dangling bond wires on silicon.

[1] T. Hitosugi, T. Hashizume, S. Heike, S. Watanabe, Y.Wada, T. Hasegawa, K. Kitazawa, Jpn. J. Appl. Phys. **36**, L361 (1997)
[2] H. Kawai, F. Ample, Q. Wang, Y. K. Yeo, M. Saeys, C. Joachim, J. Phys. Condens. Matter **24**, 095011 (2012)

DS 41.12 Thu 12:30 H23

Switchable negative differential resistance induced by quantum interference effects in porphyrin-based molecular junctions — •Daijiro Nozaki[1], Lokamani Lokamani[2], Alejandro Santana-Bonilla[2], Arezoo Dianat[2], Rafael Gutierrez[2], Gianaurelio Cuniberti[2], and Wolf Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Physik, Universität Paderborn, Paderborn, Germany — [2]Institute for Materials Science, TU Dresden, Dresden, Germany

Charge transport through a carbon-based molecular switch consisting of different tautomers of metal-free porphyrin embedded between graphene nanoribbons is studied by combining electronic structure calculations and nonequilibrium Green's function formalism. Different low-energy and low-bias features are revealed, including negative differential resistance (NDR) and antiresonances, both mediated by subtle quantum interference effects. Moreover, the molecular junctions can display moderate rectifying or nonlinear behavior depending on the position of the hydrogen atoms within the porphyrin core. We rationalize the mechanism leading to NDR and antiresonances by providing a detailed analysis of transmission pathways and frontier molecular orbital distribution.

[1] D. Nozaki, J. Phys. Chem. Lett. **6**, 3950 (2015).

DS 41.13 Thu 12:45 H23

Base alignment dependence on Seebeck coefficient of DNA: A diagrammatic non-equilibrium transport theory approach — •Yoshihiro Asai[1], Yueqi Li[2], Limin Xiang[2], Julio L. Palma[2], and Nongjian Tao[2] — [1]Research Center for Computational Design of Advanced Functional Materials, AIST, Central 2, Umezono 1-1-1, Tsukuba, Ibaraki 305-8568, Japan — [2]Center for Bioelectronics and Biosensors, Biodesign Institute, Arizona State University, Tempe, Arizona 85287-5801, USA

Theoretical calculation of temperature dependence of transport properties at finite bias voltage and/or at finite temperature gradient requires careful description of low energy excitations. Incorporation of phonon transport and its coupling to electron transport by no means should play a crucial role to describe the low energy physics. One of the authors succeeded to describe theoretically the temperature cross over behavior of the electric conductance found in the experiment of a long oligothiophene single molecular wires. The diagrammatic non-equilibrium transport theory is useful to describe the problem qualitatively. While the necessity of the non-perturbative approach to the problem is clear, it would be interesting to know how far we could go within the perturbative framework given that any reliable non-perturbative approach for the problem is not available at present. Here, we apply the theory to discuss the base alignment dependence of the Seebeck coefficient of DNA in the hopping temperature region. We will make comparative discussions on our theoretical results with our experimental ones.

DS 42: Organic Electronics and Photovoltaics II (Joint session of CPP, DS, HL and O, organized by CPP)

Time: Thursday 9:30–12:45 Location: H40

Invited Talk DS 42.1 Thu 9:30 H40

Patterned organic ferroelectric memory diodes by solution micromolding — •Paul Blom, Thomas Lenz, Simon Benneckendorf, Kamal Asadi, and Dago de Leeuw — Max Planck Institute for Polymer Research, Ackermannweg 10, Mainz, Germany, D-55128

Ferroelectric polymers are promising candidates for memory technology, since they provide two bistable non-volatile polarization states corresponding to a Boolean 1 and 0, which can repeatedly be switched by an external field. The most widely investigated organic ferroelectric is the copolymer of poly(vinylidene fluoride) and trifluoroethylene (P(VDF-TrFE)). However, implementation of ferroelectric capacitors into integrated circuits is hampered by the read-out of the information being destructive. This problem can be overcome by using phase separated blends of P(VDF-TrFE) with a semiconducting polymer. The bistable polarization state of the P(VDF-TrFE) yields the binary information that can be read-out non-destructively by the current through the semiconducting columns. Phase separation however is a random process that yields a spatially undefined microstructure. Here we use solution micromolding to obtain a linear grating of P(VDF-TrFE). he space in between the lines is backfilled with a semiconducting polymer, resulting in a binary array between two electrodes. The resulting ferroelectric diode can be programmed reversibly in a low resistive on-state and high resistive off-state. When the bias is turned off, the information is retained. The performance can be optimized by down scaling the lateral dimensions of the binary array.

DS 42.2 Thu 10:00 H40

A new Figure of Merit for Organic Solar Cells with Transport-limited Photocurrents — •Dieter Neher[1], Juliane Kniepert[1], Arik Elimelech[1], and L. Jan Anton Koster[2] — [1]University of Potsdam, Potsdam, Germany — [2]Zernike Institute for Advanced Materials, Groningen, The Netherlands

Organic semiconductors exhibit superior absorption properties but suffer from low mobilities. Organic solar cells, therefore, display non-ideal JV-curves. Here, we present a closed-form analytical expression for the JV-curves of organic solar cells, based on the model in reference [1]. The expression is able to reproduce simulated JV-curves for a wide range of mobilities, generation rates and recombination parameters. Most importantly, the model delivers a novel figure of merit α to express the balance between free charge recombination and extraction in low mobility photoactive materials. This figure of merit is shown to determine critical device parameters such as the apparent series resistance and the fill factor. We also find α to be related to the parameter θ as defined in reference [2], showing that the approaches published in [1] and [2] are closely related. With that, we can accurately reproduce the gradual decrease of the fill factor with increasing recombination coefficient, decreasing mobility and increasing thickness.

[1] U. Würfel, D. Neher, A. Spies, S. Albrecht, Nat Commun 2015, 6, 6951 [2] D. Bartesaghi et al., Nat Commun 2015, 6, 7083

DS 42.3 Thu 10:15 H40

Design Rules for Organic Donor-Acceptor Heterojunctions: Pathway for Charge Splitting and Detrapping — •Carl Poelking and Denis Andrienko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Organic solar cells rely on the conversion of a Frenkel exciton into free charges via a charge-transfer state formed on a molecular donor-acceptor pair. These charge-transfer states are strongly bound by Coulomb interactions and yet efficiently converted into charge-separated states. A microscopic understanding of this process, though crucial to the functionality of any solar cell, has not yet been achieved. Here we show how long-range molecular order and interfacial mixing generate homogeneous electrostatic forces that can drive charge separation and prevent minority carrier trapping across a donor-acceptor interphase. Comparing a variety of small-molecule donor-fullerene combinations, we illustrate how tuning of molecular orientation and interfacial mixing leads to a trade-off between photovoltaic gap and charge-splitting and detrapping forces, with consequences for the design of efficient photovoltaic devices.

[1] J. Am. Chem. Soc., 2015, **137**, 6320-6326
[2] Nature Materials, 2015, **14**, 434-439

DS 42.4 Thu 10:30 H40

Investigation of the hybrid charge transfer state at ZnO/organic interfaces — •Fortunato Piersimoni[1], Stefan Zeiske[1], Johannes Benduhn[2], Raphael Schlesinger[3], Norbert Koch[3], Koen Vandewal[2], and Dieter Neher[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — [2]Institut für Angewandte Photophysik, Technische Universität Dresden, Dresden, Germany — [3]Institut für Physik & IRIS, Adlershof Humboldt-Universität zu Berlin, Berlin, Germany

This contribution aims to study the Charge Transfer States (CTS) in hybrid systems based upon organic small molecules and ZnO. Those systems were investigated by means of spectrally resolved electroluminescence (EL) and external quantum efficiency (EQE). The presence of Hybrid CTSs is proven by the appearance of a distinct peak in the EL and EQE spectra located below the energy gap of the molecules or ZnO. The energy gap (Egap) between the ZnO conduction band and the donor HOMO was tuned either by varying the ZnO work function through self-assembled monolayers of polar molecules, or by employing organic donors with different HOMO energy. The correspondence between the EL peak position and the Egap attributes this emission to radiative recombination between an electron on the ZnO and a hole on the organic material. Notably all samples displayed a linear relation between the maximum of the EL spectrum and the 2/3 power of the electric field F, in accordance to the confinement of the HCTS in a rectangular electrostatic potential well, implying a certain degree of delocalization perpendicularly to the donor/acceptor interface.

DS 42.5 Thu 10:45 H40

PBDT[2F]T: Insight into the Secrets of a Wide Band-Gap Polymer with 7% Power Conversion Efficiency — •Julien Gorenflot[1,2], Andreas Paulke[3], Fortunato Piersimoni[3], Federico Cruciani[2], Dieter Neher[3], Pierre M Beaujuge[2], and Frédéric Laquai[2] — [1]Max Planck Institut für Polymerforschung, Mainz, Germany — [2]Universität Potsdam, Potsdam, Germany — [3]King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

PBDT[2F]BT:fullerene blends exhibit performance up to 75% higher than the reference P3HT:PCBM solar cells [1]. Using femto- to microsecond transient absorption, we investigate the origin of those outstanding properties. We find that geminate recombination losses of photogenerated charge carriers are nearly absent in PBDT[2F]BT:fullerene blends. Field-dependent measurement as well as morphological and energy levels characterization reveal efficient and field-independent charge generation, enabling excellent short-circuit current and fill factor. Strikingly, this outstanding generation is achieved in spite of a rather low offset between the polymer's excitons and the blend's charge transfer state energy levels, which allows for an open circuit voltage as high as 0.9 V. Replacing the fluorine substituents by hydrogen in those polymers results in only moderate performances, thus highlighting the importance of molecular design. This is discussed in terms of energy levels and blends morphology.

[1] J. Wolf et al., Chem. Mater. 27, 2015

15 min. break

DS 42.6 Thu 11:15 H40

The Meaning of Charge Carrier Density in Charge Extraction Experiments — •Juliane Kniepert, Edgar Nandayapa, and Dieter Neher — University of Potsdam, Potsdam, Germany

Charge extraction experiments are a powerful tool to extract important information on the charge carrier dynamics, such as the effective charge carrier mobility and the order and coefficient of nongeminate recombination, from charge carrier densities under steady state conditions. However, it is often neglected that the extracted carrier density in these experiments is highly sensitive to the actual carrier distribution in the device, which can be very inhomogeneous due to high carrier injection at the contacts, imbalanced mobilities or fast recombination. This is particularly true for organic solar cells, which usually have thin active layers and low intrinsic carrier densities. These conditions may lead to an erroneous interpretation of the results. We show with numerical simulations and experiments how the extracted carrier density is influenced by intrinsic (mobility, recombination coefficient, injection barriers) and extrinsic (layer thickness, illumination, bias) parameters. From these results we deduce experimental conditions for which reliable values for the carrier density, mobility and recombination coefficient can be obtained.

DS 42.7 Thu 11:30 H40

Rapid non-geminate recombination in organic solar cells — •Jona Kurpiers[1], John Love[1], Christopher Proctor[2], Thuc-Quyen Nguyen[2], and Dieter Neher[1] — [1]Institute of Physics and Astronomy, Soft Matter Physics, University of Potsdam, Germany — [2]Department of Chemistry & Biochemistry, University of California, Santa Barbara, USA

In the last years a dramatic increases in the efficiency of solution processed bulk heterojunction (BHJ) solar cells have been reported. However, the fundamental processes involved in the conversion of absorbed photons to free charges are still not fully understood. In this work, we use time delayed collection field (TDCF) experiments with exceptionally high time resolution to investigate the charge carrier dynamics in polymer-fullerene and small molecule-fullerene systems. TDCF experiments reveal rapid non-geminate recombination on the 20 ns time-scale, even for charge carrier densities comparable to one sun illumination. This loss becomes significantly accelerated at higher pulse fluences for the polymer-fullerene device. To identify the reason for this rapid loss, the recombination dynamics were further investigated on devices with different thicknesses. It is concluded that the primary reason for the nongeminate loss observed at the short time scale in the polymer blend is recombination of charges close to the contacts. In the small-molecule system however, the loss mechanism differs completely. Specifically, we find a rapid filling of traps on short time scales. Our work shows evidence that these rapid loss channels are essential to understand and can dramatically affect device operation.

DS 42.8 Thu 11:45 H40

Temperature dependent competition between different recombination channels in organic heterojunction solar cells — •Theresa Linderl, Ulrich Hörmann, Sergej Beratz, Mark Gruber, Stefan Grob, Alexander Hofmann, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg

A modification of the Shockley-Queisser theory is presented with a special focus on constellations, where a linear extrapolation of the temperature dependence of the open circuit voltage V_{OC} results in the optical gap of the absorber rather than in the intermolecular charge transfer (CT) gap. Depending on the electronic coupling strength between donor and acceptor molecules, either singlet or CT recombination is dominant in different temperature regimes. These regimes are separated by a transition temperature T_{tr} that is, in the case of small energy level offset and weak electronic coupling, around 300 K or even below. For α-sexithiophene (6T)/diindenoperylene (DIP) solar cells with elevated substrate temperature during 6T deposition the linear extrapolation of the temperature dependent V_{OC} yields a value of 2.07 eV, whereas the extrapolation for the device evaporated at room temperature results in a value of 1.90 eV. Heating the substrate during 6T deposition leads to a molecular configuration at the interface where the coupling between donor and acceptor molecules is strongly reduced compared to the device evaporated at room temperature. This results in a transition temperature well below room temperature which is confirmed by temperature dependent electroluminescence measurements.

DS 42.9 Thu 12:00 H40

Ambipolar Charge Transfer In Single-Wall Carbon Nanotube Based Bulk-Heterojunctions — •Michael Auth[1], Andreas Sperlich[1], Florian Späth[2], Tobias Hertel[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg — [2]Institute of Physical and Theoretical Chemistry, Julius Maximilian University of Würzburg, — [3]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

The exceptional electrical conductivity of Single-Wall Carbon Nanotubes (SWNT) makes them potentially interesting to improve charge transport in organic photovoltaics (OPV). Additionally, their near infrared absorption bands can improve the spectral response of conventional polymer-fullerene bulk-heterojunctions. Until now, only few OPV devices containing purified semiconducting SWNTs were reported regarding the charge transfer properties of solar cell absorbers. For this study we prepared highly purified semiconducting (6,5)-SWNT samples, which we investigated in combination with known OPV donors and acceptors, namely the fullerene acceptor $PC_{60}BM$ and the conjugated polymer P3HT. Using Electron Paramagnetic Resonance, we found specific signatures for charge carriers localized on either SWNTs, P3HT or $PC_{60}BM$ and revealed the potential ambipolarity of SWNTs, leading to either hole transfer from $PC_{60}BM$ or electron transfer from P3HT. Furthermore our measurements confirmed exceptional SWNT purity, with respect to doping, dangling bonds or catalyst residue. In conclusion, we see a high application potential of (6,5)-SWNTs in OPV and, generally, in optoelectronic devices.

DS 42.10 Thu 12:15 H40

Influence of the Heterojunction's Interface on the Dynamics of Separated Charges Recombination in Organic Photoactive Materials — •Julien Gorenflot[1,2], Niva Alina Ran[3], Mike Heiber[3], Guillermo Bazan[3,4], Thuc-Quyen Nguyen[3,4], and Frédéric Laquai[1,2] — [1]Max Planck Institut für Polymerforschung, Mainz, Germany — [2]King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia — [3]University of California Santa Barbara, Santa Barbara, California, United States — [4]Faculty of Science King Abdulaziz University, Jeddah, Saudi Arabia

A recent study has indicated that the energetic density of shallow trap states, specifically at the interface between the electron donor and the electron acceptor, could be responsible for the apparent high recombination order observed in organic photoactive blends [1]. In order to elucidate this issue, we carried out investigations on a material system that allows for well-controlled donor/acceptor interactions. Films of the small-molecule donor, H1, can be processed such that H1 molecules are either stacking with their pi-face perpendicular or parallel to the substrate. By evaporating a layer of the acceptor molecule C60 on the films, we study the effect of molecular orientation at the donor/acceptor interface on charge recombination using transient absorption spectroscopy. We compare the two bilayer systems to a bulk heterojunction also using H1, which is expected to have a mixture of face-on and edge-on donor/acceptor interactions as well as a much larger interface area. [1] J. Gorenflot et al., J. Appl. Phys.115, 144502 (2014)

DS 42.11 Thu 12:30 H40

Resonant GISAXS on ternary thin film systems — •Mihael Coric[1], Nitin Saxena[2], Jan Wernecke[3], Stefanie Langner[3], Peter Müller-Buschbaum[2], Michael Krumrey[3], and Eva M. Herzig[1] — [1]Technische Universität München, Munich School of Engineering, 85748 Garching, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [3]Physikalisch-Technische Bundesanstalt (PTB), Abbestraße 2-12, 10587 Berlin, Germany

Using additives to influence the properties of a material is an extensively used method in material science. It is also an approach to achieve morphological control in binary thin film systems like in organic photovoltaic systems. If the third component is also a polymer the morphological characterization poses a challenge since the sophisticated thin film characterization methods like grazing incidence small angle x-ray scattering (GISAXS) carried out a high x-ray energies can only distinguish between different electron densities. Using x-ray energies near the absorption edges of certain elements contained in the polymers enables a much higher contrast between the different materials, increasing the distinguishability of the different components within the active film of the organic solar cell. However, it is also challenging to interpret the scattering data correctly since some approximations routinely carried out in the theory used for interpretation of hard x-rays are no longer valid. We show our systematic measurements at the sulphur and chlorine edge and explain the advantages we can take out of the measurements to analyze the morphology of this ternary thin film.

DS 43: Frontiers of Electronic Structure Theory: Focus on Topology and Transport IV (Joint session of DS and O, organized by O)

Time: Thursday 10:30–13:15 Location: H24

Topical Talk DS 43.1 Thu 10:30 H24

Transport phenomena in broken-symmetry metals: Geometry, topology, and beyond — •Ivo Souza — Universidad del País Vasco, San Sebastián, Spain

While topological quantization is usually associated with gapped systems – Chern insulators and topological insulators – it can also occur in broken-symmetry metals, where the Fermi surface (FS) consists of disjoint sheets: the Berry-curvature flux through each sheet is quantized, defining an integer Chern index. Using ferromagnetic bcc Fe as an example, I will describe how the FS Chern numbers are related to the chiral degeneracies ("Weyl points") in the bandstructure. When placed in a static magnetic field, a Weyl (semi)metal will display the chiral magnetic effect (CME), where an electric field pulse $\mathbf{E} \parallel \mathbf{B}$ drives a transient current $\mathbf{j} \parallel \mathbf{B}$. Weyl semimetals with broken inversion and mirror symmetries can also display a "gyrotropic magnetic effect" (GME), where an oscillating magnetic field drives a current and, conversely, an electric field induces a magnetization. The GME is the low-frequency limit of natural optical activity. It is governed by the intrinsic magnetic moment (orbital plus spin) of the Bloch electron on the FS, in much the same way that the anomalous Hall effect and CME are governed by the FS Berry curvature. Like the Berry curvature, the intrinsic magnetic moment should be regarded as a basic ingredient in the Fermi-liquid description of transport in broken symmetry metals.

Topical Talk DS 43.2 Thu 11:00 H24

Dirac Fermions in Antiferromagnetic Semimetal — •Peizhe Tang, Quan Zhou, Gang Xu, and Shou-Cheng Zhang — Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045, USA

The analogues of elementary particles in condensed matter systems have been extensively searched for because of both scientific interests and technological applications. Recently massless Dirac fermions are found to emerge as low energy excitations in the materials named Dirac semimetals. The currently known Dirac semimetals are all nonmagnetic with both time-reversal symmetry T and inversion symmetry P. Here we show that Dirac fermions can exist in one type of antiferromagnetic systems, where T and P are broken but their combination PT is respected. We propose orthorhombic antiferromagnet CuMnAs as a candidate, analyze the robustness of the Dirac points with symmetry protections, and demonstrate its distinctive bulk dispersions as well as the corresponding surface states by ab initio calculations. Our results give a new routine towards the realization of Dirac materials, and provide a possible platform to study the interplay of Dirac-related physics and magnetism.

DS 43.3 Thu 11:30 H24

Spin Hall effect in non-collinear antiferromagnets Mn3X (X=Sn, Ge, Ga) — •Yang Zhang[1,3], Yan Sun[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany

Recently, large anomalous Hall effect (AHE) was realized in non-collinear antiferromagnetic (AFM) compounds Mn3X (X=Sn, Ge, Ga). We have found that the nonzero Berry curvature – origin of the AHE observed – will lead to another topological effect, the spin Hall effect (SHE) in the titled compounds. We have systematically investigated the intrinsic SHE and revealed large spin Hall conductivity [˜1000 ((*/e)*(S/cm)], which is comparable to that of the well-know SHE material Pt. Our work present a new family of AFM compounds for the room-temperature spintronic applications.

DS 43.4 Thu 11:45 H24

Electronic reconstruction and anomalous Hall conductivity in $3d$-oxide honeycomb lattices within the corundum structure — •santu baidya and rossitza pentcheva — Fakultät für Physik and Center of Nanointegration (CENIDE), Universität Duisburg-Essen, 47057 Duisburg

The electronic structure of $3d$ transition metal oxide honeycomb layers confined in the corundum structure (α-Al_2O_3) along the [0001] direction is investigated using density functional theory including an on-site Coulomb term (GGA+U). While in some cases (e.g. $(M_2O_3)/(Al_2O_3)_5$, M=Fe, Co, V, Cr, Ni) the confined geometry preserves the magnetic and electronic ground state properties of the corresponding bulk corundum compound $M_2\mathrm{O}_3$, strong deviations from the bulk behavior are observed in the case of $\mathrm{Ti_2O_3}$ and $\mathrm{Mn_2O_3}$ bilayers. Our results indicate a formation of a quasi two-dimensional electron gas with a vertical confinement of $\sim$5 Å for $\mathrm{Ti_2O_3}$ and $\sim$8.5 Å for $\mathrm{Mn_2O_3}$. As a function of lateral strain $(\mathrm{Ti_2O_3})/(\mathrm{Al_2O_3})_5$ undergoes a metal-to-insulator transition associated with a switching of orbital polarization. In the metallic state the Dirac point can be tuned to the Fermi level by variation of the c/a ratio. Including spin-orbit coupling a finite anomalous Hall conductivity is observed in $(M_2\mathrm{O}_3)/(\mathrm{Al_2O_3})_5$ (M=Ti, Mn).

DS 43.5 Thu 12:00 H24

Anomalous hall effect in triangular antiferromagnetic ordered structure — •Hao Yang[1], Sun Yan[2], Felser Claudia[2], Parkin Stuart[1], and Binghai Yan[2] — [1]Max Planck Institute of Microstructure Physics, 06120 Halle(Saale), Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

The anomalous Hall effect (AHE), a fundamental transport phenomenon of electrons in solids, has been believed to appear in ferromagnetic materials. Very recently AHE is revealed in noncollinear antiferromagnetic compounds. In this work, we have systematically investigated the AHE in antiferromagnetic materials Mn3X (X=Ir, Ge, Sn, Ga), where noncollinear 120-degree type antiferromagnetic spin order exists in the quasi-layered lattice. Assisted by the symmetry analysis, we demonstrate the strong anisotropy of the intrinsic anomalous Hall conductivity that is determined by the Berry curvature in the band structure. Our work well interprets recent experiment observations and predicts novel antiferromagnetic material candidates for the spintronic application.

DS 43.6 Thu 12:15 H24

Anomalous Hall conductivity and orbital magnetization as local quantities — •Antimo Marrazzo[1] and Raffaele Resta[2] — [1]THEOS, EPF Lausanne, Switzerland — [2]Dipartimento di Fisica, Univ. Trieste, Italy

Anomalous Hall conductivity (AHC) and orbital magnetization (OM) are—from a theorist's viewpoint—closely related: both have an expression as **k**-space integrals of the appropriate geometrical quantity. The **k** space is an artificial construct: all bulk properties are embedded in the ground state density matrix in **r** space, independently of the boundary conditions. Is it possible to address AHC and OM as local properties, directly in **r** space? For insulators, two recent papers have proved that the answer is affirmative: both AHC (quantized in insulators) and OM can be evaluated from a local formula over bounded samples. A rationale can be found in the "nearsightedness" of the density matrix: but since this is *qualitatively* different in insulators and metals (exponential vs. power law) it is not obvious that the same successful approach can be extended to metals. Using model Hamiltonians, we have performed simulations over 2D bounded metallic flakes, where the T-invariance is broken in two alternative ways: either à la Haldane, or by a macroscopic **B** field. In both cases, our simulations show that the relevant quantity can be extracted from a knowledge of the electron distribution in the bulk region of the sample only. This looks counterintuitive because the OM of a magnetized sample owes to currents localized near its surface; but the key reason for the success of the local approach to AHC and OM is that the formulas are *not* based on currents.

DS 43.7 Thu 12:30 H24

Laser induced DC photocurrents in a Topological Insulator thin film — •Thomas Schumann[1], Nina Meyer[1], Gregor Mussler[4], Eva Schmoranzerová[2], Dagmar Butkovicova[2], Helena Reichlová[3], Lukas Braun[5], Christian Franz[6], Michael Czerner[6], Pertr Němec[2], Detlev Grützmacher[4], Tobias Kampfrath[5], Christian Heiliger[6], and Markus Münzenberg[1] — [1]IfP, EMA University Greifswald, Germany — [2]MFF, Charles University, Prague, Czech Republic — [3]FZU, Prague, Czech Republic — [4]PGI-9, Jülich, Germany — [5]FHI Berlin, Germany — [6]University of Gießen, Germany

Topological Insulators (TI) open up a new route to influence the transport of charge and spin in a surface film via spin-momentum locking [1,2]. It has been demonstrated experimentally [2] that illumination by circularly polarized light can result in excitation of a helicity-dependent photocurrent.We report our recent results on laser induced photocurrents in a terniary 3D TI thin film. The resulting photocurrents are classified after [1,2] and we show that there are at least two signals visible, for example in time dynamics, which behave different in the suggested parameters.

We acknowledge the funding of the DFG via the SPP 1666 Topological Insulators and the joint DAAD PPP Czech Republic project FemtomagTopo. [1]S.D.Ganichev,W.Prettl,J.Phys.: Condens. Matter 15 (2003) R935-R983

[2]J.W.McIver,D.Hsieh,H.Steinberg,P.Jarillo-Herrero and N.Gedik, Nature Nanotechnology 7, 96-100 (2012)

DS 43.8 Thu 12:45 H24

Robustness of exchange protocols of Majorana fermions in quantum wire networks — •Christian Tutschku[1], Rolf W. Reinthaler[1], Chao Lei[2], Allan H. MacDonald[2], and Ewelina M. Hankiewicz[1] — [1]Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany — [2]Department of Physics, University of Texas at Austin, USA

The interface between topological non-trivial, one-dimensional, spinless p-wave superconductors and the vacuum is connected to the appearance of Majorana edge-modes [1], whose non-trivial exchange statistics makes them promising candidates for topological quantum computation [2]. Via T-Bar structures build of 1D-nanowires we can manipulate and exchange the Majorana fermions by purely electrical means [3]. By applying a tight binding approach we solve the time dependent Bogoliubov-de Gennes equations for the Kitaev chain model [1] and also cure the problem of an appearing additional Majorana-boundstate located at the T-Bar crossing point for small lattice constants. Furthermore we analyze how the robustness of the exchange protocols is affected by non-adiabatic effects or by a finite overlap of the Majorana bound states.

We acknowledge financial support by the DFG within SFB 1170 ToCoTronics.

[1] A. Y. Kitaev, Physics-Uspekhi **44**, 131 (2001)
[2] D. A. Ivanov, PRL **86**, 268 (2001)
[3] J. Alicea et al., Nature Physics **7**, 412 (2011)

DS 43.9 Thu 13:00 H24

Unpaired Majorana modes in Josephson junctions arrays with gapless bulk excitations — •Manuel Pino Garcia — Department of Physics and Astronomy, Rutgers The State University of New Jersey, 136 Frelinghuysen rd, Piscataway, 08854 New Jersey, USA

The search for Majorana bound states in solid-state physics has been limited to materials which display a gap in their bulk spectrum. We will show that such unpaired states appear in certain quasi-one-dimensional Josephson junctions arrays with gapless bulk excitations. The bulk modes mediate a coupling between Majorana bound states via the Ruderman-Kittel-Yosida-Kasuya mechanism. As a consequence, the lowest energy doublet acquires a finite energy difference. For realistic set of parameters this energy splitting remains much smaller than the energy of the bulk eigenstates even for short chains of length L ~ 10. In this talk, we first explain the JJA system and how to model it with an Ising-like Hamiltonian. Then, a qualitative argument is employed to obtain the low-energy effective theory using unpaired Majorana modes. We will show numerical results which confirm the validity of this effective theory and discuss problems that may arise in the experimental realization of our proposal.

DS 44: Physics and Application of Emergent 2D-semiconductors and their Heterostructures I (Joint session of DS and HL, organized by DS)

Time: Thursday 11:15–13:15 Location: H8

DS 44.1 Thu 11:15 H8

Defects in two-dimensional materials: their production under irradiation, evolution and properties from first-principles calculations — •Arkady Krasheninnikov — Helmholtz Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Germany — Department of Applied Physics, Aalto University, Finland

Following isolation of a single sheet of graphene, many other 2D systems such as hexagonal BN and transition metal dichalcogenides (TMDs) were manufactured. Among them, TMD sheets have received particular attention, as these materials exhibit intriguing. Moreover, the properties can further be tuned by introduction of defects and impurities. In my talk, I will present the results [1] of our first-principles theoretical studies of defects (native and irradiation-induced) in inorganic 2D systems obtained in collaboration with several experimental groups. I will further discuss defect- and impurity-mediated engineering of the electronic structure of 2D materials.

[1] Nature Comm. 6 (2015) 6736; ACS Nano 9 (2015) 3274; ACS Nano (2015) DOI: 10.1021/acsnano.5b04851; Phys. Rev. B 91 (2015) 125304; Adv. Mater. 26 (2014) 2857; Phys. Rev. X 4 (2014) 031044; see http://physics.aalto.fi/~ark/publist.html for complete list of publications.

DS 44.2 Thu 11:30 H8

Phonon induced line broadening and population of the dark exciton in a deeply trapped localized emitter in monolayer WSe2 — •Yu-Ming He[1,3], Chao-Yang Lu[3], Jian-Wei Pan[3], Sven Höfling[1,2,3], and Chrisitian Schneider[1] — [1]Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS,United Kingdom — [3]Hefei National Laboratory for Physical Sciences at the Microscale and Department of Modern Physics, & CAS Center for Excellence and Synergetic Innovation Center in Quantum Information and Quantum Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

We study locally trapped single excitons in a mechanically exfoliated WSe2 monolayer semiconductor with respect to their temperature stability, spectral diffusion and decay dynamics. We identify strong signatures of phonon induced spectral broadening in these emitters for elevated temperatures accompanied by temperature induced luminescence quenching. A direct correlation between the drop in intensity at higher temperatures with the phonon induced population of dark states in WSe2 is established.

DS 44.3 Thu 11:45 H8

Gate voltage dependence of the electron mobility in monolayer $\mathrm{MoS_2 - LiNbO_3}$ field effect transistors — •Wladislaw Michailow[1], Edwin Preciado[2], Florian Schülein[1], Benjamin Möller[1], Ariana Nguyen[2], David Barroso[2], Miguel Isarraraz[2], Gretel von Son[2], I-Hsi Lu[2], Velveth Klee[2], John Mann[2], Andreas Hörner[1], Achim Wixforth[1], Ludwig Bartels[2], and Hubert Krenner[1] — [1]Insitut für Physik, Universität Augsburg, Germany — [2]University of California, Riverside, USA

In field effect transistors (FETs) based on novel two-dimensional semiconductor materials, detailed knowledge of the density and the mobility of charge carriers in the conducting channel is of paramount importance. In the most common approach the field effect mobility and charge carrier density are determined by a simple parallel-plate capacitor model. In this model the carrier mobility is assumed to be independent of the gate potential. Here we report on investigations of monolayer $\mathrm{MoS_2 - LiNbO_3}$ FETs [1] in which we determined the source-drain current and the capacitance as function of gate voltage. We analyze both using a theoretical model of a two-dimensional free electron gas. This analysis allows us to derive both the charge carrier density and the mobility over the full $\pm 40\,\mathrm{V}$ range of gate voltage. Using our advanced analysis we show that for our structure the established parallel-plate capacitor model is oversimplified and overestimates the carrier mobility by a factor of $\gtrsim 4$.

[1] E. Preciado et al., Nat. Commun. **6**, 8593 (2015).

DS 44.4 Thu 12:00 H8

Resistivity switching in chalcogenide based interfacial phase change materials — •Nicki F. Hinsche and Kristian S. Thygesen — Center for Atomic-scale Materials Design, Technical University of Denmark, 2830 Kgs. Lyngby, Denmark

Chalcogenide based phase change materials (PCM) are emerging candidates for next generation non-volatile, ultra-fast memories. In contrast to conventional amorphous-crystal phase transition driven PCM, e.g. $\mathrm{Ge_2Sb_2Te_5}$, recently a new type of PCM device named *interfacial phase change memory* (iPCM) was proposed [1]. Here the electrical pulse induced movement of the atoms is limited to the interface, therefore substantially reducing the switching energies and allowing for shorter switching times.

By means of DFT electronic-structure [2] and Boltzmann transport calculations [3], we discuss for an iPCM GeTe-$\mathrm{Sb_2Te_3}$ heterostructure the electrical resistivity change caused by the structural switching at the interface. With a close relation of the material system to the family of topological insulators, ferroelectrics [4] and thermoelectrics, the possibility of a ferroelectric controllable topological phase transition and the ultra-fast modification of the thermoelectric properties, applicable for fast thermal switches, will be analysed additionally.

[1] R. E. Simpson *et al.*, Nature Nanotechnology **6** 8501(2011); [2] J. Enkovaara *et al.*, J. Phys.: Condens. Matter **22** 253202 (2010); [3] N. F. Hinsche *et al.*, ACS Nano **9** 4406 (2015) [4] A. V. Kolobov *et al.*, APL Mater. **2** 066101 (2014)

DS 44.5 Thu 12:15 H8

Electrical properties of CVD Molybdenum disulfide — •Wajid Awan[1], Tommy Schönherr[1], Artur Erbe[1], Stefan Facsko[1], and Xinliang Feng[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]Technische Universität Dresden

Two dimensional materials are attractive for the use in next-generation nanoelectronic devices as compared to one dimensional material because it is relatively easy to fabricate complex structures from them. Recently the layered 2D semiconducting Transition metal dichalcogenides came into the picture and got a place in a wide range of novel applications as well as in basic research. Strikingly, MoS_2 receives significant attention since it undergoes transition from indirect bandgap (bulk form) to a direct bandgap (1.2eV) semiconductor if thinned out to a single atomic layer. The bandgap is an essential property for tunable 2-D nanodevices. We performed electrical transport measurements at room temperature for CVD grown MoS_2 on SiO_2/Si substrate. Standard Electron beam lithography (EBL) was used to pattern Gold (Au) metal contacts on MoS_2 flakes. For the purpose of sample characterization, we performed the Atomic Force Microscopy (AFM) and Raman Spectroscopy techniques, respectively, which confirm that the thickness of the CVD grown MoS_2 triangular flakes corresponds to single layers. Low temperature characterization of the electrical properties of the layers elucidates the exact mechanisms of charge transport in the 2d-layers. This knowledge will be used to modify the electrical properties in a controlled way, for example by ion irradiation.

DS 44.6 Thu 12:30 H8

Nonlinear Optics in a Rydberg-Excited Semiconductor Cavity — •Valentin Walther, Robert Johne, and Thomas Pohl — Max Planck Institute for the Physics of Complex Systems, Dresden

Recent experiments have demonstrated excitons with extraordinarily large binding energies in some two-dimensional semiconductors (TMDCs), whose Rydberg states give rise to giant interactions and, therefore, hold great promise for optical utility.

We evaluate the optical response under conditions of electromagnetically induced transparency (EIT), accounting for the full excited level structure and numerous decoherence mechanisms in a semiconductor. Strong exciton-exciton interactions result in enormous effective photon-photon potentials. Using experimental parameters, we show that the photonic nonlinearity exceeds that of traditional semiconductors by several orders of magnitude and we assess the material properties required for coherent optical applications.

Further, we investigate interesting optical effects in the transverse mode structure of a driven-dissipative cavity arising from the unusually large nonlinearity.

DS 44.7 Thu 12:45 H8

Thermal expansion and transport in van-der-Waals solids from first-principles — •Daniel Lindroth, Per Hyldgaard, and Paul Erhart — Chalmers University of Technology, Gothenburg, Sweden

We have performed first-principles calculations for lattice thermal expansion and transport in the bulk of the transition metal dichalcogenides (TMDCs) MoS2, MoSe2, MoTe2, WS2, WSe2 and WTe2 using density functional theory (DFT) and the semi-classical phonon Boltzmann transport equation (BTE) within the relaxation time approximation (RTA).

Proper modeling of the lattice thermal conductivity is important for an accurate prediction of the thermoelectric figure of merit and better understanding of potentially high performing novel materials such as van der Waals heterostructures based on TMDCs. To this end, we have conducted a thorough investigation of the mentioned TMDCs based on DFT calculations using a recently published van der Waals density functional (vdW-DF-cx) in conjunction with anharmonic modeling of phonon lifetimes using third order interatomic force constants that allows for solutions to the BTE within the RTA as implemented in the phono3py code. We found that our calculations agrees with theoretical expectations as well as with experimental data where available. The methods used thus provide a promising framework for further investigation of more complex systems with potentially novel thermal properties.

DS 44.8 Thu 13:00 H8

Enabling a new class of electronic devices using self-aligned nanodomain boundaries to open a charge transport gap in trilayer graphene — •Victor Aristov[1,2,3], Olga Molodtsova[1,4], Sergey Babenkov[1], Tsung-Wei Huang[5], Askar Syrlybekov[6], Mourad Abid[7], Dmitry Marchenko[8], Jaime Sánchez-Barriga[8], Partha Sarathi Mandal[8], Andrei Varykhalov[8], Yuran Niu[9], Barry Murphy[6], Sergey Krasnikov[6], Olaf Lübben[6], Alexander Chaika[2,6], and Han-Chun Wu[6] — [1]DESY, Hamburg, Germany — [2]ISSP RAS, Chernogolovka, Russia — [3]TU Bergakademie, Freiberg, Germany — [4]ITMO, Saint Petersburg, Russia — [5]National Taiwan University, Taipei, Taiwan — [6]Trinity College, Dublin, Ireland — [7]King Saud University, Riyadh, Saudi Arabia — [8]BESSY, Berlin, Germany — [9]Max-lab, Lund, Sweden

Trilayer graphene reveals unique electronic properties interesting for fundamental science and technological applications. The ability to achieve a high on-off current ratio is the central question in this field. We propose a simple method to achieve a current with high on-off ratio by opening a transport gap in trilayer graphene with self-aligned periodic nanodomain boundaries (NBs). Our low temperature transport measurements clearly demonstrate that the self-aligned periodic NBs induce a huge charge transport gap, more than 1.3 eV at 10 K. As a result of our study the feasibility of creating new electronic nanostructures with high on-off current ratios using graphene on cubic-SiC/Si wafers was shown. This work was supported by the RAS, RFBR grants No 140200949 and 140201234, by SPP 1459 of DFG.

DS 45: Hybrid and Perovskite Photovoltaics IV (Joint session of CPP, DF, DS and HL, organized by HL)

Time: Thursday 14:45–18:30 Location: H2

DS 45.1 Thu 14:45 H2

Synthesis of perfectly oriented and micrometer-sized MAPbBr3 perovskite crystals for thin film photovoltaic applications — •Nadja Giesbrecht[1], Johannes Schlipf[2], Andreas Binek[1], and Pablo Docampo[1] — [1]Department of Chemistry and Center for NanoScience (CeNS), University of Munich (LMU), Butenandtstr. 5-13, 81377 Muenchen,Germany — [2]Lehrstuhl fuer Funktionelle Materialien, Physik-Department, Technische Universitaet Muenchen, James-Franck-Str. 1, 85748 Garching, Germany

Wide band-gap perovskites such as methylammonium lead bromide (MAPbBr3) are interesting materials for photovoltaic applications due to their potentially high open-circuit voltage. However, the fabrication of high quality planar films has not been investigated in detail for this material. We report a new synthesis approach for the fabrication of bromide based perovskite planar films based on the control of the deposition environment. The correlation of photocurrent and perovskite crystal properties in photovoltaic devices is studied. We achieve dense layers with large and perfectly oriented crystallites, as confirmed with grazing incidence wide angle X-ray scattering (GIWAXS). This represents the first solution-processed MAPbBr3 perovskite film with such a high degree of order. The current output was found to depend on crystal order in the perovskite film with internal quantum efficiencies approaching unity. Hence, our work not only gives a new pathway to tune morphology and crystal orientation, but demonstrates its importance for planar perovskite solar cells.

DS 45.2 Thu 15:00 H2

Structural properties of hybrid perovskites from first principles — •Jingrui Li[1], Jari Järvi[1,2], Hugo Levard[1], and Patrick Rinke[1] — [1]Aalto University, Helsinki, Finland — [2]University of Helsinki, Finland

Hybrid perovskites have received rapidly growing interest in recent years as promising photoactive materials in emergent photovoltaic technologies. We present a first-principles analysis of the atomistic structure of the methylammonium lead triiodide ($CH_3NH_3PbI_3$) perovskite in this work, with a particular focus on the orientation of $CH_3NH_3^+$ cations and its interplay with the inorganic matrix. Relativistic density functional theory calculations were performed using the all-electron local-atomic-orbital code `FHI-aims`. Our results indicate that (i) the lattice constants obtained by incorporating the long-range van der Waals interactions (using the Tkatchenko-Scheffler method) in the PBE exchange-correlation functional agree well with experiments; (ii) hydrogen bonding between the ammonium group and the I^- anions plays the decisive role in the position of the $CH_3NH_3^+$ cation and the shape of the PbI_3^{2-} framework; (iii) the reorientation of $CH_3NH_3^+$ is limited due to the high barriers ($\sim$ 80 meV). Based on these findings we establish a self-consistent multiscale model, in which the energetically favorable alignment of $CH_3NH_3^+$ dipoles in the material is determined by combining classical electrostatics and statistics with structure relaxation in DFT. Our procedure produces representative “pseudo random” methylammonium lead triiodide supercells that will form the basis of further first-principles work.

DS 45.3 Thu 15:15 H2

Micrometer size grains of hybrid perovskite through rapid melting procedure — •Oleksandra Shargaieva, Felix Lang, Jörg Rappich, Carola Klimm, Manuela Klaus, Bernd Rech, and Norbert Nickel — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Kekuléstr. 5, 12489 Berlin (Germany)

Interest in hybrid perovskites as an absorber has flared since the first successful attempts in dye solar cells (DSCs) and continues to grow as a promising material for solar cells application. The usage of such compounds is often associated with the opportunity to substitute existing materials due to the remarkable simplicity of the production process and its low costs. On the other hand, solution based processing of solid perovskite layers often includes difficulties with crystallization, which could result in the formation of grain boundaries. This type of crystalline defect has a strong impact on the performance of devices and tends to lower the power conversion efficiency.

In our work, we propose a new solvent-free approach to produce perovskite type compounds based on its melting process. This simple technic allows to obtain bulk material with grain sizes of several micrometers. Melting process enables the control of the crystallization of hybrid perovskite and by that suppresses grain boundaries formation. Furthermore, the procedure was optimized and successfully introduced into thin-film fabrication. Consequently, melting of perovskites gives a possibility to decrease non-radiative recombination and therefore, can improve the performance of the device.

DS 45.4 Thu 15:30 H2

J-V Hysteresis Observed in Methylammonium Lead Halide Perovskite Films at Different Voltage Scales — •Martina

Stumpp, Raffael Ruess, Jonas Horn, Jan Tinz, Christoph Richter, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen, GERMANY

Hysteresis in the current-voltage curves of methylammonium lead halide films deserves detailed investigation because it can affect their applicability in perovskite solar cells. In the current study, J-V hysteresis of $CH_3NH_3PbI_3$ and $CH_3NH_3Pb(I_{0.95}Br_{0.05})_3$ prepared via different established deposition techniques was studied in a symmetric contact geometry of microstructured gold electrode arrays on SiO_2/Si wafers. The measured J-V characteristics showed a different behavior of hysteresis depending on the applied voltage range. Residual currents at zero applied bias were observed following positive or negative poling showing persistent polarization of the perovskite films. At higher bias voltages, additional inverted hysteresis loops were measured pointing at a decrease in barrier height and width at blocking perovskite/metal contacts, presumably caused by migrating iodide ions. The net J-V characteristics in this voltage range can be simulated by two diodes operated back-to-back. Time-dependent studies were performed to analyze the decay of the different observed polarization phenomena in the films during either short-circuit or continuous sweeping of the bias.

DS 45.5 Thu 15:45 H2

Water infiltration in methylammonium lead iodide: fast and inconspicuous — •Christian Mueller[1,2,3], Bernd Epding[2,3], Tim Helder[2,3], Michael Sendner[2,3], Annemarie Pucci[2,3], Wolfgang Kowalsky[1,2,3], and Robert Lovrincic[1,3] — [1]IHF, TU Braunschweig, Germany — [2]KIP, Universität Heidelberg, Germany — [3]InnovationLab, Heidelberg, Germany

Extensive research efforts over the last few years led to a significant increase in power conversion efficiency of organometal-halide perovskite (such as $\mathrm{CH_3NH_3PbI_3}$) solar cells up to over 20%. However, our understanding of physical/chemical processes in the material lags behind device progress. For instance, the impact of water on $\mathrm{CH_3NH_3PbI_3}$-based devices, despite being well documented, is still not well understood and as such remains controversial.

Herein we use IR spectroscopy in controlled atmosphere to demonstrate that water infiltration into $\mathrm{CH_3NH_3PbI_3}$ occurs much faster and at much lower humidity than previously thought. We show that the exposure of $\mathrm{CH_3NH_3PbI_3}$ to ambient environment leads to an increase of the photocurrent by more than one order of magnitude in lateral devices. Based on transient photocurrent measurements we speculate that the effect is associated with enhanced proton conduction when light is combined with water and oxygen exposure. Our results suggest that water infiltration plays an important role in the optoelectronic properties of $\mathrm{CH_3NH_3PbI_3}$ based devices, well beyond the known water triggered degradation processes[1].

[1] C. Mueller et al., Chem. Mater., 27 (22), p. 7835-7841, 2015

DS 45.6 Thu 16:00 H2

Graphene on Hybrid Solar Cells: from Silicon and Perovskite towards Tandem Solar Cells — •Felix Lang, Matthias Zellmeier, Marc A. Gluba, Steve Albrecht, Jörg Rappich, Lars Korte, Bernd Rech, and Norbert H. Nickel — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekuléstr. 5, 12489 Berlin, Germany

A variety of hybrid solar-cell architectures require the deposition of a highly transparent and conductive contact. However, deposition techniques for conventional transparent conductive oxides typically degrade the topmost organic layers. A non-destructive wet transfer process of large area graphene from the growth substrate onto the desired sample is the clear choice to tackle this challenging problem.

Here, we present for the first time the implementation of graphene on hybrid crystalline silicon/P3HT solar cells. Despite identical V_{OC} and superior external quantum efficiency, device performance is limited by graphene sheet resistance. To overcome this limitation we combined in-situ graphene doping with an absorber with a higher band gap. Both measures reduce the impact on the device performance.

Implementation of graphene on the perovskite $\mathrm{CH_3NH_3PbI_3}$ therefore enabled a semi-transparent device concept showing superior internal quantum efficiency compared to conventional Au-contacted solar cells. The graphene contact enabled an optical sub-band gap transmission of around 60 % for the complete device. This paved the way for the development of a four terminal crystalline silicon/perovskite tandem solar cell with a power conversion efficiency of 13.2 %.

DS 45.7 Thu 16:15 H2

GW for transition metal perovskites — •Zeynep Ergonenc, Bongjae Kim, Peitao Liu, Georg Kresse, and Cesare Franchini — University of Vienna, Faculty of Physics and Center for Computational Materials Science

The ab initio calculation of quasiparticle (QP) energies beyond density functional theory is a technically and computationally challenging problem. In condensed matter physics the most widely used approach to determine QP energies is the GW approximation. The GW method has been widely applied to many elemental and binary semiconductors, but its application to more complex compound such as perovskites is less abundant. In this work we apply the GW technique to transition metal perovskites with different occupancies of d orbitals. We show that much care must be taken to obtain converge QP band structure in terms of number of unoccupied orbitals and k-points sampling. Accurate extrapolation procedures to the infinite-basis-set limit and infinite-k-point limit are necessary.

30 min. Coffee Break

DS 45.8 Thu 17:00 H2

Controlling the optical properties of organic/inorganic halide perovskites by means of size and composition — •Verena A. Hintermayr, Lakshminarayana Polavarapu, Alexander S. Urban, and Jochen Feldmann — Chair for Photonics and Optoelectronics, Department of Physics, Ludwig-Maximilians-Universität (LMU), Amalienstaße 54, 80799 Munich, Germany

Organic/Inorganic halide perovskites display a huge potential for not only photovoltaic, but also light emitting applications. In order to improve the efficiency and functionality of applications based on this material a better control of their optical properties is desirable. Here, we present a general colloidal synthesis method for the preparation of hybrid organic/inorganic halide perovskite nanocrystals (NCs) with different size and composition. We have prepared highly stable perovskite NCs that show strong quantum confinement and NCs that exhibit bulk like optical properties. We additionally investigate the tunability of the optical properties of the NCs by systematically modifying their halide content (I, Br and Cl). This work opens up a simple synthetic route for the preparation of perovskite NCs with controllable dimensionality and composition.

DS 45.9 Thu 17:15 H2

Dynamics and nature of photo-excited carriers in $\mathbf{(CH_3NH_3)PbI_3}$ organic-inorganic perovskite — •Daniel Niesner[1,2], Haiming Zhu[1], Tyler J. S. Evans[1], Bryan J. Kudisch[1], Prakriti P. Joshi[1], Kiyoshi Miyata[1], M. Tuan Trinh[1], Manuel Marks[1], and X.-Y. Zhu[1] — [1]Department of Chemistry, Columbia University, New York, NY 10027, USA — [2]Festkörperphysik, FAU Erlangen-Nürnberg, D-91058 Erlangen, Germany

Thin film solar cells based on organic-inorganic perovskites are the rising star in photovoltaics. The photophysics and transport mechanism behind the outstanding device performance remain a matter of debate. I will present the results of a study on carrier dynamics in vapor-deposited thin films of $\mathrm{(CH_3NH_3)PbI_3}$, combining time-resolved two-photon photoemission, transient absorption, and photoluminescence.

After optical excitation with sufficient photon energy ($\geq$ 2.15 eV), highly excited electrons relax quickly ($\leq$ 0.3 ps) to a region of the conduction band with a low density of states, located 0.3 eV above the band minimum. In parallel, polaron formation takes place on a time scale of 0.28 ± 0.04 ps, matching the time scale of cation motion. Polaronic screening suppresses further energy relaxation and thermalization. The polaron maintains a significant excess energy for more than 60 ps.

The excess energy can be utilized to overcome energy barriers at grain boundaries and contacts. Harvesting it directly would result in a solar cell with an efficiency exceeding the Shockley-Queisser limit.

DS 45.10 Thu 17:30 H2

Infrared spectroscopic study of vibrational modes and water infiltration in methylammonium lead halide perovskites — •Michael Sendner[1,2], Christian Mueller[1,2,3], Tobias Glaser[1,2], Annemarie Pucci[1,2], Wolfgang Kowalsky[1,2,3], and Robert Lovrincic[2,3] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab GmbH, Heidelberg — [3]Institut für Hochfrequenztechnik, TU Braunschweig

The interactions of the organic cation with the inorganic lattice in organo-metallic halide perovskites influence the vibrational properties of the cation which can be measured in the mid infrared (IR) spectral region. We determined the infrared optical properties of different methylammonium lead halide perovskite films ($CH_3NH_3Pb(I/Br/Cl)_3$) and derived the full dielectric function [1]. The peaks of the vibrational modes are assigned by means of the comparison with MP2 calculated modes of the free methylammonium cation. The influence of the inorganic cage and the processing is discussed. Furthermore, we utilize IR spectroscopy to investigate the influence of water onto perovskite thin films. We show that the infiltration of water into $CH_3NH_3PbI_3$ appears much faster and at much lower humidity than previously known [2]. We suggest a molecular picture of this infiltration where water molecules have a strong impact on the hydrogen bonding between the methylammonium cations and the surrounding Pb-I cage. [1] T. Glaser et al. J. Phys. Chem. Lett. 2015, 6 (15), 2913-2918 [2] C. Müller et al. Chem. Mater., 2015, 27 (22), 7835-7841

DS 45.11 Thu 17:45 H2

Temperature and excitation density dependence of two-photon photoluminescence of perovskite CH3NH3PbBr3 — •Heiko Linnenbank[1], Michael Saliba[2], Lili Gui[1], Bernd Metzger[1], Giuseppe Nasti[2], Jeanette Kadro[2], Anders Hagfeldt[2], Michael Graetzel[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Laboratory of Photonics and Interfaces, École polytechnique fédérale de Lausanne, Station 6, 1015 Lausanne, Switzerland

Recently solution processed organometallic halide perovskites have attracted much attention due to their simple processability, strong light absorption and favorable emission properties, which promises the realization of efficient on chip lasers. While several studies have been focused on one-photon excited luminescence processes like amplified spontaneous emission or lasing, only less attention has been paid to two-photon excited processes. In contrast to the usually expected quadratic dependence upon the excitation density in the case of two-photon photoluminescence, we rather measure a 4th power dependence at room temperature in the case of CH3NH3PbBr3. Such an excitation density dependence is a strong hint for a biexcitonic or exciton collision processes, which are rather unlikely at room temperature. To clarify the origin of the 4th power dependence, we investigate the form as well as the excitation density dependence of the photoluminescence spectra with respect to the sample temperature, revealing a suppression of the 4th power dependence with decreasing temperature.

DS 45.12 Thu 18:00 H2

Dark field photoluminescence and scanning electron beam measurements on single organic/inorganic halide perovskites of varying geometry and composition — •Alexander Richter, Verena Hintermayr, Lakshminarayana Polavarapu, Alexander Urban, and Jochen Feldmann — Chair for Photonics and Optoelectronics, Department of Physics, Ludwig-Maximilians-Universität (LMU), Amalienstaße 54, 80799 Munich, Germany

During recent years organic/inorganic halide perovskites have become a promising candidate for photovoltaic applications and also show a huge potential for light emitting applications. In case of two dimensional crystals quantum confinement affects the optical properties. Here, we present results on individual nanocrystals. Perovskites fabricated with varying halide content and geometry are embedded in a polymer matrix film to prevent degradation. Dark field photoluminescence and scanning electron beam measurements on individual spots of the sample are carried out. This yields a direct link between shape, halide composition and photoluminescence of these particles.

DS 45.13 Thu 18:15 H2

Luminescence blue-shift with decreasing size of perovskite needles. — •Amala Elizabeth and Katrin F.Domke — Molecular Spectroscopy Department,Max Planck Institute for Polymer Research, Mainz, 55128, Germany

Despite revolutionizing the photovoltaic industry by helping create highly efficient thin film solar cells, many intrinsic properties of organometallic halide perovskites still remain unknown. A complete understanding of the interplay of size, structure and electronic nature in determining the optical properties of thin film perovskites is crucial to fully exploit them for solar cell applications.

We studied methylammonium lead iodide perovskite thin films of ordered needles of varying submicron size. Energy-dispersive X-ray and IR spectroscopies reveal that the needles are chemically identical. While crystallinity is preserved in all samples, XRD and Raman spectra show a relative increase in the crystalline lead iodide content with decreasing needle size. Interestingly, we observe a blue-shift of 40 meV in both luminescence peak position and UV-vis absorption onset with decreasing needle size. Here, we discuss possible origins of the unexpected band gap increase with decreasing perovskite needle size, such as methyl ammonium cation orientational ordering [1] and lead iodide content [2].

References:

1. C. Quarti et al., J.Phys.Chem Lett. 5 (2014), 279-284.
2. Q.Shen et al., Nano Lett. 14 (2014), 4158-4163.

DS 46: Topological Insulators I (Joint session of DS and HL, organized by HL)

Time: Thursday 14:45–17:15 Location: H10

DS 46.1 Thu 14:45 H10

Topological Dirac Semimetal in strained HgTe — •Tomáš Rauch[1], Steven Achilles[1], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle (Saale), Germany

HgTe, one of the most intensively investigated materials in the context of topological insulators, is a semimetal with zero energy band gap when considered as a three-dimensional material. Applying uniaxial strain in [001] direction changes the situation dramatically [1]. Under compressive strain HgTe becomes a strong topological insulator featuring typical Dirac cone shaped surface states at the $\overline{\Gamma}$ point of the surface Brillouin zone. On the other hand, applying a tensile strain makes HgTe a topological Dirac semimetal with a pair of doubly-degenerate Dirac cones located along the k_z axis of the bulk Brillouin zone.

By combined *ab initio* and tight-binding electronic structure calculations we investigate the bulk and surface electronic properties of three-dimensional HgTe in the topological Dirac semimetal phase. This includes calculating the bulk band structure, topological invariants, and the electronic structure of the (100) surface, at which the associated non-trivial surface states emerge.

[1] T. Rauch *et al.*, Phys. Rev. Lett. **114**, 236805 (2015)

DS 46.2 Thu 15:00 H10

Tight-Binding Approach towards an Effective Model for InAs/GaSb Quantum Wells — •Matthias Sitte[1], Karin Everschor-Sitte[1], and Allan MacDonald[2] — [1]Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudingerweg 7, 55128 Mainz — [2]The University of Texas at Austin, Department of Physics, 2515 Speedway, Austin, TX 78712-1192

Topological insulators have attracted a great deal of attention as a new quantum state of matter in the last decade. The first realizations of 2D TIs were HgTe/CdTe quantum well heterostructures, but in recent years another class of semiconductor heterostructures — namely InAs/GaSb quantum wells — was shown to yield 2D TIs as well. Compared to the HgTe/CdTe-based systems they have many advantages, most prominently a continuously tunable band structure via external electric fields and stronger proximity coupling to superconductors. We perform empirical tight-binding calculations on these systems to study how topological properties are changed by varying external control parameters such as electric fields or well thicknesses.

DS 46.3 Thu 15:15 H10

Negative Magnetoresistance of $TlBi_xSb_{1-x}Te_2$ — •Oliver Breunig, Zhiwei Wang, Fan Yang, Alexey Taskin, and Yoichi Ando — II. Physikalisches Institut, Universität zu Köln

In the family of the ternary II-V-VI$_2$ compounds several materials have been identified as topological insulators. In the n-type TlBiTe$_2$ a topological surface state has been found, yet it is hardly accessible for transport studies due to the overlap with the bulk bands. Theoretical studies suggest that upon substituting Bi by Sb a narrow bulk band gap opens while preserving a single Dirac cone at the Γ point, leading to a possible realization of a bulk-insulating system with an exposed Dirac point.

Single crystals of TlBi$_x$Sb$_{1-x}$Te$_2$ were grown by a modified Bridgman technique using high-purity starting materials. They were characterized by ICP/EDX as well as transport measurements. For intermediate values x we find insulating transport properties and a surprisingly strong negative magnetoresistance. We present our crystal growth results of TlBi$_x$Sb$_{1-x}$Te$_2$ and discuss the origin of the observed large negative magnetoresistance.

DS 46.4 Thu 15:30 H10

Landau level spectroscopy of the 3D topological insulator Sb$_2$Te$_3$ — •Stefan Wilfert[1], Oliver Storz[1], Paolo Sessi[1], Thomas Bathon[1], Konstantin Kokh[2], Oleg Evgen'evich Tereshchenko[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Novosibirsk State University, 630090 Novosibirsk, Russia

Sb$_2$Te$_3$ is a prototypical three-dimensional topological insulator (TI) with intrinsic p-doping, which leads to a Dirac point lying well above the Fermi level [1]. We performed energy-dependent quasi-particle interference mapping and scanning tunnel spectroscopy in high magnetic fields up to 12 T on this compound, where both methods allow to obtain the energy dispersion. In contrast to the much more studied TIs Bi$_2$Te$_3$ [2] and Bi$_2$Se$_3$ [3], Sb$_2$Te$_3$ shows Landau levels with both negative and positive Landau level indices. This enables to analyze in more detail the energetic broadening of the Landau levels, which may lead to a better understanding of the physical limits of quantum coherence in this type of materials.
[1] C. Seibel *et al.*, Phys. Rev. Lett. **114**, 066802 (2015).
[2] Y. Okada *et al.*, Phys. Rev. Lett. **109**, 166407 (2012).
[3] T. Hanaguri *et al.*, Phys. Rev. B **82**, 081305 (2015).

30 min. Coffee Break

DS 46.5 Thu 16:15 H10

Aharonov-Bohm effect in the 3D topological insulator HgTe — •Johannes Ziegler[1], Dmitriy Kozlov[1,2,3], Dmitry Kvon[2,3], Nikolay Mikhailov[2], Sergey Dvoretsky[2], and Dieter Weiss[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]A.V. Rzhanov Institue of Semiconductor Physics, Novosibirsk, Russia — [3]Novosibirsk State University, Russia

We present our progress in the investigation of the Aharonov-Bohm effect in ring and nanowire structures, fabricated from high-mobility strained 80 nm HgTe films with a wet etching technique. The nanostructures are equipped with topgates to allow tuning of the Fermi level E_f and are measured in a dilution cryostat.

The focus lies on Topological Insulator nanowires, where it is expected that the magnetic flux Φ through the wire leads to both Φ_0 and $\Phi_0/2$ periodic oscillations [1]. Φ_0 $(= h/e)$ periodic oscillations are expected to occur in the ballistic regime for a large range in E_f. For ballistic devices, both minima and maxima of the conductance are expected at $\Phi = \Phi_0/2$ with varying E_f. In the case of diffusive transport, Φ_0 periodic oscillations are expected for E_f close to the Dirac point, while tuning E_f away from the Dirac Point leads to $\Phi_0/2$ $(= h/2e)$ periodic oscillations.

[1] J.H. Bardarson *et al.*, Phys. Rev. L **105**, 156803 (2010)

DS 46.6 Thu 16:30 H10

Emergence of quantum spin Hall and half-topological states at Graphene/TMDC heterostructures — •Denis Kochan, Martin Gmitra, Petra Högl, and Jaroslav Fabian — Institute for Theoretical Physics, University of Regensburg, Germany

We discuss orbital and spin-orbital proximity effects emerging in graphene deposited on a monolayer transition-metal dichalcogenides (TMDCs: MoS2, MoSe2, WS2, WSe2) and analyze the impact on spin transport in such graphene/TMDC heterostructures. First-principles investigations show that graphene on MoS2, MoSe2, and WS2 has a topologically trivial band structure, while graphene on WSe2 exhibits inverted bands. The essential low energy physics can be well described by a symmetry inspired realistic tight-binding Hamiltonian. We predict topologically protected helical edge states for graphene zigzag nanoribbons on WSe2, demonstrating the emergence of the quantum spin Hall effect. Our model also features "half- topological states", which are protected against time-reversal disorder on one edge only. Unlike in pristine graphene, the proximity spin-orbit coupling in graphene on TMDCs is significant (orders of meV), making the predicted effect testable experimentally.

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

DS 46.7 Thu 16:45 H10

Chiral Magnetic Effect in an Interacting Weyl Semimetal — •Matthias Puhr, Semen Valgushev, and Pavel Buividovich — Universität Regensburg, D-93053 Regensburg, Deutschland

We present results of a mean-field study of the chiral magnetic effect in a simple model of a parity-breaking Weyl semimetal. Our model is given by the lattice Wilson-Dirac Hamiltonian with on-site repulsive interaction and a constant chiral chemical potential term. We find a non-trivial behaviour of the chiral magnetic conductivity (CMC) and observe an increase, a decrease and even a change of sign depending on the interaction strength. The absolute value of the CMC never exceeds the value for the non-interacting gapless Hamiltonian. Our model exhibits a phase transition to a phase with spontaneously broken parity (Aoki phase, axionic insulator phase) and we observe a strong suppression of the CMC in the parity broken phase.

DS 46.8 Thu 17:00 H10

Negative magneto-resistivity in finite-size samples of Weyl semimetals — Pavel Buividovich, Matthias Puhr, and •Semen Valgushev — University of Regensburg, Regensburg, Germany

We numerically study Chiral Magnetic Effect and magneto-resistivity in a slab of parity-breaking Weyl semimetal modeled by Wilson-Dirac hamiltonian with open boundary conditions and subjected to the external magnetic field parallel to the boundaries. We find that the density of CME current is locally non-zero and strongly localized near the boundaries, where it approaches conventional value $j = \mu_5 B/2\pi^2$. We calculate the magneto-resistivity in a physical setup when parallel magnetic and electric fields are applied to the sample and discuss our results in the context of recent experiments on negative magnetoresistivity in Weyl semimetals.

DS 47: Focussed Session: Physics and Application of Emergent 2D-semiconductors and their Heterostructures II
(Joint session of DS and HL, organized by DS)

Atomically thin two-dimensional materials have advanced to the point where they are becoming highly appealing for the study of novel quantum physics and for constructing emergent photonic, electronic and photochemical devices using tailored 2D-heterostructures. The most prominent monolayer 2D material, graphene, has a bandstructure in its pristine form without an electronic bandgap. In contrast, monolayers of transition metal dichalcogenides (TMDCs) tend to be direct gap semiconductors with a bandgap in the visible to near-infrared spectral range. Moreover, the two-dimensional nature of these monolayered semiconductors give rise to very strong excitonic effects, even at ambient conditions and their strong light-matter interactions and spin-valley properties make them highly interesting for e.g.

opto-valleytronics and novel coherent light sources. Intriguingly, TMDC crystals can host strongly localized excitons, which result in the possibility to emit quantum light. In this symposium the current status and prospects of the very rapidly evolving field of TMDC research will be summarised including materials properties and synthesis and the exploration of phenomena such as quantum light emission, coherent laser action, spinor excitonics and cavity quantum electrodynamics.

Organizers: Sven Höfling (U Würzburg), Christian Schneider (U Würzburg) and Jonathan Finley (WSI München)

Time: Thursday 15:00–17:00 Location: H8

Topical Talk DS 47.1 Thu 15:00 H8
Bright and dark excitons in transition metal dichalcogenide monolayers — Cedric Robert[1], Gang Wang[1], Aslihan Suslu[2], Bin Chen[2], Sije Yang[2], Sarah Alamdari[2], Iann Gerber[1], Thierry Amand[1], Sef Tongay[2], Bernhard Urbaszek[1], and •Xavier Marie[1] — [1]Universite de Toulouse, INSA-CNRS-UPS, LPCNO, 135 avenue de Rangueil, 31077 Toulouse cedex, France — [2]School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, AZ 85287, USA

Highly crystalline Mo(1-x)WxSe2 has been synthetized to show engineering of the direct optical bandgap and the spin-orbit (SO) coupling in ternary alloy monolayers. We have investigated the impact of the tuning of the SO splitting on the optical and polarization properties. In particular, we have measured the effect of tuning of the conduction band SO splitting on the bright versus dark exciton state population i.e. photoluminescence (PL) intensity. We show that the MoSe2 PL intensity decreases as a function of temperature by an order of magnitude, whereas for WSe2 we measure surprisingly an order of magnitude increase over the same temperature range (T=4-300K). The ternary material shows a trend between these two extreme behaviors [1]. These results are interpreted on the basis of the reversal of the sign of the spin-orbit splitting in the CB for MoSe2 and WSe2 leading to different temperature dependences of the emission yield. The additional role of the electron-hole exchange interaction on the bright/dark exciton states splitting will also be discussed on the basis of ab-initio calculations. [1] G. Wang, et al, Nature Com. 6, 10110 (2015)

Topical Talk DS 47.2 Thu 15:30 H8
Exciton fine structure in transition-metal dichalcogenides monolayers — •Mikhail Glazov — Ioffe Institute, St.-Petersburg, Russia

Strong spin-orbit interaction in transition-metal dichalcogenides monolayers (TMDCs) such as MoS_2 or WSe_2 results in the spin-valley locking effect: The states of electrons and holes in $\mathbf{K}_\pm$ valleys of the Brillouin zone are spin-split. This makes spin and valley dynamics of charge carriers and their complexes, neutral and charged excitons, in TMCDs non-trivial and interesting. In my talk, an overview of recent theoretical results on exciton and trion fine structure in TMDCs is given. It is shown that the spin/valley dynamics of bright exciton doublet is governed by the long-range exchange interaction between an electron and a hole. The latter provides efficient spin depolarization mechanism of excitons. The developed theory is illustrated by comparison with recent experimental results on time-resolved polarized photoluminescence and Kerr-rotation spectroscopy.

Topical Talk DS 47.3 Thu 16:00 H8
Photonics and polaritonics with van der Waals heterostructures — •Alexander Tartakovskii — Department of Physics and Astronomy, University of Sheffield, Sheffield, S3 7RH, UK

Monolayer films of van der Waals crystals of transition metal dichalcogenides (TMDCs) are direct band gap semiconductors exhibiting excitons with very large binding energies and small Bohr radii, leading to a high oscillator strength of the exciton optical transition. Together with graphene as transparent electrode and hexagonal boron nitride (hBN) as an insulator, TMDC monolayers can be used to produce so-called van der Waals heterostructures. Here we use this approach to make electrically pumped light-emitting quantum wells (LEQWs) and single-photon emitters. We combine this new technology with optical microcavities to demonstrate control of the emitter spectral properties and directionality, making first steps towards electrically injected TMDC lasers. By embedding MoSe2/hBN structures in tuneable microcavities, we enter the regime of the strong light-matter interaction and observe formation of exciton-polaritons. We demonstrate that the magnitude of the characteristic anti-crossing between the cavity modes and the TMDC excitons can be enhanced by embedding a multiple-QW structure, containing two TMDC monolayers separated by an hBN barrier. This work opens a new avenue in the use of van der Waals crystals and heterostructures with a potential for polariton devices operating at room temperature.

Topical Talk DS 47.4 Thu 16:30 H8
van der Waals Epitaxy of 2D materials — •Sefaattin Tongay — Arizona State University, USA

Van der Waals (vdW) epitaxy is a common technique used for production of 2D materials systems. Owing to their chemically passivated surfaces, vdW epitaxy does require any lattice match and a number of 2D transition metal dischalcogenide (TMDCs) and post-transition metal chalcogenides (PTMCs) can be deposited onto various oxide surfaces. Since the underlying substrate and 2D materials weakly interact with each other, vdW epitaxy anticipated to produce 2D systems with material properties closely similar to that of exfoliated ones. This talk will focus on how underlying substrates influence the material properties through interation with 2D layered materials, and introduce colossal band renormalization in some unique systems.

DS 48: Oxide Semiconductors for Device and Energy Applications II (Joint session of DS and HL, organized by DS)

Time: Thursday 15:00–16:45 Location: H11

DS 48.1 Thu 15:00 H11
How Seebeck coefficient measurements help determine oxide transport properties — •Alexandra Papadogianni[1], Oliver Bierwagen[1], Mark E. White[2], James S. Speck[2], Zbigniew Galazka[3], Kelvin H. L. Zhang[4], Yingge Du[4], and Scott A. Chambers[4] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, D-10117 Berlin, Germany — [2]Materials Department, University of California, Santa Barbara, California 93106, USA — [3]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, D-12489 Berlin, Germany — [4]Pacific Northwest National Laboratory, Richland, Washington 99352, USA

Measuring the Hall effect is a common and convenient method to investigate the electrical transport properties of thin samples, providing us with an estimate of integral sheet carrier concentration. In low-mobility p-type semiconducting oxides, such as the Sr-doped $LaCrO_3$, however, Hall measurements fail. For such instances, studying thermoelectric properties, namely the Seebeck coefficient, can be a simple alternative, which provides us with the carrier type and volume carrier concentration. A combination of Seebeck and Hall measurements can moreover be used for estimating the actual thickness of a carrier system within a semiconductor. As an example, an application on n-type SnO_2 shows how this method can help distinguish bulk carriers, with homogeneous depth distribution, from sheet carriers accumulated within a thin layer.

DS 48.2 Thu 15:15 H11
Metal incorporation and reaction-kinetics for the molecular beam epitaxial growth of $(Ga_xIn_{1-x})_2O_3$ — •Patrick Vogt and

Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5–7, 10117 Berlin, Germany

This contribution presents the metal incorporation and reaction-kinetics study of the plasma-assisted molecular beam epitaxial (MBE) growth of the transparent semiconducting oxide alloy $(\mathrm{Ga}_x\mathrm{In}_{1-x})_2\mathrm{O}_3$. By using MBE, an impinging Ga- (Φ_{Ga}), In- (Φ_{In}), and oxygen-flux (Φ_{O}) react amongst others to $(\mathrm{Ga}_x\mathrm{In}_{1-x})_2\mathrm{O}_3$ on a heated, single-crystalline substrate under ultra-high vacuum conditions. The data obtained were measured *in-situ* by a laser reflectometry (LR) set-up and a line-of-sight quadrupole mass spectrometer (QMS) or *ex-situ* by energy dispersive X-ray spectroscopy (EDX). The LR allowed measuring the growth-rate (ρ), the QMS enabled identifying the species that desorbed off the substrate which are not incorporated into the alloy, and the EDX measurements revealed the In incorporation x and the reciprocal Ga incorporation 1-x.

We present the growth rate dependencies of the binary grown $\mathrm{In}_2\mathrm{O}_3$ and $\mathrm{Ga}_2\mathrm{O}_3$ as function of growth temperature (T_{G}). Furthermore, we show the dependence of ρ and x for the ternary grown alloy on T_{G}, the metal-to-oxide ratio ($r_{\mathrm{MeO}} = (\Phi_{\mathrm{In}} + \Phi_{\mathrm{Ga}})/\Phi_{\mathrm{O}}$) , and the In-to-Ga ratio ($r_{\mathrm{InGa}} = \Phi_{\mathrm{In}}/\Phi_{\mathrm{Ga}}$).

The measured discrepancy of ρ for the binary grown oxides compared to x for the ternary grown alloy can be explained by the different adhesion energies for In and Ga on the $(\mathrm{Ga}_x\mathrm{In}_{1-x})_2\mathrm{O}_3$ surfaces.

DS 48.3 Thu 15:30 H11

Application of Cr_2O_3 and Cr_2O_3:Mg as a Buffer Layer in Organic Solar Cells — •Daragh Mullarkey[1], Elisabetta Arca[1], Linda Cattin[2], Jean Christian Bernède[3], and Igor Shvets[1] — [1]School of Physics and CRANN, Trinity College Dublin, University of Dublin, Ireland — [2]Université de Nantes, Institut des Matériaux Jean Rouxel, France — [3]Université de Nantes, MOLTECH-Anjou, France

The use of undoped Cr_2O_3 and p-type Cr_2O_3:Mg as an anode buffer layer in organic solar cells is explored. The effects of buffer layer thickness, roughness, and growth conditions on the properties of the solar cell were studied. These effects were investigated for solar cells grown on both indium tin oxide and fluorine doped tin oxide. In both cases, Cr_2O_3 and Cr_2O_3:Mg were found to improve the efficiency of the solar cell.

The band offsets between the anode material and the buffer layer, as well as between the buffer layer and the organic absorber were studied by X-ray Photoelectron Spectroscopy (XPS) and Ultra Violet Photoelectron Spectroscopy (UPS). The efficiency of the solar cells is discussed in terms of the experimentally determined band alignment.

DS 48.4 Thu 15:45 H11

TiO2 laminated Silicon microstructures based stable photocathode for water splitting — •Chittaranjan Das[1], Massimo Tallarida[2], and Dieter Schmeisser[3] — [1]Angewantde Physik / Sensorik ,BTU Cottbus-Senftenberg, Germany — [2]ALBA-Barcelona — [3]Angewantde Physik / Sensorik ,BTU Cottbus-Senftenberg, Germany

The photoelectrochemical (PEC) water splitting is one of the most efficient ways to obtain hydrogen from water using solar power which can be used as carbon free fuel. The PEC device can bedesigned using semiconducting material that will convert solar radiation to H2. Silicon can be one of the best choices for PEC due to its success in solar cells technology. There are certain issues with Si such as stability in electrochemical medium [1] and higher surface reflectance (25%) which limits the Si as an ideal candidate for PEC technique [2].

In the present work we addressed these issues by surface structuring and laminating the surface with metal oxide. The microstructuring of Si was done by electrochemical method. The Si microstructure photocathode was stabilized by thin layer of ALD grown TiO2 film. The microstructuring and lamination of Si photocathode by ALD layer of TiO2 decreased the reflectance ofthe surface and shift the onset potential towards anodic direction by 350 mV with a prolonged stability over 60 hours[3].

[1] C. Levy-Clement, J. Electrochem. Soc 1991, 12, 69 [2] J. Oh, et al. Energy Environ. Sci., 2011, 4, 1690 [3] C. Das, et al. Nanoscale 2015,7, 7726

DS 48.5 Thu 16:00 H11

Optical and Magneto-Optical Investigation of Normal and Disordered $ZnFe_2O_4$ in Relation to Magnetic Properties — •Vitaly Zviagin[1], Peter Richter[2], Yogesh Kumar[1], Israel Lorite[1], Michael Lorenz[1], Dietrich R.T. Zahn[2], Georgeta Salvan[2], Pablo Esquinazi[1], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany — [2]Technische Universtät Chemnitz, Semiconductor Physics, Reichenheiner Str. 70, Germany

We present the magneto-optical dielectric tensor of normal and disordered $ZnFe_2O_4$ grown at different temperatures on MgO (100) and $SrTiO_3$ (100) substrates by pulsed laser deposition. Optical transitions in the diagonal element of the dielectric function, obtained by spectroscopic ellipsometry, are identified as transitions from O_{2p} to Fe^{3+} 3d and 4s bands. Via the off-diagonal element, obtained by magneto-optical Kerr effect spectroscopy, the observed features are confirmed to be similar to the mentioned transitions. One transition in particular, namely a transition from O_{2p} to tetrahedrally coordinated Fe^{3+} cation, located at $\sim 3.5\,\mathrm{eV}$, suggests disorder of the normal crystal structure. Its amplitude is highest for the sample grown at the lowest temperature in both the diagonal and off-diagonal elements of the dielectric tensor. Furthermore, the overall magnetic response, measured by SQUID, is highest for the sample grown at the lowest temperature, suggesting that the presence of Fe^{3+} on the tetrahedral sites is directly related to the ferrimagnetic order of the crystal due to the dominating nature of the oxygen mediated coupling between the two lattice sites.

DS 48.6 Thu 16:15 H11

Monitoring Proton Diffusion in Thin Films of Tungsten Oxide — •Simon Burkhardt[1], Sabrina Darmawi[1], Matthias T. Elm[1,2], and Peter J. Klar[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 17, 35392 Gießen

The reversible change of the optical properties of materials due to the electrochemical insertion of ions is called electrochromism. Tungsten-VI oxide (WO_3) and its electrochromic properties have been intensively studied since 1969 as a model system which nowadays can be found in applications like smart window systems or other coated glasses. However fundamental questions concerning the colouration mechanism are still under discussion. A combination of electrochemical proton insertion and *in situ* UV/Vis-transmission spectroscopy is applied to provide new insights. With the developed set up it is not only possible to investigate the time-dependence of the colouration behaviour, but it also allows a spatially resolved analysis of the colouration process and thus the ion diffusion in electrochromic thin films. To investigate the diffusion of protons, thin films of WO_3 are deposited on TCO-coated substrates via electron beam evaporation and coated with a structured PMMA layer to enable local ion insertion. Significant differences in the colouration behaviour of amorphous and crystalline WO_3 films can be observed which will be compared with a simulation of lateral 1D diffusion processes.

DS 48.7 Thu 16:30 H11

Oxygen Vacancies in the Ultrathin SiO_2 Interfacial Layer of High-K/Metal Gate CMOS Devices — •Florian Lazarevic[1,2], Roman Leitsmann[1,2], Philipp Plänitz[1], and Michael Schreiber[2] — [1]MATcalc, AQcomputare GmbH, Annaberger Str. 240, 09125 Chemnitz, Germany — [2]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

We study oxygen vacancy defect levels in ultrathin SiO_2 layers in metal-oxide-semiconductor devices. First principles calculations were performed to model a $Si/SiO_2/HfO_2$ gate stack and a SiO_2 bulk reference system. The extremely thin SiO_2 layer thickness and dissimilar structural and electronic properties of the adjacent layers (namely Si and HfO_2) result in a degeneration and stabilization of certain SiO_2 bulk defects. We find that partial H passivation of the vacancies additionally stabilizes defects energetically which are related to the leakage current in CMOS devices. Furthermore the incorporation of F atoms has a large influence on the stability of H passivated SiO_2 defects.

DS 49: Transport: Molecular Electronics and Photonics II (Joint session of CPP, DS, HL, MA, O and TT, organized by TT)

Time: Thursday 15:00–16:00 Location: H23

DS 49.1 Thu 15:00 H23

First-principles calculation of the thermoelectric figure of merit for [2,2]paracyclophane-based single-molecule junctions — •Marius Buerkle[1], Fabian Pauly[2], and Yoshihiro Asai[1] — [1]AIST Tsukuba — [2]University Konstanz

Here we present a theoretical study of the thermoelectric transport through [2,2]paracyclophane-based single-molecule junctions [1]. Combining electronic and vibrational structures, obtained from density functional theory (DFT), with nonequilibrium Green's function techniques allows us to treat both electronic and phononic transport properties at a first-principles level. Paracyclophane derivatives offer a great flexibility in tuning their chemical properties by attaching different functional groups. We show that, for the specific molecule, the functional groups mainly influence the thermopower, allowing us to tune its sign and absolute value. We predict that the functionalization of the bare paracyclophane leads to a largely enhanced electronic contribution ZelT to the figure of merit. Nevertheless, the high phononic contribution to the thermal conductance strongly suppresses ZT. Our work demonstrates the importance to include the phonon thermal conductance for any realistic estimate of the ZT for off-resonant molecular transport junctions.
[1] M. Buerkle et al., PRB **91**, 165419 (2015)

DS 49.2 Thu 15:15 H23

Switching the conductance of a molecular junction by proton transfer — •Dominik Weckbecker, Pedro B. Coto, Chriszandro Hofmeister, and Michael Thoss — Institut für Theoretische Physik, Staudtstraße 7/B2, 91058 Erlangen, Germany

The idea of designing switches or diodes using single molecules has motivated intensive experimental and theoretical research on the conductance properties of these systems. In particular, it has been demonstrated that a molecular junction may be used as a nanoswitch if the molecular bridge has two stable states with different conductance that can be reversibly transformed into each other [1]. In this contribution, we explore the possibility of switching a molecular junction using a proton transfer reaction triggered by an external electrostatic field [2]. The study uses transport theory based on first-principles electronic structure calculations [2,3] and considers molecular junctions with graphene or gold as material for electrodes. We show that for the systems investigated, proton transfer can be used for the reversible interconversion between two states, which exhibit different degrees of delocalization of the π-electrons and therefore very different conductance.
[1] S. J. van der Molen et al., J. Phys.: Cond. Mat. **22**, 133001 (2010)
[2] C. Hofmeister et al., J. Mol. Model. **20**, 2163 (2014)
[3] M. Brandbyge et al., PRB **65**, 165401 (2002)

DS 49.3 Thu 15:30 H23

Design rules for molecular electronics: Diarylethene molecules und derivatives — •Lokamani Lokamani[1], Torsten Sendler[1], Peter Zahn[1], Sibylle Gemming[1,2], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01314 Dresden, Germany. — [2]Instiute of Physics, Technische Universität, 09107 Chemnitz, Germany.

Diarylethenes, a class of photosensitive molecules which exhibit photochoromism, can be switched between open- and closed-ring isomers. In break-junction experiments diarylethene derivatives[1] in open and closed-ring forms can be distinguished by a low and high conductance state respectively with a difference in current levels of about one order of magnitude. In addition, these molecules exhibit stable electrical characteristics in both conductance states. Here, we study the electronic transport properties of such derivatives at the level of single molecules. In particular, we analyze the effect of various electron accepting and donating groups on the conductance properties of single molecules attached to gold electrodes. We explore the underlying design rules for molecular electronics comparing break-junction experiments and the theoretical investigations on diarylethene molecules and derivatives.
[1] T. Sendler et al., Advanced Science **2**, 1500017 (2015)

DS 49.4 Thu 15:45 H23

Experimental investigation of the role of electron-phonon-coupling on the Mott critical behavior in the organic charge-transfer salts κ-(BEDT-TTF)$_2$X — •E. Gati[1], M. Garst[2], R.S. Manna[1], U. Tutsch[1], B. Wolf[1], S. Hartmann[1], L. Bartosch[3], T. Sasaki[4], H. Schubert[1], J.A. Schlueter[5], and M. Lang[1] — [1]Physikalisches Inst., Goethe Uni, SFB/TR49, Frankfurt, DE — [2]Inst. f. Theo. Physik, Universität zu Köln, DE — [3]Inst. f. Theo. Physik, Goethe Uni, FfM, DE — [4]IMR, Tohoku University, Sendai, Japan — [5]Materials Science Division, Argonne National Laboratory, USA

The Mott transition is one of the key phenomena of strongly correlated electron systems. Of fundamental interest is the determination of its critical behavior and the underlying universality class. Despite intensive experimental efforts, the universality class is still unresolved. A key aspect, which has not been addressed in these approaches, is the role of electron-phonon-coupling as it is supposed to alter the critical properties to Landau criticality [1]. We will present thermal expansion studies under pressure [2] on the organic charger-transfer salt κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl. This technique is a very sensitive tool to detect critical behavior [3] as well as influences of the lattice on the electronic subsystem [1]. Our results clearly show a breakdown of Hooke's law of elasticity which is a direct evidence for significant electron-phonon-coupling. Furthermore, we will discuss its effect on the critical exponents determined by this thermodynamic probe.
[1] Zacharias et al., PRL **109**, 176401 (12)
[2] Manna et al., Rev. Sci. Instrum. **83**, 085111 (2012)
[3] de Souza et al., PRL **99**, 0370031 (2007)

DS 50: Frontiers of Electronic Structure Theory: Focus on Topology and Transport V (Joint session of DS and O, organized by O)

Time: Thursday 15:00–18:15 Location: H24

DS 50.1 Thu 15:00 H24

Zero-point renormalization of the electronic structure: trends across chemical and structural space — •Honghui Shang[1], Christian Carbogno[1], Patrick Rinke[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Aalto University, Helsinki, Finland

The importance of the renormalization of the electronic structure due to the zero-point nuclear motion (ZPR) has been discussed since long [1,2], but only recent advances in the first-principles treatment of electron-phonon coupling (EPC) enabled an accurate assessment of this effect for simple, prototypical materials, e.g., diamond [3] and Si [4]. However, it is largely unknown how chemical and structural properties affect the ZPR. To shed light on this question, we compute the EPC and ZPR for the octet binaries in both the zincblende and NaCl structure. Computationally, this is achieved by exploiting our recent implementation of density-functional perturbation theory in real-space, which provides considerable computational advantages with respect to numerical costs, parallelization, and especially scalability with respect to the number of atoms. We demonstrate the validity of our implementation by comparing with existing studies and finite difference results, investigate the trends across chemical/structural space, and critically discuss the role of the exchange-correlation functional.
[1] P. B. Allen and V. Heine, J. Phys. C **9**, 2305 (1976).
[2] M. Cardona, Solid State Commun. **133**,3 (2005).
[3] F. Giustino,*et.al.* Phys. Rev. Lett. **105**, 265501 (2010).
[4] S. Poncé, *et.al.* J. Chem. Phys. **143**, 102813 (2015).

DS 50.2 Thu 15:15 H24

All-Electron Many-Body Approach to X-Ray Absorption Spectroscopy — •Christian Vorwerk, Caterina Cocchi, and Claudia Draxl — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

We present an all-electron approach of the many-body perturbation theory to describe X-ray absorption spectroscopy (XAS) in solid-state materials. In this formalism, the electron-hole interaction is explicitely included by solving the Bethe-Salpeter equation. A fully relativistic description of core states, as implemented in the all-electron full-potential code `exciting`[1], enables the explicit treatment of the effects of spin-orbit coupling in the spectra. We investigate the XAS for prototypical systems, such as TiO_2 and MgO, considering excitations from oxygen K and metal L edges. Our results, in good agreement with experiments, allow us to gain insight into the nature of the core-level excitations of these materials.

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

DS 50.3 Thu 15:30 H24

Cohesive properties from all-electron RPA total energies — •Markus Betzinger[1], Christoph Friedrich[1], Andreas Görling[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

We present an all-electron implementation of the RPA total energy within the full-potential linearized augmented plane-wave (FLAPW) method. An incomplete basis-set correction (IBC) [1] is employed to improve the convergence of the total energy with respect to the basis-set and the number of unoccupied states. To some extent the IBC incorporates an infinite number of bands and enables a virtually exact treatment of the core electrons.

We demonstrate that the core electrons give rise to a sizeable contribution to the RPA total energy. Their individual contribution is comparable to that of the valence electrons. All-electron RPA lattice constants and bulk moduli are shown for a set of prototype materials and compared to experimental results. An excellent agreement with experiment is observed.

[1] M. Betzinger *et al.*, Phys. Rev. B (accepted, 2015); **88**, 075130 (2013); **85**, 245124 (2012).

DS 50.4 Thu 15:45 H24

Explicitly correlated self consistent field theory — •Christian Lasar and Thorsten Klüner — Universität Oldenburg

Explicitly correlated correlation methods are an interesting field of current research since they are able to drastically improve the otherwise slow basis set convergence of conventional correlation methods. Therefore, chemical accuracy can be achieved with rather small basis sets.[1] The new correlation method presented in this contribution has already been developed for two-electron systems a long time ago[2]. We present the generalization of this ansatz to N-electron systems.

The basic idea is to augment a single slater-determinant with an explicitly correlated prefactor which then takes care of the correlation effects and the basis set convergence. Another interpretation of this ansatz would be a contracted CISD with orbital optimization in a complete basis set. The contraction is achieved by the explicitly correlated prefactor whose choice therefore defines the possible accuracy of the method. In principle, the generalization to any pair method i.e. CCSD and MP2 will be possible.

The big advantage of this kind of ansatz for the wave function is the drastic reduction of matrix elements needed for the optimization of the wave function. As a result, the presented method will be applicable to large molecules.

[1] Chem. Rev. 112, p. 4 (2012) [2] J. Chem. Phys. 99, p. 8830 (1993)

DS 50.5 Thu 16:00 H24

Representing energy landscapes by combining neural networks and the empirical valence bond method — •Sinja Klees[1], Ramona Ufer[2], Volodymyr Sergiievskyi[2], Eckhard Spohr[2], and Jörg Behler[1] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Duisburg-Essen, D-45141 Essen, Germany

In recent years, artificial neural networks (NNs) have become a powerful method to develop reactive interatomic potentials for large systems. However, the construction of NN potentials can become computationally very demanding due to the high dimensionality of the configuration space, which needs to be mapped by reference electronic structure calculations. Combining NN potentials with the empirical valence bond (EVB) method offers a promising approach to derive the potential energy of complex systems with substantially reduced effort, since the size of the reference structures can be strongly decreased. Preliminary results will be discussed and compared to density functional theory data.

DS 50.6 Thu 16:15 H24

CELL: a python package for cluster expansions with large parent cells — •Santiago Rigamonti[1], Maria Troppenz[1], Christopher Sutton[2], Luca M. Ghiringhelli[2], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft

The discovery of new materials for applications in areas such as energy harvesting, relies more and more on the accurate theoretical description of complex structures with large unit cells. The properties of interest are often tuned by substitutional dopants. Due to the vast configurational dopant space, a wide-spread approach is the cluster expansion (CE) technique. Most available CE codes are designed for alloys based on small parent cells, with usually 1 to 4 atoms. For the many important materials with much larger parent cells such approaches can't be applied. We devise an iterative scheme, based on efficient samplings of the configurational space, avoiding full structure enumerations. CELL consists of several modules that can be used independently, enabling to design CEs for specific purposes. Various CE schemes are available, offering ℓ_2 and ℓ_1 norms as penalization terms and different cross-validation strategies. Methods such as LASSO and split Bregman iteration are available for dealing with the ℓ_1 norm (compressive sensing). Access to finite-temperature properties and the characterization of phase transitions is possible through the Wang-Landau and diffusive nested sampling modules. Examples are presented for type-I thermoelectric clathrates, with 46 sites in the parent cell.

DS 50.7 Thu 16:30 H24

Structural and electronic properties of the thermoelectric clathrates $Ba_8Al_xSi_{46-x}$ and $Sr_8Al_xSi_{46-x}$ — •Maria Troppenz, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

Clathrate compounds are promising candidates for high-efficiency thermoelectric applications. Their cage-like structure containing guest atoms allows for exploiting the idea of the phonon-glass electron-crystal and reaching a large figure of merit. We study $Ba_8Al_xSi_{46-x}$ and $Sr_8Al_xSi_{46-x}$ ($6 \leq x \leq 16$), where optimal electronic properties are expected close to the Zintl composition ($x = 16$). Cluster expansions on various quantities are performed, thus having access to ground-state as well as finite-temperature properties. A linear increase of the lattice constant with the number of Al substituents is obtained (0.019 Å per Al addition) confirming experimental observations (0.02 Å). The calculated bond distances between high-symmetry sites agree well with experiment for the full compositional range [1,2]. We find a close correlation between bond distances and fractional Al occupancies. This helps improving models used by experimentalists to estimate fractional occupancies. The substitutional configurations present an order-disorder transition around $600 - 900\,\mathrm{K}$, which is further analyzed applying the Wang-Landau method. An important finding is the semiconducting behavior of the low-temperature ordered phase at the Zintl composition, which points out the technological relevance of these compounds.

[1] J. H. Roudebush *et al.*; *Inorg. Chem.* **51**, 4161 (2012)

[2] M. Bobnar *et al.*; *Dalton Trans.* **44**, 12680 (2015)

DS 50.8 Thu 16:45 H24

***Ab-initio* calculation of Raman spectra of graphene-based materials** — •Albin Hertrich, Caterina Cocchi, Pasquale Pavone, and Claudia Draxl — Department of Physics, Humboldt-Universität zu Berlin, Germany

Raman scattering is an important non-destructive method for characterizing carbon-based materials. The main features of experimental Raman spectra of pristine graphene and graphite are the first-order G-band at ≈1580 cm^{-1} and the dispersive second-order 2D-band at ≈2700 cm^{-1}. We calculate first- and second-order Raman spectra fully *ab-initio* using the full-potential all-electron DFT package `exciting` [1], which allows for the calculation of both phonon dispersion, within the frozen-phonon approximation, and frequency-dependent dielectric tensors, from time-dependent DFT and the Bethe-

Salpeter equation. In our approach [2], we expand the dielectric tensor with respect to the phonon normal coordinates. By taking its derivatives and by computing vibrational matrix elements, we calculate Raman scattering intensities. Applying this scheme to monolayer graphene, bilayer graphene, and graphite, we obtain the G-band in good agreement with experiment [3]. Furthermore, we explore the influence of both the stacking sequence and the laser energy on the 2D-band.
[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[2] C. Ambrosch-Draxl *et al.*, Phys. Rev. B **65**, 064501 (2002).
[3] A. C. Ferrari *et al.*, Phys. Rev. Lett. **97**, 187401 (2006).

DS 50.9 Thu 17:00 H24

Exciton dispersion in layered and 2D systems — •Francesco Sottile[1,2], Giorgia Fugallo[1,2], Pierluigi Cudazzo[1,2], and Matteo Gatti[1,2,3] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-IRAMIS, Université Paris-Saclay, F-91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility — [3]Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, Boîte Postale 48, F-91192 Gif-sur-Yvette, France

The study of the exciton dispersion is of paramount importance for all applications involving light harvesting, beside providing fundamental knowledge about exciton mobility and migration. Using state-of-the-art ab initio many-body approach, like the Bethe-Salpeter equation [1], we present a first principle study of exciton dispersions in layered materials and 2D systems. Results for the former systems (on the prototypical hBN and MoS2) have been recently confirmed by experiments carried out at the Synchrotron ESRF [2]. For the latter (2D) systems we investigate exciton dispersion in graphane and hBN. From our results we provide a general picture of the mechanisms governing the dispersion of neutral excitations in 2D systems, and of the role played by the confinement of the electronic charge in setting the exciton binding energy. In particular we found that due to the strongly reduced screening of the Coulomb interaction in low- dimensional materials, the binding energy of both Wannier and Frenkel excitons in the optical spectra is large and comparable in size[3]. [1] M. Gatti et al., Phys. Rev. B 88, 155113 (2013) [2] G. Fugallo et al. Phys. Rev. B 92, 165122 (2015) [3] P. Cudazzo et al. submitted to Phys. Rev. Lett.

DS 50.10 Thu 17:15 H24

Electronic structure of selected superheavy elements (Z>104) — •Hana Cencarikova[1] and Dominik Legut[2] — [1]Institute of Experimental Physics, SAS, Kosice, Slovakia — [2]IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

The electronic structure of selected super-heavy elements (Z>104) have been determined from the first-principle calculations based on the density functional method. To determine the ground-state structure we have calculated number of basic phases including the face-centered cubic, body-centered cubic, simple cubic as well as hexagonal closed packed structures. Our results were obtained using local density approximation for the exchange and correlation effects and without and with the spin-orbit interaction for the band states. The analysis has been focused on the determination of the electronic density of states, electronic band structure dispersion relation, mechanical properties (elastic constants) and selected thermodynamical properties.

DS 50.11 Thu 17:30 H24

Layer-resolved calculated vibrations at gold surfaces — •Andrei Postnikov[1] and Kamil Moldosanov[2] — [1]Université de Lorraine, LCP-A2MC, Metz, France — [2]Kyrgyz-Russian Slavic University, Bishkek, Kyrgyzstan

Vibration modes at (001), (011) and (111) surface of gold are calculated from first principles, using the Siesta method [1] and the frozen phonon approach. Calculations are done on thick slabs of moderate lateral size – (2×2) for (001), (2×3) for (011), (3×3) for (111). This allows to resolve the vibration patterns layer by layer into the depth, in dependence on the in-plane wavevector component, and discriminating the polarisation of vibration modes. One notes the softening of modes at the surface, and an appearance of specifically surfacial modes. The bulk behaviour is largely recovered from the 5th or 6th layer downwards.

This study was driven by an intention to grasp the properties of longitudinal acoustic modes propagating at some depth under the surface of gold nanoparticles, which were an important element of our recent work related to the mechanism of radiofrequency absorption and hence resulting heating of nanoparticles of $\gtrsim 5$ nm size [2]. Since it is difficult to meaningfully incorporate the diversity of the nanoparticles' shapes in a practical calculation, the vibrations beneath the most common facets occurring at the nanoparticles' surface were studied instead.

1. The Siesta method, `http://departments.icmab.es/leem/siesta/` .
2. A. Postnikov and K. Moldosanov, `http://arxiv.org/abs/1508.00735` .

DS 50.12 Thu 17:45 H24

Electronic structure, mechanical and thermodynamic properties of Actinium from first-principles — •Zuzana Grosmanova[1] and Dominik Legut[2] — [1]Nanotechnology, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic — [2]IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

In this work, the mechanical (elastic constants) and thermodynamic properties of actinium were investigated using first-principle calculations. Our results were obtained using density functional theory employing local density and general gradient approximation for the electronic exchange-correlation effects and including the spin-orbit interaction for the band states. The ground-state structure were determined among simple phases like the face-centered cubic, body-centered cubic, simple cubic as well as hexagonal closed packed structures.

DS 50.13 Thu 18:00 H24

Interaction of Tritium and Chlorine 36 with defects in Graphite: Insights from Theory — •Christoph Lechner[1], Philippe Baranek[1], and Holger Vach[2] — [1]EDF Lab Les Renardières, Avenue des Renardieres, F-77818 Moret-sur-Loing Cedex, France — [2]CNRS-LPICM, Ecole Polytechnique, F-91128 Palaiseau Cedex, France

In order to optimize the waste management of nuclear graphite used in power plants, it is important to understand the properties of the activated impurities it contains, such as tritium and chlorine 36. Therefore, a computational study of the interaction of tritium and chlorine 36 with defects in graphite has been achieved at the density functional theory (DFT) level by using the functionals PBE and PBE0 with Grimme's D3 dispersion correction. The physisorption and chemisorption of atomic and molecular hydrogen or chlorine on graphite surfaces, (001), (100), and (110) with or without mono- and divacancies, have been investigated. The stabilities of the formed complexes are interpreted in terms of the formation energy. To obtain insight into the nature of the bonding a population analysis of the systems has been performed. While the bonding of hydrogen is mostly covalent for chemisorption and van der Waals for physisorption, the behavior of chlorine is much more complex. Depending on the defect site, both, dominantly covalent and dominantly charge transfer bonding, is observed. Raman spectra for selected structures have been investigated, in order to evaluate, if the experimentally observed defect bands can be reproduced.

DS 51: Transport: Spintronics and Magnetotransport (Joint session of DS, HL, MA and TT, organized by TT)

Time: Thursday 16:15–18:30 Location: H23

Invited Talk DS 51.1 Thu 16:15 H23

Non-Abelian gauge theory description of (dynamical) spin-orbit coupling effects in Fermi gases. — •Cosimo Gorini — Institut für Theoretische Physik, Universität Regensburg, Germany

Spin-orbit coupling heavily influences the dynamics of charge carriers in a solid, where its strength can be enhanced by orders of magnitude as compared to the vacuum. Remarkable consequences are phenomena such as the spin Hall and inverse spin galvanic (or Edelstein) effects, where spin currents and polarizations are generated by purely electrical means. The intricacies of such rich spin-charge coupled dynamics can be described within a non-Abelian gauge theory approach [1], based on Keldysh non-equilibrium formalism [2]. Thanks to a symmetric treatment of spin and charge degrees of freedom, and the removal of ambiguities related to spin non-conservation in the presence of (static or dynamical) spin-orbit coupling, a physically transparent picture is achieved [3]. Furthermore, the non-Abelian language, by virtue of its universal character, treats on the same footing standard spin-orbit interaction in solid state systems and exotic forms of (pseudo) spin-orbit coupling which arise, or can be engineered, in different contexts.

[1] H. Mathur and A. D. Stone, PRL **68**, 2964 (1991)
I. V. Tokatly, PRL **101**, 106601 (2008).
[2] C. Gorini et al., PRB **82**, 195316 (2010).
[3] C. Gorini et al., PRL **109**, 246604 (2012)
C. Gorini et al., PRL **115** , 076602 (2015).

DS 51.2 Thu 16:45 H23

Shot noise in magnetic tunnel junctions: effect of the geometric phase — •Tim Ludwig[1] and Alexander Shnirman[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]L. D. Landau Institute for Theoretical Physics RAS, Kosygina street 2, 119334 Moscow, Russia

We analyze the current driven dynamics of magnetization and voltage in a magnetic tunnel junction. As predicted in [1, 2], the magnetization can be driven by spin currents. This effect can also be reversed, such that an externally driven magnetization generates a dc voltage [3]. Although both effects are intimately related, so far they have been treated separately. We generalize the approach of [4] to derive an action that contains both effects simultaneously. We employ the Keldysh formalism, which allows us to derive stochastic Landau-Lifshitz-Gilbert-Langevin equations describing the angular dynamics of the magnetization coupled with the voltage dynamics. We identify two low-temperature regimes. In one regime the voltage fluctuations are governed by the applied current only, as expected for the shot noise. In the other regime an excess noise arises, which is governed by the geometric phase of the precessing magnetization.

[1] L. Berger, PRB **54**, 9353 (1996)
[2] J. C. Slonczewski, J. Magn. Magn. Mater. **159**, L1 (1996)
[3] L. Berger, PRB **59**, 11465 (1998)
[4] A. Shnirman, Y. Gefen, A. Saha, I. S. Burmistrov, M. N. Kiselev, A. Altland, PRL **114**, 176806 (2015)

DS 51.3 Thu 17:00 H23

Electron transport through the helical molecules in the presence of spin-orbit coupling — •Volodymyr V. Maslyuk, Rafael Gutiérrez, and Gianaurelio Cuniberti — Institute for Material Science and Max Bergmann Center for Biomaterials, Dresden University of Technology, Hallwachstr. 3, 01069 Dresden, Germany

Recently it was shown [1] that electron transport through systems with helical symmetry shows spin selectivity. Here we present a theoretical investigation of the transport properties through helical molecules placed between magnetic and nonmagnetic leads by using the DFT and NEGF approach. The performed analysis of the data allow us to show that the systems show spin-polarization only because of spin-orbit interaction and the spin polarization is clearly related to the helical symmetry since a change in handedness of the helix changes the sign of the spin-polarization and a linear chain does not display any sizeable polarization.

[1] B. Göhler, V. Hamelbeck, T. Z. Markus, M.Kettner, G. F. Hanne, Z. Vager, R. Naaman, and H. Zacharias, Science **331**, 894 (2011).

15 min. break

DS 51.4 Thu 17:30 H23

Magnetic impurities on Bi thin films - conductivity and surface diffusion — •Philipp Kröger[1], Sergii Sologub[2], Andreas Lücke[3], Nora Vollmers[3], Uwe Gerstmann[3], Wolf Gero Schmidt[3], Herbert Pfnür[1], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Inst. für FKP, Appelstr. 2, 30167 Hannover — [2]Inst. of Ph., Nat. Acad. of Sc., Nauky Av. 46, 03028 Kyiv, Ukraine — [3]Universität Paderborn, Theoretische Materialphysik, Pohlweg 55, 33098 Paderborn

The semimetal bismuth has attracted a lot of interest because of its unique electronic properties such as low carrier concentration and large mobility. The surface states reveal a pronounced Rashba splitting. The surface conductivity can well be discriminated from bulk contributions for ultra-thin films grown epitaxially on Si(111) substrates, so that surface related effects are accessible even in macroscopic conductance measurements.
In this context, the adsorption of Cr with its high magnetic moment on the Bi(111) surface will be discussed. Cr induces a transition from Weak Anti- to Weak Localization. This indicates strong impurity scattering that mixes spin and orbit momenta, with corresponding symmetry breaking on the Bi surface (TRS), in agreement with results from DFT calculations. Contrary to other impurities adsorbed at subsurface sites (Fe,Co,Cr, Sb), Cr shows signs of diffusion processes at low T (T ≈ 10 K), as previously observed for Tb which adsorbes on the surface.

DS 51.5 Thu 17:45 H23

Spin-vibronics in interacting nonmagnetic molecular nanojunctions — •Stephan Weiss[1], Jochen Brüggemann[2], and Michael Thorwart[2] — [1]Theoretische Physik, Universität Duisburg-Essen & CENIDE — [2]1. Institut für Theoretische Physik, Universität Hamburg

We show that in the presence of ferromagnetic electronic reservoirs and spin-dependent tunnel couplings, molecular vibrations in nonmagnetic single molecular transistors induce an effective intramolecular exchange magnetic field[1]. It generates a finite spin-accumulation and -precession for the electrons confined on the molecular bridge and occurs under (non)equilibrium conditions. The effective exchange magnetic field is calculated here to lowest order in the tunnel coupling for a nonequilibrium transport setup. Coulomb interaction between electrons is taken into account as well as a finite electron-phonon coupling. For realistic physical parameters, an effective spin-phonon coupling emerges. It is induced by quantum many-body interactions, which are either electron-phonon or Coulomb-like.

[1] S. Weiss, J. Brüggemann and M. Thorwart,
PRB **92**, 045431 (2015).

DS 51.6 Thu 18:00 H23

Coherent Dynamics of Quantum Spins in Magnetic Environments — •Lars-Hendrik Frahm[1], Christoph Hübner[1], Benjamin Baxevanis[1,2], and Daniela Pfannkuche[1] — [1]1. Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg, Germany — [2]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands

We investigate equilibration and transport effects of a magnetic atom that is exchange coupled to two electron reservoirs. An effective crystal field, which arises from the substrate the atom is living on gives the spin of the atom an easy axis for alignment. Further, a spin-polarized electron reservoir breaks the rotation symmetry around the spin quantization axis. A proper description of the dynamics of the quantum spin requires to consider the complete density operator, where its knowledge allows to calculate magnetization dynamics and transport properties on an equal footing. We discuss the electron transport through the atomic system by especially focusing on the non-linear influence of the spin torque effect.

DS 51.7 Thu 18:15 H23

Colossal Magnetoresistance observed in Natural Graphite — •Jose Barzola-Quiquia[1], Mahsa Zoraghi[1], Markus Stiller[1], Christian Precker[1], Ana Champi[2], and Pablo Esquinazi[1] — [1]Institute for Experimental Physics II, University of Leipzig, 04103 Leipzig, Germany — [2]Centro de Ciencias Naturais e Humanas Universidade Federal do ABC, Sao Paulo- Brasil

In this work, the electrical transport properties of a bulk natural graphite flake extracted from a mine in Brazil were investigated. The sample showed metallic behavior and the changes in the magnetoresistance (MR) at 5 K and 7 T shows 1123600% change when the field was applied parallel to the *c*-axis. This value was not yet reported in any graphite sample in the literature. Applying constant magnetic field, resistance measurements as a function of the temperature show also a magnetic field induces metal-insulator transition (MIT), with a small critical field $B_0 \approx 10$ mT compared to literature. We observed also that at fields B > 0.2 T a metallic reentrance was observed that remains up to ≈ 50 K. STEM measurements reveal the presence of interfaces in the investigated material. Therefore, the observed transport properties are not an intrinsic behavior of the graphite sample but due to the presence of these interfaces. Interfaces in the sample are formed at the interfaces between two crystalline regions inside the sample where a two dimensional electron gas (2DEG) system appears. Raman measurements reveal that our samples are free from any other defects.

DS 52: Ion and Electron Beam Induced Processes

Time: Thursday 17:00–18:15 Location: H11

DS 52.1 Thu 17:00 H11

High Current LMIS for Ion Implanters and Single-ended Accelerators — •Philipp Laufer[1], Daniel Bock[1], Wolfgang Pilz[1], Lothar Bischoff[2], and Martin Tajmar[1] — [1]Technische Universität Dresden, 01062 Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden

An ion source module based on high current Liquid Metal Ion Sources (LMIS) will be presented for optional use of mon - or polyatomic ion currents of metallic or semiconducting elements [1, 2, 3]. Total emitted ion currents in the order of 100 μA can be reached which are formed to a nearly parallel ion beam of 2 mm diameter using an asymmetric ion-optical Einzel lens. Cluster ion fractions are in the range of per mil up to a few percent dependent on the emitted elements. A mass separation system (Wien filter) selects the desired ions while a quadrupole is used for beam adjustment. Few-atomic cluster ions are of interest to be implanted for an effective surface modification [4]. High cluster ion currents enable the formation of different nanostructures or even smooth surfaces over an area in cm^2-range. The LMIS preparation and the performance of the ion beam module at certain experiments will be presented and discussed.

[1] M. Tajmar, et al., Ultramicroscopy 111 (2010) 1
[2] D. Bock, et. al., DPG Conference Dresden (2014) DS 17.6
[3] P. Laufer, et al., DPG Conference Berlin (2015) DS 19.9
[4] L. Bischoff, et al., Nucl. Instr. and Meth. B 272 (2012) 198

DS 52.2 Thu 17:15 H11

Milling and imaging techniques at the helium ion microscope for sub 2 nm nanopore fabrication — •Daniel Emmrich[1], Emanuel Marschewski[1], Jani Kotakoski[2], Achim Nadzeyka[3], Frank Nouvertné[3], Jannik Meyer[2], André Beyer[1], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems, Bielefeld University, Germany — [2]Physics of Nanostructured Materials, University of Vienna, Austria — [3]Raith GmbH, Dortmund, Germany

The helium ion microscope (HIM) is a charged particle microscope employing helium ions for probing the sample. In the low dose regime, the HIM operates as microscope, high doses enable material modification and sputtering. Compared to conventional focussed ion beams (FIB) using metal ions like gallium, the HIM offers a very small focal spot size down to 0.35 nm and a strongly localized sputter interaction with the material. We employ the HIM for both milling nanopores in free standing membranes as well as for the inspection of pores. The helium ion beam with its unique properties overcomes the resolution limit of conventional FIB tools as we show in a comparison with a high resolution gallium FIB. We investigated three different materials: 30 nm thick silicon nitride, graphene and 1 nm thick carbon nanomembranes (CNM) made from aromatic self-assembled monolayers by electron-induced cross-linking. By HIM milling and imaging we can detect smallest nanopores at 3 nm diameter in all membranes. Further studies on CNM with an atomic resolution STEM revealed even nanopores with diameters of less than 2 nm made by ion beam exposure.

DS 52.3 Thu 17:30 H11

Tuning pattern symmetry by choosing the substrate in reverse epitaxy — •Martin Engler[1], Xin Ou[2], and Stefan Facsko[1] — [1]Institute for Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, Shanghai, China

Ion beam erosion of solid surfaces is long known to yield regular surface morphologies, like periodic ripples or hexagonal dot patterns. At room temperature, semiconductors are amorphized by the ion beam. Pattern formation under these conditions has been studied extensively in the last decades.

Ion beam erosion above a material dependent dynamic recrystallization temperature allows the formation of crystalline nano scale patterns on semiconductor surfaces. At these elevated temperature pattern formation is driven by diffusion of vacancies created by sputtering of atoms. Anisotropic diffusion on the surface and diffusion barriers across step edges lead to the formation of pattern reflecting the symmetry of the irradiated surface. We will discuss how the surface symmetry determines the pattern symmetry.

DS 52.4 Thu 17:45 H11

Energy loss and charge exchange of slow highly charged ions in graphene — •Richard Wilhelm[1], Elisabeth Gruber[2], Valerie Smejkal[2], Janine Schwestka[2], Roland Kozubek[3], Anke Hierzenberger[3], Marika Schleberger[3], Stefan Facsko[1], and Friedrich Aumayr[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]TU Wien, Institut für Angewandte Physik, Wien, Österreich — [3]Universität Duisburg-Essen, FB Physik, Duisburg, Deutschland

Slow highly charged ions (e.g. Xe^{q+} with $q = 10 - 40$) enable studies of ion-solid interaction far from equilibrium. These ions neutralize quickly in a solid, i.e. typically within the first nm of the solid. The neutralization is associated with the deposition of the ion's potential energy in a small volume (nm^3) during a short time (fs). To study the neutralization dynamics in more detail and also to study charge state enhanced kinetic energy loss we used graphene as the thinnest target material there is for ion transmission experiments. We observe even in freestanding single layer graphene strong charge exchange and extracted a surprisingly short neutralization time of around 2-3 fs. Additionally we see a strong enhancement of the energy loss (stopping) with charge state and with charge exchange.

DS 52.5 Thu 18:00 H11

Properties of TiO2 films grown by reactive ion beam sputter deposition — •Thomas Lautenschläger, Eric Thelander, Daniel Spemann, and Carsten Bundesmann — Leibniz-Institut für Oberflächenmodifizierung, Permoserstr. 15, 04318 Leipzig

Ion beam sputter deposition is a versatile technique for tailoring thin film properties as it provides several ways of varying the properties of the film-forming, secondary particles. TiO2 films were deposited by reactive ion beam sputter deposition under systematic variation of ion beam and geometrical parameters. The films were characterized concerning thickness, growth rate, structural properties, mass density, composition and optical properties. Film thickness and growth rate show an over-cosine angular distribution that is tilted in forward direction. The growth rate was found to increase with increasing ion energy and ion incidence angle, which can be explained by the known dependence of the sputter yield. The TiO2 films are amorphous and show systematic variations in the mass density and index of refraction. Mass density and index of refraction reveal a strong correlation. The systematic variations in mass density and index of refraction are assigned to the properties of the backscattered primary particles. Furthermore, a considerable amount of primary particles was found in the films. The atomic fraction of inert gas particles depends on the scattering geometry, i.e. it increases with increasing sum of ion incidence angle and polar emission angle, but seems to be unaffected by the ion energy.

DS 53: Postersession DS/HL

Presenters are kindly requested to be near their poster for at least one hour during poster session or leave a note about their availability for discussions.

Time: Thursday 16:00–19:00 Location: Poster A

DS 53.1 Thu 16:00 Poster A

Metallic Chains on Ge (001) Surface and Their Manipulation — •Deniz Aşan Acar[1], Umut Kamber[1], Dilek Yildiz[2], and Oğuzhan Gürlü[1] — [1]Istanbul Technical University, Istanbul, Turkey

— [2]University of Basel, Basel, Switzerland

One dimensional, single atom thick wires present an exotic playground. We investigate the surface structure formed by adsorption of Pt and Au on Ge(001) surface. It is well known that upon annealing of Pt deposited Ge(001) surface at 1000 K atomic chains form along with two different types of terraces. Similar structures form due to Au deposition on Ge(001). In this study we have experimented on the co-deposition of Au and Pt on to Ge(001) surfaces. We will report on our findings related to the formation of novel atomic scale structures. (This study was funded by a TUBITAK 1001 project with grant number 112T818.)

DS 53.2 Thu 16:00 Poster A

Mask-less Selective Area Epitaxy of self-catalyzed GaN-microrods on silicon — •Christian Blumberg, Dennis Jansen, Werner Prost, and Franz-Josef Tegude — University Duisburg-Essen, Faculty of Engineering, Solid-State Electronics Department, Duisburg, Germany

3D GaN microrod structures offer the potential to fabricate electro-optical devices that may outperform their 2D counter parts. Promising candidates are the GaN/InGaN microrod-LEDs. These m-planar GaN/InGaN-LEDs are not limited by quantum-confined Stark effect at the GaN/InGaN interface (long charge-carrier lifetimes and less radiative efficiency at high intensities). A major issue by producing a macro sized usable LED from microrod-structures is the inhomogeneous distribution among the microrods: length, diameter and distance between each rod changes from rod to rod. As a result each rod-device has different electro-optical properties, which leads e.g. to a broadening of emission spectrum of a LED, consisting of parallel electric-powered microrod-LEDs. In order to reach a high homogeneity selective area epitaxy (SAE) of the rods is necessary. In this work we discuss the high-density seeding of rods on Si (111). We have developed a new method of the SAE for self-catalysed GaN-rods, which is based on pattering the Si-surface by nanoimprint technology. In contradiction to other methods for SAE we did not use a dielectric mask (like SiNx or SiOx). By adapting the Si-surface pattern (depth of etched holes and surface cleaning) and the epitaxial parameters (silane-flow and V/III) we were able to grow position controlled GaN-rods on Si.

DS 53.3 Thu 16:00 Poster A

Stability of misfit dislocations in axial-heteroepitaxial 3C-SiC/c-GaN nanopillars and nanomesas — •Thomas Riedl[1], Ricarda Kemper[1], Andras Kovacs[2], Doris Meertens[2], Donat As[1], and Jörg Lindner[1] — [1]University of Paderborn, Department of Physics, Warburger Straße 100, 33098 Paderborn, Germany — [2]Ernst-Ruska Centre for Microscopy and Spectroscopy with Electrons, FZ Jülich, 52425 Jülich

GaN represents the most important compound semiconductor for realization of highly efficient blue LEDs and lasers. The cubic modification of GaN (c-GaN) has attracted growing interest due to the absence of internal electric fields. For the fabrication of high-quality semiconductor devices defect-free epilayers are essential. One way to avoid defects arising due to misfit is to reduce the lateral dimension of the layer to the nanoscale, which leads to a purely elastic relaxation in three dimensions.

In order to investigate the effect of the lateral size of axial pillar or mesa shaped heterostructures on the stability of misfit dislocations for the 3C-SiC/c GaN system, we apply various analytic approaches based on linear continuum elasticity theory. We find that the approaches of Glas and Ertekin predict the stability zone of misfit dislocations to exist at significantly smaller lateral dimensions and slightly larger layer thicknesses in comparison to the model of Zubia and Hersee. The former approaches yield a reasonable agreement with high-resolution TEM observations of c-GaN layers that have been grown on top of 3C-SiC mesa posts of different edge lengths.

DS 53.4 Thu 16:00 Poster A

Spectroelectrochemical Response of Half Cells for Solid-state Electrochromic Devices — •Christian Lupo[1], Yurong Su[2], Angelika Polity[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Heinrich Buff-Ring 16, 35392 Giessen, Germany. — [2]1st Physics Institute, Justus Liebig University Giessen, Heinrich Buff-Ring 16, 35392 Giessen, Germany

Electrochromic devices made by solid-state components only could provide longer lifetimes or faster switching speeds compared with currently produced devices ("smart windows", "smart mirrors") with polymeric or liquid electrolytes. Lithium phosphorous oxynitride ($LiPON$) is a promising candidate as a solid electrolyte for use in electrochromic devices. Thin films of $LiPON$ could replace the relatively thick electrolytes based on a Lithium salt in liquid or polymeric compounds because of a high chemical stability and good transparency of $LiPON$. In the present study, $LiPON$ is used in combination with tungsten oxide (WO_x) or nickel oxide (NiO), both well-known electrochromic materials which become colored upon chemical reduction or oxidation, respectively. On the way to an all-solid-state device, the first challenges consist in reaching a good ionic conducting solid electrolyte and well-working solid contacts. Electrochemical and spectroelectrochemical measurements are used to characterize the response and the coloration performance of electrochromic half cells consisting of combinations of $WO_x/LiPON$ or $LiPON/NiO$ solid layers prepared via combinations of sputtering and/or chemical bath deposition methods.

DS 53.5 Thu 16:00 Poster A

Spectroscopic Ellipsometry and MOKE as a Probe for Structural Properties of Spinel Oxide Thin Films — •Vitaly Zviagin[1], Peter Richter[2], Yogesh Kumar[1], Israel Lorite[1], Michael Lorenz[1], Daniel Spemann[1], Jan Meijer[1], Dietrich R.T. Zahn[2], Georgeta Salvan[2], Pablo Esquinazi[1], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany — [2]Technische Universtät Chemnitz, Semiconductor Physics, Reichenheiner Str. 70, Germany

Normal, disordered, and inverse spinel oxide ferrite and cobaltite thin films were grown at different temperatures on MgO (100), $MgAl_2O_4$ (100), and $SrTiO_3$ (100) substrates by pulsed laser deposition. Assigned electronic transitions visible in diagonal and off-diagonal elements of the dielectric tensor show a clear dependence on growth temperature corresponding to the crystal quality of the films. Silicon irradiation of $ZnFe_2O_4$ films caused inversion of normal spinel structure as well as lattice distortion with further treatment, clearly visible in the dielectric function. The $Zn_xFe_{3-x}O_4$ composition was found to contain defects such as presence of Fe^{2+} ions. Magneto-optical Kerr effect spectroscopy was employed to investigate magneto-optically active transitions, and in combination with spectroscopic ellipsometry we obtained detailed information of site occupancy related to crystal inversion and disorder. We relate optical properties to magnetic properties to show a direct correlation between site occupancy of tetrahedral sites by Fe^{3+} ions to saturation and remanence magnetization.

DS 53.6 Thu 16:00 Poster A

Growth-of p-type nickel oxide on different substrates and surface orientations — •Carsten Tschammer and Oliver Bierwagen — Paul-Drude-Institut, Hauvogteiplatz 5-7, 10117 Berlin, Germany

NiO belongs to the transparent semiconducting oxides with unintentional p-type conductivity. Currently, NiO is used in batteries and capacitors, and is considered for future applications in UV-detectors, all-oxide hetero pn-diodes, and organic solar cells. For the latter, NiO is an excellent candidate for an interfacial layer between the ITO anode and active organic layer, serving as electron blocking and hole transport layer. Doping NiO with Nitrogen as an acceptor should increase the p-type conduction.

Here NiO thin layers were grown by plasma-assisted MBE using RHEED as in situ monitoring tool. For the growth of well-defined NiO layer and surfaces MgO was chosen as substrate due to its common crystal structure and low lattice mismatch to NiO. Thus, NiO was grown on MgO(100), MgO(110), MgO(111) to help investigating the interface to the active organic layer on differently oriented surfaces. Growth on epitaxial ITO and In_2O_3 was performed to come closer to the solar cell application and application in pn-diodes, respectively. The film crystal and surface structure were investigated by AFM, XRD, XRR. The electronic properties were investigated by Raman, PL and transport measurements.

DS 53.7 Thu 16:00 Poster A

Intermediate tin oxide phases from first principles — Bianca Eifert and •Christian Heiliger — Institut für Theoretische Physik, Justus Liebig University Gießen, D-35392, Germany

The two stable tin oxides, SnO and SnO_2, are semiconductors with bandgaps of different types and sizes. Both of them are therefore of great interest for applications, and may even be used together for tin-only devices. It has also been known for over a century that when SnO disproportionates, mixed-valence oxides of other stoichiometries can be formed as intermediates. These phases are also accessible from elementary precursors, for instance through thin-film deposition techniques. The intermediate oxides have, however, eluded conclusive analysis in the past. Using density functional theory (DFT) and phonon calculations, we can predict the electronic structures and Raman spectra for different candidate crystal structures. Comparing these new insights with experimental results, we are now able to determine the identity and properties of the intermediate tin oxide.

DS 53.8 Thu 16:00 Poster A

Pseudomorphic growth and relaxation of alpha gallium oxide on sapphire substrate — •Zongzhe Cheng[1], Patrik Vogt[1], Robert Schewski[2], Oliver Bierwagen[1], Martin Albrecht[2], Achim Trampert[1], and Michael Hanke[1] — [1]Paul-Drude-Institut für Festkörperelektronik (PDI), Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung (IKZ), Berlin, Germany

Alpha phase gallium oxide is a transparent semiconducting material with an indirect wide band gap of around 5eV. The heteroepitaxial growth of alpha phase gallium oxide on insulating c-plane sapphire (band gap = 8.8ev) can be realized by molecular beam epitaxy since they have the same corundum crystal structure and small lattice mismatch (4.6% in a-axis and 3.3% in c-axis). However under ambient conditions, the beta phase gallium oxide with a monoclinic structure is thermodynamically more stable than the alpha phase, so normally beta phase gallium oxide starts to grow after a three atomic layer of alpha phase gallium oxide on the c-plane sapphire substrate in molecular beam epitaxy growth. So it is important to stabilize the growth of alpha phase gallium oxide trying to get pure alpha phase gallium oxide layer on the substrate in case of device applications (eg. 2deg). In this work, we use mainly synchrotron radiation and high resolution transmission electron microscopy in order to understand the pseudomorphic growth and relaxation of the alpha phase gallium oxide on c-plane sapphire substrate. In addition, an annealing experiment on a low-temperature-deposited amorphous gallium oxide layer is performed trying to crystallize the gallium oxide layer and stabilize the alpha phase.

DS 53.9 Thu 16:00 Poster A

Transmission Electron Diffraction on a really free-standing heterostructure and analysis of the resulting Moiré pattern — Marlene Adrian, •Arne Senftleben, Silvio Morgenstern, and Thomas Baumert — Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel

The combination of various 2D layered materials in multilayer heterostructures arises great interest in the current science. Due to the large variety of electronic properties of the group of 2D layered materials the combination opens a new pathway towards ultrasmall electronic devices. In this contribution we present a preparation method to obtain free-standing samples of multilayer heterostructures and a full characterisation of their diffraction images. A 20 nm thick MoS_2–graphite heterostructure was produced and analysed with the methods presented. Additionally, the ultrafast lattice dynamics after optical excitation of the sample will be discussed.

DS 53.10 Thu 16:00 Poster A

Silicene-based spin-filter device: Impact of random vacancies — Cesar Nunez[1], Francisco Dominguez-Adame[2], Pedro Orellana[1], Luis Rosales[1], and •Rudolf A. Römer[3] — [1]Universidad Tecnica Federico Santa Maria, Valparaiso, Chile — [2]Universidad Complutense, E-28040 Madrid, Spain — [3]University of Warwick, Coventry, CV4 7AL, UK

We propose a hybrid spin-filter device based on a silicene nanoribbon. A ferroelectric polymer grown on top of the nanoribbon splits spin-up and spin-down electron bands and gives rise to spin polarisation of the conductance. In particular, we study the effects of a random distribution of vacancies on the performance of this spin-filter device. Disorder induces Anderson localisation of electrons and we find that the localisation length strongly depends on the electron spin. By adjusting the Fermi level of the source contact, only electrons with one spin orientation can reach the drain contact because their localisation length is larger than the length of the device. Electrons with opposite spin are largely back-reflected. Electric conductance then becomes spin polarised and the device behaves as a quasi-half-metal. We conclude that a moderate concentration of vacancies has little impact on the spin-filter capabilities of the device, opening the possibility to using it as a tuneable source of polarized electrons.

DS 53.11 Thu 16:00 Poster A

Stacking different two-dimensional materials to fabricate a high mobility transistor — •Himani Arora[1,2], Gotthard Seifert[3], Gianaurelio Cuniberti[4], Manfred Helm[1,2], and Artur Erbe[1] — [1]HZDR, Bautzner Landstrasse 400, 01328 Dresden — [2]Technical University Dresden, Faculty of Mathematics and Natural Sciences, 01062 Dresden — [3]Technical University Dresden, Institute for Physical Chemistry and Electrochemistry, 01062 Dresden — [4]Technical University Dresden, Institute for Materials Science and Max Bergmann Centre of Biomaterials, 01062 Dresden

In recent years, several two-dimensional (2D) semiconducting materials like graphene, MoS2, WSe2, silicene, germanene etc. have been produced and studied. Their semiconducting properties allow the development of 2D structures, whose electronic properties can be tuned. By fabricating gate electrodes on the 2D materials, field effect transistors have been demonstrated. Further exciting possibilities open up when these materials are stacked together to achieve the desired application. The first series of experiments are carried out with graphene nanoribbons (GNRs) deposited on functionalized Si/SiO2 substrate. Prior to the deposition, the Si/SiO2 substrate is patterned with Ni alignment marks, to locate and characterize GNRs by AFM and Raman spectroscopy. Au electrodes are then fabricated on selected GNRs using electron beam lithography to measure the electrical transport properties. In future, the aim will be to fabricate a heterostructure by stacking different 2D materials, whose different properties can complement each other to fabricate a high mobility transistor.

DS 53.12 Thu 16:00 Poster A

Magnetic-field dependent photoluminescence measurements of WS_2 monolayers — •Jan Kuhnert, Simon Schmitt, Arash Rahimi-Iman, Ajanth Velauthapillai, and Wolfram Heimbrodt — Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany

Layered transition-metal dichalcogenides have attracted great interest in the last few years. Thinned down to monolayers they exhibit outstanding optical properties caused by the direct band gap. Here we present photoluminescence measurements of tungsten disulfide monolayers at low temperatures (2 K) in the presence of an external magnetic field in Faraday geometry. In the monolayer limit the inversion symmetry is broken and spin and valley are coupled. The degeneracy between the two equivalent K and K' valleys is broken by applying external magnetic fields. This causes a Zeeman shift which has already been shown in similar layered transition-metal dichalcogenides (eg. MoSe2: 0,25 meV/T (1)). We show this field-dependent Zeeman splitting in tungsten disulfide at low temperatures (2 K) and find a surprisingly large splitting of 0,8 meV/T.

(1) Nature Physics 11, 141147 (2015)

DS 53.13 Thu 16:00 Poster A

Hydrogenation of Epitaxial Silicene Studied by *in situ* Raman Spectroscopy — •Dmytro Solonenko[1], Patrick Vogt[2], Ovidiu D. Gordan[1], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany

As silicene can be only grown epitaxially on a substrate like Ag(111) single crystals, the influence of the substrate on the 2D silicene properties have been extensively discussed in literature. It was shown that the electronic properties of epitaxial silicene are altered due to the significant interaction with the substrate but it still keeps a clear semimetallic character[1], as expected for ideal freestanding silicene. On the other hand, an electronic bandgap could be opened by applying an electric field perpendicular to the sheet, or via functionalization, *e.g.* by H-adsorption. In the latter case, controlled hydrogenation of freestanding silicene might open a bandgap up to the UV edge of the visible spectral region[2]. In order to examine if the silicene structure is preserved upon hydrogenation, we grew silicene monolayer sheets on Ag(111) substrate and hydrogenated them by supplying activated atomic H. *In situ* Raman spectroscopy study was carried out in order to follow structural changes of the silicene layer upon H-adsorption. We find that the silicene hydrogenation is reversible by heating the sample, at temperatures expected to be sufficient for breaking the H-Si bonds. [1] Johnson, N. W. *et al.*, *Adv. Func. Mat.* **24**, 5253-5259 (2014). [2] Osborn, T. H. *et al.*, *Chem. Phys. Lett.* **511**, 101 (2011).

DS 53.14 Thu 16:00 Poster A

Electrical properties of CVD Molybdenum disulfide — •Wajid

Awan[1], Tommy Schönherr[1], Artur Erbe[1], Stefan Facsko[1], and Xinliang Feng[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]Technische Universität Dresden

Two dimensional materials are attractive for the use in next-generation nanoelectronic devices as compared to one dimensional material because it is relatively easy to fabricate complex structures from them. Recently the layered 2D semiconducting Transition metal dichalcogenides came into the picture and got a place in a wide range of novel applications as well as in basic research. Strikingly, MoS_2 receives significant attention since it undergoes transition from indirect bandgap (bulk form) to a direct bandgap (1.2eV) semiconductor if thinned out to a single atomic layer. The bandgap is an essential property for tunable 2-D nanodevices. We performed electrical transport measurements at room temperature for CVD grown MoS_2 on SiO_2/Si substrate. Standard Electron beam lithography (EBL) was used to pattern Gold (Au) metal contacts on MoS_2 flakes. For the purpose of sample characterization, we performed the Atomic Force Microscopy (AFM) and Raman Spectroscopy techniques, respectively, which confirm that the thickness of the CVD grown MoS_2 triangular flakes corresponds to single layers. Low temperature characterization of the electrical properties of the layers elucidates the exact mechanisms of charge transport in the 2d-layers. This knowledge will be used to modify the electrical properties in a controlled way, for example by ion irradiation.

DS 53.15 Thu 16:00 Poster A

Molecular beam epitaxy growth and in situ analysis of transition metal dichalcogenides — •Avanindra Kumar Pandeya, Amilcar Bedoya Pinto, Ilya Kostanovskiy, Kai Chaang, and Stuart Parkin — Max Plank Institute for Microstructure Physics, Halle, Germany

Atomically thin transition metal dichalcogenides (TMDCs), layered materials which have captured great attention due to their tunable electronic properties [1], are commonly fabricated via exfoliation of high-quality bulk crystals. Although there has been tremendous progress in fabricating devices out of exfoliated heterostructures [2], there are other effects, such as spin transfer, that need atomically clean interfaces for an optimum harvesting. Our approach is to grow TMDCs layers by molecular beam epitaxy and assess the layer and interface quality using in-situ characterization (RHEED, LEED, XPS, AES and STM). The fabrication of high-quality TMDCs heterostructures by UHV methods opens new prospects for the design of interface-sensitive electronic and spintronic devices.

1. J. Kang, et al. Applied Physics Letters, 102, 012111 (2013)
2. C. Lee, et. al. Nature Nanotechnology 9, 676-681, (2014)

DS 53.16 Thu 16:00 Poster A

Si(553)-Au surface functionalized by small molecules — •Svetlana Suchkova[1], Eugen Speiser[1], Sandhya Chandola[1], Conor Hogan[2], Friedhelm Bechstedt[3], and Norbert Esser[1] — [1]Leibnitz-Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Schwarzschildstr. 8-10, 12489 Berlin, Germany — [2]Universita di Roma Tor Vergata, Via della Ricerca Scientifica 1, 00133 Roma, Italy — [3]Friedrich-Schiller-University Jena, Institut für Festkörpertheorie und optik, Helmholtzweg 3, 07743 Jena

We discuss the adsorption of toluene-3,4-dithiol molecules on the Si(553)-Au surface. In contrast to the highly reactive clean Si surface, Au-passivated surfaces offer the potential for a more selective adsorption, eventually yielding molecular layers that are essentially self-ordered on the underlying silicon substrate. The calculations of Potential Energy Surface (PES) by Density Functional Theory (DFT) in combination with reflectance anisotropy spectroscopy (RAS) provide us with the information on molecular orientation on the surface.

DS 53.17 Thu 16:00 Poster A

Preparation-dependent viscoelastic properties of ultra-thin glass-forming polymer films. — •Pierre Chapuis[1,2], Anne Rubin[2], Freddy Anstotz[3], Paul Montgomery[3], and Günter Reiter[1] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Germany — [2]Institut Charles Sadron, Strasbourg, France — [3]ICube/IPP, Strasbourg, France

Properties of ultra-thin glassy polymers films differ from bulk behavior. Many studies stated that it is a consequence of confinement and/or interfacial physics. Another possible explanation is suggested: the preparation process of the film by spin-coating entails an out-of-equilibrium state of the chains [1].

To give insight on this phenomenon we explore the influence of the preparation process of ultra-thin glassy freestanding polymer films on their viscoelastic response. Ultra-thin polymer films are obtained by spin-coating technique and transferred onto a silicone substrate containing an array of 5 μm. Using the nanobubble inflation method [2], a static pressure was applied and the resulting deformation was probed with time by 4D interferometric microscopy which is a non-contact method (3D + real time) developed at ICube.

We discuss the results of creep compliance measurements on poly(vinyl acetate) (PVAc) films of thicknesses below 100 nm for different molecular weights.

[1] M.Chowdhury et al., PRL 109, 136102 (2012) [2] P.A. O Connell et al., Science 18, 1750 (2005).

DS 53.18 Thu 16:00 Poster A

Transparent white AC/DC OLEDs — •Felix Fries, Markus Fröbel, Simone Lenk, and Sebastian Reineke — Institut für Angewandte Photophysik, Technische Universität Dresden, Germany

Future lighting applications will strongly benefit from transparent luminescent devices. In this contribution, we demonstrate transparent organic light-emitting diodes (OLEDs), which allow for flexible adjustment of the emission color. We extend the AC/DC concept, that was only recently presented for bottom-OLEDs, to transparent devices. Since two units are stacked on each other and the cathode of one is connected to the anode of the other, they can be addressed independently via an AC-signal. Comprising blue and yellow emission units leads to the possibility to tune the color between deep blue over cold and warm white to yellow emission.

Based on optical simulation, we build OLEDs that show an overall transparency of 62% when switched off and emit warm white light to both sides (top, bottom) with an overall power efficacy of 11.8 lm/W at a brightness of 1000 cd/m^2 when switched on. Moreover, devices without indium-tin oxide (ITO) are presented, which exclusively rely on highly transparent ultra-thin metal electrodes. These ITO-free devices achieve a power efficacy of 18.4 lm/W at 1000 cd/m^2 for warm white emission and 56% transmission.

Using an emitter combination providing red, green, and blue emission, we were also able to achieve a high color-rendering index (CRI) of 84, which further expands the range of possible applications for this promising device concept.

DS 53.19 Thu 16:00 Poster A

Influence of temperature on the interaction of excitons with electron-hole pairs in organic bulk heterojunction structures — •Jędrzej Szmytkowski — Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gdańsk, Poland

Nowadays, a great attention is focused on organic photovoltaics. Bulk heterojunction structures based on donor-acceptor materials are treated as very promising systems to obtain high efficiencies of organic solar cells. The main effect which causes a loss of photocurrent is a recombination of charge carriers. Recently, it has been shown that an order of recombination depends on temperature. The aim of this work is to describe this process in the case when it occurs at a donor-acceptor interface due to excitons annihilation on electron-hole Langevin pairs. Additionally, a theoretical consideration based on the role of disorder is also presented.

DS 53.20 Thu 16:00 Poster A

Polarization-dependent Differential Reflectance Spectroscopy for real-time monitoring of organic thin film growth — •Andrea Navarro-Quezada, Markus Aiglinger, Ebrahim Ghanbari, Thorsten Wagner, and Peter Zeppenfeld — Institute of Experimental Physics, Johannes Kepler University, Altenbergerstr. 69, 4040 Linz, Austria

Optical spectroscopy is a powerful tool to study physical processes occurring in molecular thin films and at their interfaces with inorganic materials. In particular, differential reflectance spectroscopy (DRS) records the change in the reflectance of a surface upon physical or chemical modification. Therefore, it allows real-time monitoring of the deposition of organic thin films. In this work, we present an extended DRS setup that allows the simultaneous detection of both linear polarization states (s and p) of the reflected light [1]. The setup exhibits a signal to noise ratio better than 1000:1 as well as high signal stability, thus we detect changes in the reflectance in the order of 10^{-3}. As a proof of principle, we have implemented polarization-dependent DRS to monitor the growth of perfluoropentacene thin films on a Ag(110) single crystal in combination with photoelectron emission spectroscopy. From the analysis of the different DRS transients for s and p polarized light, we follow the alignment of the molecules on the Ag(110) surface during growth.

[1] A. Navarro-Quezada, M. Aiglinger, E. Ghanbari, Th. Wagner, and P. Zeppenfeld, *Rev. Sci. Inst.* 86, 113108 (2015)

DS 53.21 Thu 16:00 Poster A

Improved color stability of white OLEDs with tandem structure and new host material — •Yuan Liu[1,2], Zuo-Quan Jiang[1], and Liang-Sheng Liao[1] — [1]Institute of Functional Nano & Soft Materials, Soochow University, 215123 Suzhou, China; — [2]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany;

Tandem structures can improve the efficiency and lifetime of organic light-emitting diodes (OLEDs) simultaneously. More importantly, this is also an effective strategy to reduce the color shift with increasing current density in white OLEDs. High performance tandem OLEDs require highly efficient emitting units along with an efficient charge generation layer. To improve the performance of single emitting unit, two novel host materials SF2BCz and SF3BCz which combine spirobifluorene and carbazole units via meta- and para-bonding are designed for phosphorescent OLEDs (PhOLEDs). The meta-linkage of spirobifluorene enables SF3BCz to possess high triplet energy, suitable energy levels, and good thermal stability. Blue PhOLEDs featuring SF3BCz as a host show high performance and low efficiency roll-off, with an efficiency of 41.4 cd/A (18.0%, 39.8 lm/W) at 100 cd/m2 and 39.7 cd/A (17.2%, 29.8 lm/W) at 1000 cd/m2. In addition, SF3BCz is adopted as a universal host for tandem white OLEDs, achieving an external quantum efficiency of 40% and a color stable emission spectrum.[1]

References: [1] Y. Liu, L. Cui, X. Shi, Q. Li, Z. Jiang and L. Liao, J. Mater. Chem. C, 2014, 2, 8736.

DS 53.22 Thu 16:00 Poster A

Controlling Nanostructures by Templated Templates: Inheriting Molecular Orientation in Binary Heterostructures — •Tobias Breuer and Gregor Witte — AG Molekulare Festkörperphysik, Philipps-Universität Marburg

Precise preparation strategies are required to fabricate nanostructures of specific arrangement. In bottom-up approaches, where nanostructures are gradually formed by piecing together individual parts to the final structure, the self-ordering mechanisms of the involved structures are utilized. In order to achieve the desired structures regarding morphology, grain size and orientation of the individual moieties, templates can be applied, which influence the formation process of subsequent structures. However, this strategy is of limited use for complex architectures, as the templates only influence the structure formation at the interface between the template and the first compound. Here, we discuss the implementation of so-called templated templates and analyze, in which extent orientations of initial layers are inherited in top layers of another compound to enable structural control in binary heterostructures. To that purpose we have prepared crystalline templates of the organic semiconductors pentacene and perfluoropentacene in different exclusive orientations. We observe that for templates of both individual materials the molecular orientation is inherited in the top layers of the respective counterpart.

[1] T. Breuer & G. Witte ACS Applied Materials & Interfaces 7 (36), 20485-20492 (2015)

DS 53.23 Thu 16:00 Poster A

Preparation and Characterization of Mixed Organic Thin Films Containing Sexithiophene and Perfluorinated Sexithiophene — •Berthold Reisz, Simon Weimer, Rupak Banerjee, Christopher Lorch, Johannes Dieterle, Giuliano Duva, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — Universität, Tübingen, Deutschland

We study molecular mixed thin films of α-Sexithiophene (6T), a well known organic p-type semiconductor with high hole mobility, together with its perfluorinated counterpart, the so far rarely studied n-type tetradecafluoro-α-sexithiophene (PF6T). Thin films of this donor-acceptor system with various mixing ratios have been grown on several substrates in ultrahigh vacuum by coevaporation. The films have been examined with x-ray and ultraviolet photoelectron spectroscopy (XPS/UPS), atomic force microscopy (AFM), x-ray diffraction (XRD), absorption measurements and variable angle spectroscopic ellipsometry (VASE). Connections between mixing ratio, morphology, crystalline structure and optical properties are discussed, following previous studies [1].

[1] A. Hinderhofer, F. Schreiber. Organic-Organic Heterostructures: Concepts and Applications. ChemPhysChem, 13(3):628-643, 2012.

DS 53.24 Thu 16:00 Poster A

Surface morphology of vapor deposited chitosan thin films — •Maria Jose Retamal[1,3], Tomas Corrales[2], Marcelo Cisternas[3,6], Nicolas Moraga[3,6], Sebastian Gutierrez[4], Tomas Perez-Acle[4], Patrick Huber[5], and Ulrich Volkmann[3,6] — [1]Facultad de Química, PUC, Santiago, Chile — [2]IAI Universidad de Tarapacá, Arica, Chile — [3]CIEN-UC, Santiago, Chile — [4]DLab, Fundación Ciencia y Vida, Santiago, Chile — [5]Hamburg U. of Technology, D-21073 Hamburg, Germany. — [6]Instituto de Física, PUC, Santiago,Chile

Chitosan is a useful biopolymer with several industrial and biological applications. In spite of the many applications of chitosan, there is a lack of studies regarding the morphology and growth mechanisms of thin films of this biopolymer. We present a study of thin chitosan films prepared using PVD with in-situ ellipsometric monitoring. The prepared films are studied using AFM in order to correlate surface morphology with evaporation parameters. We find that the surface morphology of our final thin films depends both on the ellipsometric optical thickness as well as the evaporation rate. We find the correct evaporation parameters in order to obtain homogeneous thin films of chitosan, which are relevant for future chitosan based nano-devices. AFM images on samples prepared as a function of film thickness at constant evaporation rate, as well as AFM topographies of samples prepared as a function of evaporation rate for reaching identical film thickness show both very strong similarities to images reported as spinodal dewetting of thin metal and polymer films as a function of temperature.

DS 53.25 Thu 16:00 Poster A

XPS study of Tetraphenylporphyrin layers on Au(111) — •Peter Roese[1,2], Philipp Espeter[1,2], Christoph Keutner[1,2], Dominique Krull[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4a, 44221 Dortmund, Germany — [2]DELTA, Technische Universität Dortmund, Maria-Goeppert-Mayer-Straße 2, 44221 Dortmund, Germany

Porphyrins are important building blocks of life. Furthermore, the interest in applying porphyrins as technical devices increased in recent years. Applications such as organic solar cells [1], organic LED's [2] or the usage of porphyrins as a photosensibilisator in cancer treatment [3] utilize the strong absorption properties of porphyrins in the visible spectrum. Here, we present the investigation of multilayers of metal-free meso-tetraphenylporphyrin (2HTPP) on an Au(111) surface using x-ray photoelectron spectroscopy (XPS) at the U55 beamline 11 at DELTA. In this study we report on a possible bonding between the molecules in the first interface layer to the Au(111) substrate while the upper molecule layers are deposited in their original form without bonding. References: [1] J. P. Collman et al., Chemical Reviews 104, 561 (2004). [2] J. M. Olson, Biochimica et Biophysica Acta (BBA) - Reviews on Bioenergetics 594, 33 (1980). [3] W. M. Campbell et al., The Journal of Physical Chemistry C 111, 11760 (2007).

DS 53.26 Thu 16:00 Poster A

Interface Analysis of PTCDI-C1 thin films on polycrystalline silver surfaces — •Guangcheng Huang, Carolin C. Jacobi, Julia Rittich, Cathy Jodocy, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Aachen, Germany

Electronic devices based on organic thin films, such as organic solar cells (OSCs) and organic thin film transistors (OTFTs), have been greatly improved in the last decade. Understanding the interface effects between organic thin films and metal surfaces is one of the crucial steps to further improve these devices. The organic material N,N'-Dimethyl-3,4,9,10-perylenetetracarboxylic diimide (PTCDI-C1) is a promising n-type semiconductor for the application in OSCs and OTFTs. In this work, thin films of PTCDI-C1 are deposited by organic molecular beam deposition (OMBD) with varying film thicknesses onto polycrystalline silver surfaces. The energy level alignment and binding state between the metal surface and the organic molecule are determined in-situ by photoelectron spectroscopy (PES) and inverse photoelectron spectroscopy (IPES). In addition, the morphology of the organic thin films is investigated by atomic force microscopy (AFM) and the structure by X-ray diffraction (XRD).

DS 53.27 Thu 16:00 Poster A

Optical and Structural Properties of Thin Films of Difluoro-anthradithiophene — •Timo Storzer[1], Alexander

Hinderhofer[1], Giuliano Duva[1], Alexander Gerlach[1], John E. Anthony[2], and Frank Schreiber[1] — [1]Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — [2]Department of Chemistry, University of Kentucky, Lexington, Kentucky, 40506, USA

We report on the optical and structural properties of the novel functionalized anthradithiophene derivative difluoro-anthradithiophene (diF-ADT). Anthradithiophene (ADT) is isoelectronic with pentacene, which is one of the most studied organic semiconductors. A fluorinated anthradithiophene derivative with (triethylsilyl)ethynyl side groups (diF-TES-ADT) has been studied in recent years and showed high charge carrier mobilities in solution-cast thin-film transistors [1]. We present a study of thin films of diF-ADT prepared by organic molecular beam deposition (OMBD). We show how the growth conditions (e.g. substrate temperature, deposition rate) influence the optical and structural properties based on UV-Vis absorption, spectroscopic ellipsometry, photoluminescence (PL), X-ray reflectivity (XRR) and AFM measurements.

[1] Gundlach, D. J.; Anthony, J. E. et al., Nat. Mater. 2008, 7, 216.

DS 53.28 Thu 16:00 Poster A

Nanomechanical investigation of a thin-film multi-layered electroceramic/metal-organic framework optical device — •James P Best[1], Engelbert Redel[2], Hartmut Gliemann[2], Christof Wöll[2], and Johann Michler[1] — [1]EMPA, Thun, Switzerland — [2]KIT-IFG, Karlsruhe, Germany

Thin-film multilayer stacks of mechanically hard magnetron sputtered indium tin oxide (ITO) and mechanically soft highly porous surface anchored metal-organic framework (SURMOF) HKUST-1 were studied using nanoindentation. Crystalline, continuous, and monolithic surface anchored MOF thin films were fabricated using a liquid-phase epitaxial growth method. Control over respective fabrication processes allowed for tuning of the thickness of the thin film systems with a high degree of precision. It was found that the mechanical indentation of such thin films is significantly affected by the substrate properties; however, elastic parameters were able to be decoupled for constituent thin-film materials. For indentation of multilayer stacks, it was found that as the layer thicknesses were increased, while holding the relative thickness of ITO and HKUST-1 constant, the resistance to deformation was significantly altered. Such an observation is likely due to small, albeit significant, changes in film texture, interfacial roughness, size effects, and controlling deformation mechanism as a result of increasing material deposition during processing. Such effects may have consequences regarding the rational mechanical design and utilization of MOF-based hybrid thin-film devices.

DS 53.29 Thu 16:00 Poster A

Adsorption study of terephthalic and benzoic acids on HOPG with Metastable Induced Electron Spectroscopy (MIES) — •Marcel Marschewski[1], Harun Tas[2], Christian F. Otto[2], Wolfgang Maus-Friedrichs[1], Andreas Schmidt[2], and Oliver Höfft[3] — [1]Institut für Energieforschung und Physikalische Technologien, Technische Universität Clausthal, Deutschland — [2]Institut für Organische Chemie, Technische Universität Clausthal, Deutschland — [3]Institut für Elektrochemie, Technische Universität Clausthal, Deutschland

The adsorption behavior of benzoic acids on conducting interfaces like HOPG is of high interest for the understanding of the building mechanism of 2D and 3D frameworks on surfaces. Thus, the knowledge about the molecular orientation and the molecule-substrate interaction is of great importance. Here we present our results on the adsorption of 4-substituted benzoic acids (R = hydroxy-, methoxy-, propoxy-, pentyloxy- and decyloxy-chains) and terephthalic acid (TPA) on HOPG. The molecular films were studied with Metastable Induced Electron Spectroscopy (MIES) and Ultraviolet Photoelectron Spectroscopy (UPS(HeI)). For the TPA monolayer we find hints for a more planar orientation of the molecules. The benzoic acid molecules show a similar adsorption behavior on HOPG. For the 4-(decyloxy) benzoic acid we assume a possible reorientation of the alkyl chains after the first monolayer.

DS 53.30 Thu 16:00 Poster A

The study of interaction, nonlinear and dissipation effects in nanomembranes by investigating the dispersion relations of bending waves — •Fan Yang, Elke Scheer, and Reimar Waitz — Universitaetsstrasse.10 Fach 681, 78457 Konstanz, Germany

Deciphering the mode shapes of vibrations of nanopatterned membranes is paving the way for applications of nanoscale membrane which rely on particular properties of vibrational excitations. The mode shape of bending waves in thin silicon, silicon carbide, silicon nitride and ultrathin carbon nanomembranes is measured as a function of space and time, using a phase-shift interferometer with continuous and stroboscopic light [1,2]. We develop a method to obtain the contribution of the membrane itself, the eigen-frequencies and the Q factor of the membrane. The contributions of a superposition of the mode corresponding to the excitation frequency and several higher harmonics can be separated and be imaged up to the eighth harmonic of the excitation frequency. We can determine the dispersion relation of membrane oscillations in a frequency range from ground mode up to 12 MHz. The study of the temperature-dependent vibration behavior reveals an unexpected temperature dependence of the mechanical properties of a prestressed nanomembrane. At variance to expectations based on classical continuum mechanics we observe that Young's modulus increases with increasing temperature.

[1] R. Waitz, et al., Phys. Rev. B 86, 039904 (2012).

[2] X. H. Zhang, et al., Appl. Phys. Lett. 2015, 106(6): 063107.

DS 53.31 Thu 16:00 Poster A

Growth of pinholes in metal electrodes of organic photovoltaic cells — •Daniel Fluhr[1], Burhan Muhsin[1], Rolf Öttking[1], Roland Rösch[1], Marco Seeland[2], and Harald Hoppe[1] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena) & Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Technische Universität Ilmenau, 98693 Ilmenau, Germany

Lifetime is still a major problem of organic photovoltaic (OPV) cells. There are many reasons for solar cell degradation varying from shunts induced by impurities or electromigration over photoinduced oxidation of active layer materials to corrosion and delamination of the metal contact both induced by oxygen or water ingress. One issue concerns so-called pinholes through the metal back electrode of the device. These pinholes offer pathways for ingress of water and oxygen which may attack the metal-organic interface by introducing delamination through formation of insulating metal oxides or hydrogen evolution. As charge injection and extraction is suppressed at delaminated areas, the active area taking part in power conversion - and hence the overall efficiency - becomes reduced. We investigated the influence of different environmental conditions on the reduction of the active area of the OPV cell. Spatially resolved measurements give information on location and size of insulated areas induced by pinholes in the metal back contact. Time resolved measurements during degradation of the devices revealed the dynamics and rate of growth of these individual defects.

DS 53.32 Thu 16:00 Poster A

Formation of noble metal thin films on P(VDF-TrFE) during DC-magnetron sputtering — Alexander M. Hinz[1], •Oleksandr Polonskyi[1], Franziska C. Löhrer[2], Volker Körstgens[2], Matthias Schwartzkopf[3], Stephan V. Roth[3], Peter Müller-Buschbaum[2], Thomas Strunskus[1], and Franz Faupel[1] — [1]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, 24143 Kiel, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [3]Deutsches Elektronensynchrotron DESY, 22607 Hamburg, Germany

In most devices using organic thin films as functional layers, e.g. organic solar cells, OLEDs or MEMS sensors, it is necessary to have an electrical contact with well-defined properties on these layers. This is often accomplished by depositing metallic electrodes onto the organic layers by physical vapour deposition (PVD) techniques. In order to control and predict the properties of the electrical contacts it is necessary to understand the interplay between the deposition process and the formation of the metallic electrodes. In this contribution we present the in-situ morphological characterization of Au thin film growth during the deposition by DC-magnetron sputtering onto P(VDF-TrFE). P(VDF-TrFE) is a versatile ferroelectric polymer used in many applications including transducers, actuators and sensors. The morphological information is obtained by grazing incidence small angle x-ray scattering (GISAXS). The in-situ information is compared with ex-situ information obtained by SEM.

DS 53.33 Thu 16:00 Poster A

Molecular order in dihexylsexithiophene thin film OFETs —

Nina Zeilmann[1], Hans-Georg Steinrück[2,3], Manuel Johnson[1], Andreas Magerl[2], and •Rainer Fink[1] — [1]FAU Erlangen-Nürnberg, Physical Chemistry 2, Erlangen, Germany — [2]FAU Erlangen-Nürnberg, LS Kristallografie, Erlangen, Germany — [3]present address: SSRL, Menlo Park, USA

The end-functionalized sexithiophene Hex6THex represents a benchmark molecule for organic electronic applications such as OFETs due to its high charge carrier mobility. The latter is mainly related to the high degree of molecular ordering and π-π-stacking within the films. We have employed several probes to investigate the morphologies, molecular order and orientations of such films (thicknesses around 10 layers) prepared by vacuum sublimation at various substrate temperatures on inert SiO2 or Si3N4 substrates. X-ray reflectivity (XRR) probes the vertical electron density distribution that provides information on the thickness and density of individual sublayers. In particular, XRR yields high quality data on the arrangements of both the hexyl functionalities and the thiophene backbone. It is found that the projected length of both film features critically depends on the substrate temperature during deposition. Based on the experimental results, a model proposing the molecular orientation of the Hex6THex molecules with respect to the substrate is derived. These results are in very good agreement with AFM and micro-NEXAFS studies. Some correlations to the electrical transport properties of the films are drawn.

DS 53.34 Thu 16:00 Poster A

Colloidal masking and ion-etched nanochannels on flexible thin foils — •Calvin Brett[1,2], Matthias Schwartzkopf[1], Stephan Roth[1], Michael A. Rübhausen[2], Patrick Kluth[3], Markus Bender[4], Daniel Severin[4], and Christina Trautmann[4] — [1]DESY, Notkestr. 85, 22607 Hamburg — [2]Universität Hamburg, Inst. f. Nanostruktur- und Festkörperforschung, CFEL, APOG, Univ. Hamburg, Luruper Chaussee 149, 22761 Hamburg — [3]Australian National University. Department of Electronic Materials Engineering, Research School of Physics and Engineering, The Australian National University, Canberra, ACT 2601 — [4]: GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, 64291 Darmstadt

The major issues in the fabrication of periodic nanostructure arrays are the high costs, low patterning speed, and small patterning area. Spray coating of polystyrene colloids (PS) and ion-etched nanochannels on a flexible, chemical resistance polymer (PDMS) thin foil, enable reusable soft masks for deposition and imprinting techniques. Spray coating leads to a self-assembled colloidal film, where every nanosphere can be used as lenses for lithographic fabrication methods. We prove the application principle and the morphology by scattering methods, contact angle analysis and spectroscopic imaging methods. This study offers a novel routine for cost effective nanofabrication which is wide applicable in nanoscale materials.

DS 53.35 Thu 16:00 Poster A

Organic thin film growth on exfoliated hexagonal boron nitride — •Jakob Alexander Genser[1], Markus Kratzer[1], Alexandar Matkovic[2], Rados Galic[2], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversität Leoben, Austria — [2]Institute of Physics, University of Belgrade, Serbia

Hexagonal boron nitride (h-BN) is a two-dimensional insulator. Especially in conjunction with graphene as ultrathin flexible electrode in organic electronics h-BN has great potential as 2D dielectric. Therefore, it is essential to understand organic thin film growth on h-BN.

Here, we use the organic semiconductor molecule para-hexaphenyl (6P) to study the growth of small, linear, conjugated molecules on h-BN. As substrates, exfoliated h-BN flakes transferred onto a SiO2 support is used. Submonolayer 6P thin films are prepared by vapor deposition in a hot wall epitaxy (HWE) system. The resulting thin film morphologies are investigated as a function of substrate temperature using atomic force microscopy. First results indicate that 6P forms needle like structures consisting of molecules with their long axes oriented parallel to the h-BN plane. The needles show preferential growth directions corresponding to the substrate symmetry.

DS 53.36 Thu 16:00 Poster A

Tailoring Bragg-gratings for light outcoupling of red top-emitting organic light-emitting diodes — •Paul-Anton Will[1], Cornelius Fuchs[1], Frank Boldt[2], Reinhard Scholz[1], Simone Lenk[1], and Sebastian Reineke[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — [2]Institut für Physik, Technische Universität Chemnitz, Germany

Introducing Bragg-gratings into OLED structures is a promising approach to increase the overall device efficiency. Here, scattering effects lead to a redistribution of internal modes, i.e. wave guided and/or surface plasmon polariton modes, with the benefit of an increased out-coupled mode fraction [1]. The overall emission characteristics of a device depend on the OLED properties like emitter spectrum, device layout, and optical micro cavity order, and also strongly on the shape, period, and height of the incorporated grating structure. We present a detailed analysis of the influence of one dimensional gratings on the emission of various red top-emitting OLEDs by using optical thin film simulations quantifying the emission from periodically perturbated optical micro cavities. AFM measurements of nanoimprinted Bragg-gratings serve as input for the optical simulations. This facilitates the comparison with experimental results from manufactured devices leading to first hints for optimal grating periods in relation to the vertical aspect ratios of the grating structure. Once the optimal parameters are found, the use of Bragg-gratings pose a cheap and up-scalable method to improve the OLED efficiency.

[1] T. Schwab *et al.*, Opt. Express 22, 7524-37, (2014)

DS 53.37 Thu 16:00 Poster A

Growth morphologies of a polar pentacene derivative on SiO$_2$ and graphene — •Benjamin Kaufmann[1], Markus Kratzer[1], Tony Lelaidier[2], Olivier Siri[2], Aleksandar Matković[3], Radoš Gajić[3], Conrad Becker[2], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversitaet Leoben, Franz Josef Straße 18, 8700 Leoben, Austria — [2]CINaM, Aix Marseille Université, Campus de Luminy Case 913, 13288 Marseille, France — [3]Institute of Physics, Department for Solid State Physics and New Materials, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

We investigated the growth morphologies of the polar organic molecule dihydrotetraazapentacene (DHTAP) on SiO$_2$ and exfoliated graphene. The morphology of ultra-thin films grown by hot wall epitaxy was analyzed using atomic force microscopy. The morphologies arising between 290K - 390K exhibit a strong temperature dependence and differ from those found for pentacene. Above substrate temperatures of 330K, the molecules tend to build curved, needle-like structures with lengths of 50nm - 1000nm and heights of a few nanometers. At lower growth temperatures, no needles are present as it is also the case for pentacene growth on SiO$_2$. On graphene, the islands are reduced in height compared to those grown on SiO$_2$. Also here, needle-like structures were found.

DS 54: Symposium on Frontiers of Electronic Structure Theory: Focus on Topology and Transport
(Joint symposium of DS, HL, MA, MM and O, organized by O)

Time: Friday 9:30–12:15 Location: H1

Invited Talk DS 54.1 Fri 9:30 H1

Intrinsic Transport Coefficients and Momentum Space Berry Curvatures — •Allan H MacDonald — University of Texas at Austin, Austin TX, USA

The response of a conductor to a bias voltage is normally dominated by repopulation of states near the Fermi level. The transport steady state is fixed by a competition between acceleration in an electric field and disorder-induced scattering which attempts to restore equilibrium. This response of observables to a bias voltage is therefore extrinsic. There is however also response of states away from the Fermi level, which are polarized by the electric field. Provided that the typical band separation is larger than the finite life-time uncertainty in Bloch state energies this response is intrinsic, and for some observables it can be dominant. Intrinsic response coefficients are attractive targets for electronic structure theory because they are readily evaluated. Examples of responses to bias voltages that are sometimes dominantly intrinsic are the anomalous Hall conductivity of ferromagnetic or antiferromagnetic conductors, the spin-Hall conductivity of heavy metals, and current-induced torques in heavy-metal/ferromagnet systems. Intrinsic transport coefficients tend to be large in crystals with large momentum-space Berry curvatures, for example in crystals with topologically non-trivial electronic structure, and remain finite when a gap opens at the Fermi level to eliminate the Fermi surface. I will discuss some important examples of transport coefficients that are dominated by intrinsic contributions, mentioning as an important case the quantum anomalous Hall effect.

Invited Talk DS 54.2 Fri 10:00 H1

Berry phase linked spin-orbit torques in Ferromagnetic and Antiferromagnetic systems — •Jairo Sinova — Johannes Gutenberg Universität Mainz, Staudingerweg 7, 55128 Mainz Germany

As current-driven torques are becoming more relevant in future MRAM technologies, in-plane current magnetization dynamics driven by the so called Rashba spin-orbit torques or through a combination of spin-Hall effect and spin-transfer torque has become more and more important. Understanding these torques is paramount to maximize their use. In recent experiments we have shown that in addition to the intrinsic SHE and STT effect there exists an intrinsic spin-orbit torque originating from the Berry phase of the spin-orbit coupled Bloch electrons analogous to the intrinsic spin Hall effect. This type of torques can be observed through SO-FMR driven experiments. We show this new type of toques in theory and experiments in GaMnAs and show that it can be of similar strength to the strong field-like torque. In addition, we extend these physics to a new type of order-parameter manipulation by currents by examining the combined effect of spin-orbit coupling and anti-ferromagnetic order. We show that in broken inversion symmetry anti-ferromagnets a current will induced a non-equilibrium Néel-order field that will act directly on the Néel order parameter, hence making the direct manipulation of anti-ferromagnets without auxiliary exchange biased coupling to other ferromagnets a new and exciting possibility. One of these type of Néel torques has been recently experimentally confirmed.

Invited Talk DS 54.3 Fri 10:30 H1

Transport in Topological Insulators and Topological Superconductors: In Search of Majorana Fermions — •Ewelina Hankiewicz — Wuerzburg University

Topological insulators (TIs) have a bulk energy gap that separates the highest occupied band from the lowest unoccupied band and the metallic gapless states at the edge [1]. Similarly, topological superconductors (TSC) have gapless zero energy states protected by the particle-hole symmetry, which in some cases form Majorana bound states. Here, we focus on the proximity-induced superconductivity in TIs [2] as well as on unusual properties of TSC [3] showing that they both can pave a road to find a Majorana state.

Concerning proximity-induced superconductivity in TIs, we describe a novel superconducting quantum spin-Hall effect, which is protected against elastic backscattering by combined time-reversal and particle-hole symmetry even in magnetic fields [2]. We discuss unusual transport properties of this effect and possible Majorana detection schemes.

Finally, we discuss new systems like TSC on the hexagonal lattices. We develop combined microscopic and macroscopic description of these materials that predicts realistic scanning tunneling microscopy signal in these superconductors [3]. Is there a way to measure Majorana state in these systems?

[1] G. Tkachov and E. M. Hankiewicz, Review in Phys. Status Solidi B 250, 215 (2013). [2] R. Reinthaler, G. Tkachov and E.M. Hankiewicz, Phys. Rev. B 92, 161303(R) (2015). [3] L. Elster, C. Platt, R. Thomale, W. Hanke, and E. M. Hankiewicz, Nature Comm. 6, 8232 (2015).

session break

Invited Talk DS 54.4 Fri 11:15 H1

Engineering Topological Quantum States: From 1D to 2D. — •Jelena Klinovaja — University of Basel, Switzerland

I will discuss low-dimensional condensed matter systems, in which topological properties could be engineered per demand. Majorana fermions can emerge in hybrid systems with proximity pairing in which the usually weak Rashba spin-orbit interaction is replaced by magnetic textures. I will discuss candidate materials such as semiconducting nanowires [1] and atomic magnetic chains [2]. One further goal is to go beyond Majorana fermions and to identify systems that can host quasiparticles with more powerful non-Abelian statistics such as parafermions in double wires coupled by crossed Andreev reflections [3,4]. Next, I will focus on 'strip of stripes model' consisting of weakly coupled one-dimensional wires [5-7], where interaction effects in the wires can be treated non-perturbatively via bosonization. Such systems can exhibit the integer or fractional quantum Hall effect, spin Hall effect, and anomalous Hall effect.

[1] J. Klinovaja and D. Loss, Phys. Rev. B 86, 085408 (2012). [2] J. Klinovaja, P. Stano, A. Yazdani, and D. Loss, Phys. Rev. Lett. 111, 186805 (2013). [3] J. Klinovaja and D. Loss, Phys. Rev. B 90, 045118 (2014). [4] J. Klinovaja, A. Yacoby, and D. Loss, Phys. Rev. B 90, 155447 (2014). [5] J. Klinovaja and D. Loss, Phys. Rev. Lett. 111, 196401 (2013); J. Klinovaja and D. Loss, Eur. Phys. J. B 87, 171 (2014). [6] J. Klinovaja and Y. Tserkovnyak, Phys. Rev. B 90, 115426 (2014). [7] J. Klinovaja, Y. Tserkovnyak, and D. Loss, Phys. Rev. B 91, 085426 (2015).

Invited Talk DS 54.5 Fri 11:45 H1

Skyrmions – Topological magnetization solitons for future spintronics — •Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Ultrathin magnetic films and heterostructures provide a fantastic playground for the stabilization, manipulation and usage of chiral magnetic skyrmions – topological magnetization solitons – magnetic entities described by a micromagnetic energy functional with particle like properties that may open a new vista for spintronics. A crucial quantity for the chiral skyrmion formation is the Dzyaloshinskii-Moriya interaction (DMI), whose presence in thin films could be established in a concerted effort of first-principles theory and spin-polarized scanning tunneling microscopy. It could be shown that the spin-orbit interaction and the structure inversion-asymmetry in these systems result in a DMI that is strong enough to give rise to one- and two-dimensional lattices of chiral spin-textures, chiral domain walls and even single skyrmions. In retrospect, it is surprising how little is known about the DMI in these metallic systems. In this talk I give insight into the DMI, relating first-principles calculations to different models, discussing the transport properties of electrons *e.g.* the topological (THE) and anomalous (AHE) Hall effect in relation to the spin texture of a skyrmion, and discuss possibilities to tailor the magnetic interactions to enlarge the materials base to stabilize single skyrmions. – I acknowledge fruitful collaborations with D. Crum, J. Bouaziz, B. Dupé, S. Heinze, N. Kiselev, S. Lounis, Y. Mokrousov, A. Nandy, and B. Zimmermann.

DS 55: Organic Thin Films III

Time: Friday 9:30–12:15 Location: H8

DS 55.1 Fri 9:30 H8

Donor-acceptor molecular interfaces in binary mixtures of organic semiconductors: Diindenoperylene(DIP):[hexafluoro]-tetracyanonaphtoquinodimethane([F6]-TCNNQ) vs Sexithiophene(6T):F6TCNNQ — •Giuliano Duva[1], Paul Beyer[2], Alexander Hinderhofer[1], Andreas Opitz[2], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen (Germany) — [2]Humboldt-Universität zu Berlin, Department of Physics, Brook-Taylor-Str. 6, 12489 Berlin (Germany)

Binary mixtures of organic semiconductors[1] involve formation of heterointerfaces between materials with different HOMO-LUMO energies. This may lead to partial or integer charge-transfer (CT) between the compounds in the form of either full ionization or frontier orbital hybridization[2]. The different size and shape of the molecular components has a great impact on the structure, leading to complex mixing scenarios from complete phase separation to mixed-crystal formation[1]. Overall, the mixing free energy can be expressed as a function of several parameters involving anisotropic interactions, implicitly taking into account the overlap between frontier orbitals. In this study we combine mixtures of DIP and [F6]TCNNQ with mixtures of 6T and F6TCNNQ in order to vary these parameters and study their impact on the CT. We demonstrate the formation of mixed co-crystal by X-ray scattering, whereas the corresponding CT states are probed by several spectroscopy methods (UV-Vis, IR, Raman).[1]A. Hinderhofer et al. Chem.Phys.Chem.13(2012);[2]H. Méndez et al. Nat.Comm.6(2015)

DS 55.2 Fri 9:45 H8

Correlating the donor/acceptor interface energetics with electronic dynamics in organic bilayer solar cells — •Michael Brendel[1], Essraa Ahmed[2], Iulia Minda[2], Heinrich Schwoerer[2], and Jens Pflaum[1,3] — [1]Exp. Physics VI, Julius-Maximilians-University Würzburg, D-97074 Würzburg — [2]Laser Research Institute, Stellenbosch University, ZA-7602 Matieland — [3]Bavarian Center for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

The crucial functional building block of any state of the art organic solar cell is the donor/acceptor (D/A) heterojunction. At this interface, the energetic offset of the frontier orbitals between donor and acceptor drives the dissociation of excitons into free charge carriers.

In this contribution we systematically tune the D/A interface energetics of bilayer cells by successive fluorination of the donor material zinc phthalocyanine, F_nZnPc (n = 0, 4, 8, 16). As evinced by ultraviolet photoelectron spectroscopy, upon fluorination energy levels of the donor are shifted towards lower energies with respect to the acceptor C_{60}. [1] The static picture of interface energetics is complemented by correlation with the excitonic and electronic dynamics accessed via ultrafast transient absorption spectroscopy. Exciton separation at the respective F_nZnPc/C_{60} interface takes place on fs-time scale, increasing in speed with increasing energetic offset at the D/A interface. After initial exciton dissociation, recombination dynamics of electrons in C_{60} remain almost unaffected by the D/A interface energetics on a ps-time scale. Financial support from SOLTECH and the DAAD.

[1] M. Brendel et al., Adv. Funct. Mater., 2015, 25, 1565.

DS 55.3 Fri 10:00 H8

Effects of Molecular Orientation in Acceptor-Donor Interfaces between Pentacene and C_{60} and Diels-Alder Adduct Formation at the Molecular Interface — •Tobias Breuer, Andrea Karthäuser, and Gregor Witte — AG Molekulare Festkörperphysik, Philipps-Universität Marburg

Interfaces between pentacene and Buckminster-Fullerene (C_{60}) have attracted interest due to their application as oligomeric model system for organic solar cells. As the actual device characteristics in such implementations are crucially controlled by the interface structure, detailed investigations of this interface on a molecular level are mandatory. Therefore, we have analyzed the influence of the orientation of the pentacene molecules in highly-ordered crystalline bottom layers on the characteristics of such interfaces. We show that the interface structure is driven by temperature-controlled diffusion of C_{60} molecules to the pentacene step-edges in the case of uprightly-oriented pentacene. For lying pentacene in the bottom layer, no step-edge decoration is observed and the wetting of the pentacene layer is enhanced. Furthermore, the stability of the interface against intercalation and re-orientation has been analyzed by means of NEXAFS spectroscopy, showing that the orientation of the pentacene molecules at the interface remains unchanged. Instead, we observe strong indication for a chemical modification of the molecular entities by the formation of Diels-Alder adducts between C_{60} and pentacene, which challenges the interpretation of this model system as chemically inert.

DS 55.4 Fri 10:15 H8

The energy level alignment at the interfaces of CoPc with ferromagnetic substrates studied by ultraviolet and inverse photoemission spectroscopies — •Jing Guo, Volodymyr Dzhagan, Georgeta Salvan, and Dietrich R.T. Zahn — Semiconductor Physics, Technische Universität Chemnitz, 09107 Chemnitz Germany

Metal-organic interfaces play a crucial role for the ever growing field of organic spintronics. Here the electronic structure of the interface between a CoPc thin film and Co or Ni foils as substrates is investigated by ultraviolet photoemission spectroscopy (UPS) and inverse photoemission spectroscopy (IPES). Both HOMO and LUMO positions of CoPc are noticeably dependent on the CoPc film thickness. Due to the image charge screening effect induced by the metallic substrate, the positions of LUMO and HOMO both shift towards lower binding energy at the interface. In addition, an interfacial state is supposed to form at the CoPc/Co interface, but not in the case of the CoPc/Ni interface. As a result, the transport band gap of CoPc on Co foil "opens" from (1.3±0.3) eV at 1 nm film thickness up to (2.2±0.3) eV above 6 nm film thickness. But for CoPc on Ni foil, its "opening" is much less pronounced from (1.9±0.3) eV to (2.2±0.3) eV. This different energetic behaviour at these interfaces is important for designing the electronic and spintronic devices.

DS 55.5 Fri 10:30 H8

The role of Induced Density of Interface States in the Interfacial Energy Level Alignment of PTCDA — •Mahdi Samadi Khoshkhoo[1], Heiko Peisert[1], Thomas Chassé[1,2], and Marcus Scheele[1,2] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 18, 72076 Tübingen, Germany — [2]Center for Light-Matter Interaction, Sensors & Analytics LISA+, University of Tübingen, Auf der Morgenstelle 15, 72076 Tübingen, Germany

We use various type of diverse substrates with different work functions and different coupling interactions to investigate the electronic structure of PTCDA using ultraviolet and X-ray photoelectron spectroscopy (UPS and XPS) as well as complementary electrostatic potential calculations. For thick enough layers of PTCDA, nearly unchanged injection barriers on all substrates are observed without any dependence on the type of substrate (unreactive, reactive or passivated metals and polymers). The Fermi level is observed to be strongly pinned at the charge neutrality level (CNL) of the organic semiconductor. For lower thicknesses of PTCDA, this universal Fermi level pinning is perturbed and differences in the work function of up to 0.8 eV are detected, depending on the nature of the substrate and the thickness. We find near-quantitative agreement between our experimental data and electrostatic potential calculations in the framework of an expanded model of induced density of interface states (IDIS). These results provide valuable information for the design and fabrication of PTCDA-based heterostructures.

15 min. break.

DS 55.6 Fri 11:00 H8

The energy levels in hole-doped molecular semiconductors — •Patrick Amsalem[1], Stefanie Winkler[1,2], Johannes Frisch[1], Martin Oehzelt[1,2], Georg Heimel[1], and Norbert Koch[1,2] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

Understanding the energy level alignment in doped organic thin films is crucial in order to achieve rational design in opto-electronic organic devices. Here, we rely on interface doping phenomena as occurring at electrode / buffer layer / organic semiconductor to hole-dope a ultra-thin film C60 [1]. The present system is investigated by direct and inverse photoemission measurements and theoretical calculations based on density functional theory. The obtained results reveal a picture which differs strongly from the traditionally conceived one, i.e. where the energy levels consist of singly occupied molecular states lying within the energy gap of the semiconductor [2]. Instead, here we demonstrate that the on-site Coulomb repulsion splits the partially unoccupied frontier molecular level in the p-doped systems into two sublevels [1]. The role of inter-site Coulomb interaction between molecular ions and neighbor molecules is further addressed and helps providing a complete picture of the electronic structure of molecular semiconductors in the presence of excess charges [1]. [1] S. Winkler, P. Amsalem, J. Frisch, M. Oehzelt, G. Heimel, N. Koch, Materials Horizons 2 (2015) 427. [2] J. L. Bredas and G. B. Street, Acc. Chem. Res. 18 (1985) 309.

DS 55.7 Fri 11:15 H8

Characterization of charge transfer in weakly interacting organic mixtures — •Valentina Belova[1], Alexander Hinderhofer[1], Alexander Gerlach[1], Frank Schreiber[1], Eduard Meister[2], Wolfgang Brütting[2], Paul Beyer[3], and Andreas Opitz[3] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Institut für Physik, Universität Augsburg, Germany — [3]Institut für Physik, Humboldt-Universität zu Berlin, Germany

To obtain a detailed understanding of the structural and energetic aspects of intermolecular interaction upon mixing we study the CT in thin films of DIP and PEN as donors and PDIR-CN2 and PDIF-CN2 as acceptors, which are relevant for organic electronic devices[1]. Mixing rigid rod-like materials (DIP, PEN) with a compound with flexible alkyl-chains (PDIR-CN2, PDIF-CN2) give rise to many different structural configurations between both species. Choosing the components in binary molecular mixtures[2] we adjust the energy gap between the donor HOMO level and the acceptor LUMO level. We characterize the CT of these mixtures upon electronic excitation (via PL and optical absorption) as well as at the ground-state (via FTIR) in combination with X-ray scattering to define the correlation with structural properties and anisotropic character of the CT.

[1] P.J. Jadhav et.al. Adv. Mater., 24, 6169 (2012); [2] A. Hinderhofer/F. Schreiber, ChemPhysChem, 13, 628 (2012)

DS 55.8 Fri 11:30 H8

Controlled UHV growth of organic-inorganic hybrid structures: Conjugated molecules on ZnO — •Mino Sparenberg[1], Anton Zykov[1], Jörg Megow[1], Viola Schmidt[1], Yves Garmshausen[2], Stefan Hecht[2], Stefan Kowarik[1], and Sylke Blumstengel[1] — [1]Humboldt Universität zu Berlin, Institut für Physik — [2]Humboldt Universität zu Berlin, Institut für Chemie

For the fabrication of inorganic-organic hybrid structures an understanding of the interaction at the interface is crucial. Therefore the growth of thin organic films is conducted in an all-UHV MBE system and analysed *in situ* via AFM and differential reflectance spectroscopy (DRS). The inorganic semiconductor examined here is epitaxially grown ZnO. Studied is the influence of chemical tuning on the growth process using the organic molecule *para*-sexiphenyl (6P). As promising candidate for usage in opto-electronic devices controlling the growth properties is critical [Phys. Rev. B, 2008, 77, 085323]. For this chemical tuning is used, as done for 6P by partial fluorination. We show that due to different terminal fluorination of 6P the growth mode could be drastically changed. Whereas symmetric fluorinated 6P-F_4 shows a smooth layer-by-layer growth [PCCP, 2014, 16, 26084], asymmetric 6P-F_2 possesses a static dipolar moment making it sensitive to the surface of ZnO. Furthermore the growth of PTCDI and NTCDA were investigated via DRS where the evolution of thin PTCDA films from monomer to aggregate was observed and successfully theoretically described [J. Phys. Chem. C 2015, 119, 5747] whereby for NTCDA the resonant overlap at the edge of ZnO is observed.

DS 55.9 Fri 11:45 H8

Organic-inorganic nanocomposites: nano-crystals of Au, Al and Ag in CuPcF4 organic molecular film — •Sergey Babenkov[1], Olga Molodtsova[1,2], Andrei Hloskovsky[1], Irina Aristova[3], Maxim Tchaplyguine[4], Ralf Nyholm[4], Karina Schulte[4], Denis Vyalikh[5], Oleg Vilkov[5], and Victor Aristov[1,3,6] — [1]DESY, Hamburg, Germany — [2]ITMO, Saint Petersburg, Russia — [3]ISSP RAS, Chernogolovka, Russia — [4]Max-lab, Lund, Sweden — [5]BESSY, Berlin, Germany — [6]TU Bergakademie, Freiberg, Germany

The morphology and electronic properties of nano-composite films based on blended aluminum, gold and silver nanoparticles into organic semiconductor of fluorinated copper phthalocyanine (CuPcF4) have been investigated by means of TEM and SR-PES measurements as function of nominal amount of metal deposition. TEM measurements reveal organic film with self-assembled nanoparticles, whose size and distribution are strongly correlated with nominal amount of deposited metal. Moreover, comparative study of electronic properties self-assembled nanoparticles detects strong interaction of metal atoms with organic substrate. This work was supported by the RFBR Grant No. 13 -02-00818 and the BMBF-Project No. 05K12GU2, PSP-Element No. U4606BMB1211.

DS 55.10 Fri 12:00 H8

μ-Photoluminescence studies on the interaction between charge carriers and excitonic states in organic semiconductors — •T. Ferschke[1], N.H. Hansen[1], T. Schmeiler[1], and J. Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Charge carrier – exciton interactions are of significant importance for the performance of organic opto-electronic devices.[1] Recently, it has been shown that the current density in an organic semiconducting matrix can be analyzed on nanometer length scales by means of the photoluminescence (PL) of single guest dye molecules.[2] Here, we transfer the aforementioned concept from single molecules to, technologically more relevant, molecular ensembles by utilizing μ-PL studies to characterize intentionally doped Tris(8-hydroxyquinolinato)aluminium (Alq3) organic light emitting diodes (OLEDs). For this purpose, Tetraphenyldibenzoperiflanthene (DBP) was embedded as dopant (0.1 wt%) via vacuum deposition at vertically defined positions within the Alq3 emitting layer. Upon applying a negative bias to the Ca/Al cathode, we observe an effective reduction in the PL of DBP by up to 14%. Varying the vertical position of the dopant and performing a 2D μ-PL-mapping we gain comprehensive information on the static and dynamic charge carrier characteristics within the recombination zone. These data provide insights in the microscopic mechanisms governing the two competing processes of PL quenching and electroluminescence.

[1] N.H. Hansen, *et al.*, *Phys. Rev. B*, **2013**, 87, 241202(R)

[2] M. Nothaft, *et al.*, *ChemPhysChem*, **2011**, 12, 2590–2595

DS 56: Focussed Session: Resistive Effects II

The phenomenon of "resistive switching" relates to the observation that in various materials the electrical resistance is not a material-specific constant, but that it can be modified by applying a voltage or current pulse. Within a microelectronic context this effect allows a resistive random access memory concept to generate highly scalable non-volatile memory elements. With silicon-based CMOS technology reaching the lower limit of scalability according to Moore's law, such concept has matured to a viable alternative with the potential to further reduce device area and power consumption. Suitable materials range from simple binary metal oxides to the higher chalcogenide based phase change materials. In a broader context the resistive property also renders a system reprogrammable and hence able to adapt to changing environments. In addition to the obvious potential for sensing applications this property is characteristic for systems which can be trained or learn. Thus, resistive elements have successfully been introduced into neural networks, which artificially mimic learning in the human brain.

Organizers: Sibylle Gemming (HZ Dresden-Rossendorf) and Peter Zahn (HZ Dresden-Rossendorf)

Time: Friday 9:30–11:45 Location: H11

Topical Talk DS 56.1 Fri 9:30 H11

Processes at the nanoscale: Recent progress in understandings on ReRAMs — •Ilia Valov — Forschungszentrum Jülich, PGI-7, 52425 Jülich, Germany

Since their re-discovery roughly 20 years ago the resistive switching memories (RRAM) turned out into one of the most exciting, innovative and multidisciplinary scientific field with a greatest potential for application in the nanoelectronics and information technology. Relating these systems to the missing memristor and pointing out the possible functionalities such as neuromorphic computing, non-volatile memories etc., pushed this topic to one of the highest priorities not only for the academic research but also for the nanoelectronics industry.

The present talk will focus on the processes at the nanoscale in memristive devices emphasizing the importance of understanding nanosize effects in order to design and control thin film device at the atomic scale. The recent achievements in the microscopic understandings of the physicochemical processes will be presented. The mobility of cations in VCM devices will be discussed in the light of bridging ECM and VCM mechanisms. The importance of interface dynamics, local charge concentration and distribution, the effects of moisture and in general the generic relevance of the counter charges will be highlighted. The nanobattery effect and its implications on both memristors theory and device stability and performance will be outlined on theoretical and experimental level.

The topic will be discussed in a more fundamental context of microscopic description of electrochemical processes at the atomic scale.

Topical Talk DS 56.2 Fri 10:00 H11

Tunnel junction based memristors as artificial synapses — •Andy Thomas — Leibniz Institute of Solid State and Materials Research (IFW Dresden), Institute for Metallic Materials, Dresden, Germany

The synapse is a crucial element in biological neural networks, but a simple electronic equivalent has been absent. This complicates the development of hardware that imitates biological architectures in the nervous system. Now, the recent progress in the experimental realization of memristive devices has renewed interest in artificial neural networks. The resistance of a memristive system depends on its past states and exactly this functionality can be used to mimic the synaptic connections in a (human) brain [1].

We prepared magnesia, tantalum oxide and barium titanate based junction structures and investigated their memristive properties. We increased the amplitude of the resistance change from 10% up to 100%. Utilizing the memristive properties, we looked into the use of the junction structures as artificial synapses. We observed analogs of long-term potentiation, long-term depression and spike-time dependent plasticity in these simple two terminal devices [2]. Finally, we prepared these junctions on top of an integrated neuromorphic circuit to store analog synaptic weights and and support the implementation of biologically plausible learning mechanisms in the future.

[1] A. Thomas, J. Phys. D: Apple. Phys. 46 (2013) 093001

[2] A. Thomas et al., Frontiers in neuroscience 9 (2015) 241

15 min. break.

DS 56.3 Fri 10:45 H11

Metastable states of HfO_2 suboxides and resistive switching — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Resistive random access memories (RRAM) are considered the next generation of memory devices, which combine the operation speed of volatile DRAM and the nonvolatile ability of flash technology in one device with good scalability. Materials used for RRAM should be compatible with silicon technology. One of these materials is hafnia (HfO_2), thin films of which have valence change memory properties. With the aim of shining light on the filamentary initial state of the memory cell after electroforming we will present results of a study of the Hf-O system combining an evolutionary-algorithm [1] for structure prediction with density functional theory. The main focus is given to suboxides in close vicinity of the HfO_2 ground state, in order to search for possible metastable structures in oxygen deficient conditions. We find metastable crystalline structures, which could occur in the electroforming process and allow for a reversible resistive switching. The obtained structures favor ionic conductivity of oxygen. We characterise electronic and vibrational properties of these phases in order to compare them with experimental data.

We acknowledge financial support by the Helmholtz Young Investigators Group Programme VH-NG-409 and by the DFG through the SFB917 (Nanoswitches).

[1] http://uspex.stonybrook.edu

DS 56.4 Fri 11:00 H11

Avalanche-discharge-induced electrical forming in Ta_2O_5 based MIM structures — •Katharina Skaja[1], Christoph Bäumer[1], Oliver Peters[1], Stephan Menzel[1], Marco Moors[1], Hongshu Du[1,2], Manuel Bornhöfft[1,2,3], Chun-Lin Jia[1,2], Joachim Mayer[2,3], Rainer Waser[1,4], and Regina Dittmann[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich , Germany — [2]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, 52425 Jülich , Germany — [3]Central Facility for Electron Microscopy, RWTH Aachen University, 52056 Aachen , Germany — [4]Institute of Materials in Electrical Engineering and Information Technology II, RWTH Aachen University, 52056 Aachen , Germany

We investigated the resistive switching characteristics of Pt/ Ta_2O_5/Ta cells prepared by sputtering. Structural changes in the top electrode develops during the electrical forming process, which can be correlated to the formation of a dendrite-like conductive structure, which is induced by an avalanche discharge between the top electrode and the Ta_2O_5 layer, which occurs instead of a local breakdown between top and bottom electrode. The dendrite-like structure evolves primarily at structures with a pronounced interface adsorbate layer. Local conductive atomic force microscopy reveals that the entire dendrite region becomes conductive. We demonstrate by in-situ spectromicroscopy that the subsequent switching is caused by a valence change between Ta^{4+} and Ta^{5+}, which takes place over the entire former Pt/ Ta_2O_5 interface of the dendrite-like structure.

DS 56.5 Fri 11:15 H11

KKRnano: A Massively Parallel KKR Green's Function Code for Large Scale Systems — •Marcel Bornemann, Rudolf Zeller, Roman Kovacik, and Stefan Blügel — Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The advent of exascale supercomputers may enable researchers to perform electronic structure calculations for systems that exceed the realm of conventional solid state physics and reach deep into the field of material sciences. In Jülich, we developed the KKRnano code [1] to facilitate the research of systems containing up to 10000 atoms and beyond. This ability is crucial to the study of effects of chemical and structural disorder, doping, single and line defects in various materials which are, from a theoretical point of view, insufficiently understood so far. In KKRnano we apply the Korringa-Kohn-Rostocker Green's function method that is already widely used in computer programs aiming at smaller system sizes. By extending its theoretical framework we were able to come up with a code whose requirements for computational resources, e.g. memory and CPU time, scale linearly with system size. In the past we have applied KKRnano 1.0 to phase change materials [2]. Currently we are developing KKRnano 2.0 that we plan to apply to oxide systems in conjunction with the understanding of the switching behavior of VCM type ReRAM.

This work is supported by the DFG via SFB 917.

References: [1] A. Thiess et al., Phys. Rev. B 85 , 235103 (2012), [2] W. Zhang et al., Nature Materials 11, 952 (2012)

DS 56.6 Fri 11:30 H11

Bipolar resistive switching of p-$YMnO_3$/n-$SrTiO_3$:Nb junctions — •Agnieszka Bogusz[1,2], Daniel Blaschke[1], Barbara Abendroth[3], Ilona Skorupa[1], Danilo Bürger[2], Oliver G. Schmidt[2,4], and Heidemarie Schmidt[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [2]Material Systems for Nanoelectronics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [3]Institute for Experimental Physics, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [4]Institute for Integrative Nanosciences, IFW-Dresden, 01069 Dresden, Germany

Resistive switching (RS) phenomena of oxides in metal-insulator-metal structures have been widely investigated due to promising applications as a non-volatile memory and in neuromorphic circuits. In our previous works, we have demonstrated unipolar RS of $YMnO_3$-based structures [1]. This work investigates the non-volatile RS switching in Au/$YMnO_3$/Nb:$SrTiO_3$/Al structures with (p-$YMnO_3$)-(n-Nb:$SrTiO_3$) junctions. The $YMnO_3$ films are deposited by pulsed laser deposition on the (100)-$SrTiO_3$ doped with 0.5 wt.% of Nb substrates and exhibit bipolar RS. Observed RS behavior is assigned to the coupled electronic and ionic processes which depend on the depletion layer extension in the p-n junction. Exploitation of RS in p-n junctions offers additional functionalities of memristive devices, e.g. related to their optical properties.

[1]A. Bogusz et al., AIP Advances 4 (2014), A. Bogusz et al., Adv. Mater. Res. 1101 (2015).

DS 57: Topological Insulators II (Joint session of DS and HL, organized by HL)

Time: Friday 9:30–12:00 Location: H15

DS 57.1 Fri 9:30 H15

Signatures of induced superconductivity in a p-n heterostructure comprised of Sb_2Te_3 and Bi_2Te_3 3D topological insulator thin films with in situ Al capping — •Peter Schüffelgen[1], Daniel Rosenbach[1], Martin Lanius[1], Jörn Kampmeier[1], Gregor Mussler[1], Markus Eschbach[1], Ewa Mlynczak[1], Lukasz Plucinski[1], Martina Luysberg[1], Stefan Trellenkamp[1], Martin Stehno[2], Prosper Ngabonziza[2], Alexander Brinkman[2], Yuan Pang[3], Li Lu[3], Thomas Schäpers[1], and Detlev Grützmacher[1] — [1]Peter Grünberg Institut and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]TNW and MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands — [3]Laboratory for Solid State Quantum Information and Computation, Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China

We investigate the transport properties of Sb_2Te_3/Bi_2Te_3 p-n heterostructure topological insulator film-superconductor junctions. The films are grown by means of molecular beam epitaxy on a Si (111) substrate and capped *in-situ* by a thin layer of aluminum to prevent thin film degradation and to preserve the Dirac-like surface states. Josephson junctions are defined by depositing two niobium electrodes, separated by a few tens of nanometers, onto the Sb_2Te_3/Bi_2Te_3 layer. The transport measurements at cryogenic temperatures showed signatures of Andreev reflections and Josephson supercurrents. For wider junctions a Fraunhofer pattern was observed for the critical current, whereas for the narrow junctions a monotonous decrease was found.

DS 57.2 Fri 9:45 H15

Teraherz-Induced Chiral Edge Photogalvanic currents in 2D HgTe Topological Insulators — •Kathrin-Maria Dantscher[1], Dimitry A. Kozlov[2], Maria-Theresia Scherr[1], Sebastian Gebert[1], Vasily V. Bel'kov[3], Nikolay N. Mikhailov[2], Sergey A. Dvoretskii[2], Ze Dong Kvon[2], and Sergey D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Institute of Semiconductor Physics, Novosibirsk, Russia — [3]Ioffe Institute, St. Petersburg, Russia

We report on the observation of a chiral photogalvanic current generated in the topological protected edge states of 2D topological insulators fabricated on the basis of 8 nm thick HgTe quantum wells. Illuminating the sample with circularly polarized terahertz radiation and picking-up the signal along the edges we detected a photocurrent whose direction reverses by switching radiation polarization from right- to left-handed one. The influence of the magnetic field, the temperature and the angle of incidence of the radiation to these photocurrents are investigated. We demonstrate that circularly polarized radiation, which, according to selection rules, excites only electrons with a certain spin, results in an imbalance of electron distribution in the k-space and causes a spin polarized electric current.

DS 57.3 Fri 10:00 H15

temperature induced shift of the chemical potential of Bi2Te2Se tetradymite topological insulators — •jayita nayak[1], gerhard h fecher[1], siham quardi[1], chandra sekhar[1], claudia felser[1], christian tusche[2], shigenori ueda[3], and eiji ikenaga[4] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden — [2]Max Planck Institute of Microstructure Physics, Halle — [3]Synchrotron X-ray Station at SPring-8National Institute for Materials Science, Hyogo 679-5148, Japan — [4]Japan Synchrotron Radiation Research Institute, SPring-8, Hyogo, 679-5198, Japan

The temperature dependent HAXPES spectra of Bi2Te2Se reveal the appearance of an additional spectral feature above the band gap at low temperature. It appears at 20 K but is absent in the 300 K spectra and the onset of the main features of the spectra is shifted to lower energies. Momentum resolved photoemission electron microscopy (k-PEEM)was carried out using in order to explain the origin of the additional spectral feature. The measurement provides the evidence of the evolution of bulk bands at low temperature which is caused by the shift of the chemical potential. The bulk sensitive HAXPES valence band spectra are in perfect agreement with first principles calculations.

DS 57.4 Fri 10:15 H15

Optical investigation of the three-dimensional Dirac semimetals $CaMnBi_2$ and $SrMnBi_2$ — •Micha B. Schilling[1], Artem V. Pronin[1], Martin Dressel[1], and Youguo Shi[2] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China

The interest in the measurements of optical conductivity in three-dimensional Dirac semimetals is based on the recent theoretical studies [1, 2], where the interband optical response of such systems has been shown to be very peculiar. Namely, the real part of the interband optical conductivity has been predicted to be linear in frequency with the slope being related to the Fermi velocity of Dirac electrons.

We investigated the optical properties of the three-dimensional Dirac semimetals $CaMnBi_2$ and $SrMnBi_2$ by means of Fourier-transform infrared spectroscopy. We measured the reflectivity over a frequency range from 50 to 25000 cm^{-1} at different temperatures down to 10 K and determined the optical conductivity from these measurements. In the presentation, we will discuss our results on the optical conductivity in comparison with theoretical predictions.

[1] P. Hosur, S. A. Parameswaran, and A. Vishwanath, Phys. Rev. Lett. **108**, 046602 (2012). [2] A. Bácsi and A. Virosztek, Phys. Rev. B **87**, 125425 (2013).

30 min. Coffee Break

DS 57.5 Fri 11:00 H15

Optoelectronic dynamics in nanocircuits based on the topological insulator Bi2Te2Se — •Mariana Hettich[1], Paul Seifert[1], Christoph Kastl[1], Kristina Vaklinova[2], Marko Burghard[2], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, D-85748 Garching, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

We report on the optoelectronic dynamics in nanocircuits made of the topological insulator Bi2Te2Se. An on-chip photocurrent pump-probe spectroscopy based on coplanar striplines allows us to identify the different ultrafast photocurrent mechanisms in topological insulators with a picosecond time resolution. We discuss non-equilibrium thermal effects as well as the circular photogalvanic current generation as contributions to the overall photocurrent.

DS 57.6 Fri 11:15 H15

Structural Study of Weak Topological Insulator Bi_1Te_1 Films on Si(111) grown by Molecular Beam Epitaxy — •Martin Lanius[1], Markus Eschbach[1], Ewa Mlynczak[1], Jens Kellner[2], Pika Gospodaric[1], Chengwang Niu[1], Elmar Neumann[1], Martina Luysberg[3], Gregor Mussler[1], Lukasz Plucinski[1], Gustav Bihlmayer[1], Stefan Blügel[1], Markus Morgenstern[2], Claus Michael Schneider[1], and Detlev Grützmacher[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [2]II. Institute of Physics B and JARA-FIT, RWTH Aachen University, Aachen, Germany — [3]Ernst Ruska-Centre for Microscopy and Spectroskopy with Electrons, Forschungszentrum Jülich, Germany

We have studied the nucleation, growth process and structural composition of the weak topological insulator Bi_1Te_1 on Si(111) substrates by STM and STEM. Bi_1Te_1 is a superlattice of predicted 2D topological insulating materials, one bilayer Bi and two Bi_2Te_3 quintuple layers per unit cell. The van der Waals growth mode of Bi_1Te_1 shows smooth surfaces and a supressed twin domain density. The thin films from several nanometers thickness down to the nucleation regime have been grown by molecular beam epitaxy. STEM measurements of the grown films reveal a high crystalline perfection. Simulations and ARPES measurements show 2D surface states originating from spin-orbit coupling, depending in their structure on the surface termination. Furthermore we will demonstrate the ability to grow n-p heterostructures of n-doped Bi_1Te_1 with the p-doped strong TI Sb_2Te_3.

DS 57.7 Fri 11:30 H15

Bi2Se3-based heterostructures including magnetic layers: the case of n-QLs Bi2Se3 ontop of Mn-doped Bi2Se3 — •J.

Honolka[1], M. Valiska[2], J. Warmuth[3], M. Michiardi[4], M. Vondracek[1], A. S. Ngankeu[4], V. Holy[2], M. Bianchi[4], G. Springholz[5], V. Sechovsky[2], P. Hofmann[4], and J. Wiebe[3] — [1]Institute of Physics, ASCR, Prague, CZ — [2]Department of Condensed Matter, Charles University, Prague, CZ — [3]INF, University of Hamburg, Hamburg, DE — [4]Department of Physics and Astronomy, iNANO, University of Aarhus, Aarhus, DK — [5]Institute of Semiconductor Physics and Solid Solid State Physics, Johannes-Kepler University, Linz, AT

Interfaces between ferromagnetic and non-magnetic Bi2Se3 phases are studied as a material platform to investigate the influence of spin degrees of freedom on 3D topological insulator (TI) properties.

An inverted geometry of n quintuple layers (QLs) Bi2Se3 ontop of Mn-doped Bi2Se3 is achieved by molecular beam epitaxy for n=0 to n=24 QLs and allows to unhamperedly monitor the development of electronic and topological properties by surface sensitive key techniques like angular resolved photoemission spectroscopy. A gap at the Dirac point is observed at small n, which is gradually filled with increasing n. The Dirac point is fully reestablished at about n = 9 QLs. Band bending effects due to the proximity of the interface with the ferromagnetic layers are discussed.

DS 57.8 Fri 11:45 H15

Observation of gapped surface states in the topological regime of the quantum-phase transition in Bi-doped Pb-Sn-Se (111) epitaxial films — •Partha Sarathi Mandal[1], Gunther Springholz[2], Valentyn Volobuev[2], Günther Bauer[2], Evangelos Golias[1], Andrei Varykhalov[1], Jaime Sa'nchez-Barriga[1], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Institut für Halbleiter und Festkörperphysik, Johannes Kepler Universität, Linz, Austria

Topological crystalline insulators are believed to show a straight forward and versatile connection between mirror symmetries and gap opening at the surface Dirac points. Here we systematically studied the trivial-to-topological insulator phase transition [1] of the $\mathrm{Pb}_{1-x}\mathrm{Sn}_x\mathrm{Se}(111)$ surface grown by molecular beam epitaxy and using angle-resolved photoemission spectorscopy (ARPES) under variation of Sn concentration (10 to 28%) and temperature. Differently from the case of the (001) surface [2], we observe two types of Dirac cones centered at $\overline{\Gamma}$ and $\overline{\mathrm{M}}$ in the surface Brillouin zone. By comparing the band structure of samples with fixed Sn concentration and different Bi doping, we demonstrate the existence of gapped surface states within the topological regime of the quantum-phase transition at low temperatures [1].

[1] Y. Ando and L. Fu Annual Review of Condensed Matter Physics Vol. 6: 361-381 (2015). [2] Y. Tanaka, T. Shoman, K. Nakayama, S. Souma, T. Sato, T. Takahashi, M. Novak, Kouji Segawa, and Yoichi Ando PHYSICAL REVIEW B 88, 235126 (2013).

DS 58: Organic Electronics and Photovoltaics III (Joint session of CPP, DS, HL and O, organized by CPP)

Time: Friday 9:30–12:00 Location: H40

DS 58.1 Fri 9:30 H40

Influence of order and disorder on some photovoltaic properties of AnE-PV polymers - a DFT study — •Chuan-Ding Dong and Wichard J. D. Beenken — Institut für Physik und Institut für Micro- und Nanotschnologie, Technische Universität Ilmenau, Germany

Recently, the copolymer poly(p-anthraceneethynylene-alt-poly(p-phenylenevinylene) (AnE-PV) has turned out to be a promising model for the effect of order and disorder in polymer-based solar cells.[1] By substituting linear octyl or branched 2-ethyl-hexyl sidechains to the conjugated backbone, the structure of AnE-PV can be tuned from order to disorder. Using Grimme's correction for dispersion in our DFT calculations, we will show that the van-der-Waals interaction between the sidechains influences the planarity of the conjugated backbones significantly. Consequently, we found order-dependent shifts of the respective absorption spectra, which are in agreement with the experimental data. Furthermore, we will demonstrate the effect of the alternative sidechain substitution on the stacking of AnE-PV copolymers to semi-crystalline aggregates, which is crucial for the efficiency of polymer solar cells.

[1] Kästner, C.; Egbe, D.; Hoppe, H.: *J. Mater. Chem. A* **3**(2015)395.

DS 58.2 Fri 9:45 H40

Influence of surface characteristics on electronic properties of polymer thin films — •Philipp Ehrenreich, Susanne Birkhold, Alexander Graf, Eugen Zimmermann, Hao Hu, Kwang-Dae Kim, and Lukas Schmidt-Mende — Department of Physics, University of Konstanz, POB M 680, Konstanz 78457, Germany

Many applications in polymer electronics demand not only for a lossfree charge percolation pathway towards electrodes, but also a highly delocalized pi-orbital system for efficient charge generation after exciton dissociation. The latter is especially important for the development of all-polymer solar cells, in order to compete with fullerene-based devices. Within this work the influence of surface characteristics on structural, or rather electronic properties of polymer thin films is investigated by means of an H/J-aggregate analysis on the model polymer Poly(3-hexylthiophene).

DS 58.3 Fri 10:00 H40

Quantum Molecular Dynamical Calculations of Poly(3,4-ethylenedioxythiophene) and its derivatives — •Amina Mirsakiyeva, Håkan W. Hugosson, and Anna Delin — KTH Royal Institute of Technology, Department of Material and Nanophysics, SE-16440, Sweden

Organic thermoelectrics (TE) are materials with the ability to produce an electrical current from a temperature gradient (the so-called Seebeck effect) and the advantages of organic compounds, such as less toxicity. Organic TE are based on conductive polymers where the conjugation between double and single bonds creates the π-bonds overlapping and consequently allows charge carriers transport along the polymer backbone. Up to this date, the most studied organic TE material is poly(3,4-ethylenedioxythiophene) (PEDOT). Its transparency, high stability in the oxidized state and ability to form water-soluble polyelectrolytes bring it to the leading position in industry. The success of PEDOT makes also its selenium (PEDOS) and tellurium (PEDOTe) derivatives promising thermoelectric materials. Here, we present theoretical calculations of PEDOS and PEDOTe. We determined structures of the polymer chains of PEDOS and PEDOTe, investigated HOMO and LUMO and calculated point-charge distributions along the polymer backbone. Our analysis aims at finding the localization of a polaron, i.e. the electronic excitation resulting in localized structural changes and charge accumulation. Such a deeper atomistic understanding of the processes inside thermoelectric materials will hopefully allow an improvement of the thermoelectric qualities of conductive polymers.

DS 58.4 Fri 10:15 H40

How Morphology Affects the Charge Transport: A Case Study for C60 — •Sebastian Schellhammer[1,2,3], Frank Ortmann[1,2], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science, Technische Universität Dresden, 01062 Dresden, Germany — [3]Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany

The performance of organic electronic devices is significantly influenced by the morphology of the individual layers. However, theoretical studies can cover mostly only highly ordered or completely amorphous systems.

We present a computational algorithm for the construction of arbitrarily ordered films ranging from amorphous to polycrystalline and highly crystalline. We demonstrate its application for a systematic study of the electron mobility in C60 systems depending on the degree of ordering which is based on a full parameterization of the electronic properties. Additionally, we present a generalization for other molecular materials such as pentacene as well as organic blends.

DS 58.5 Fri 10:30 H40

Intermolecular hopping transfer between DPP-based donor-acceptor polymers: A first principle study — •Florian Günther[1,2], Sibylle Gemming[1,3], and Gotthard Seifert[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Physical Chemistry and Electrochemistry, Dresden University of Technology, Dresden, Germany — [3]Institute of Physics, Technical University Chemnitz, Germany

Diketopyrrolopyrrole (DPP) based materials have recently been considered as promising candidates for novel organic electronics. Here, we report about our investigation on intermolecular charge transfer between DPP-based polymers. We utilize Marcus transfer theory and evaluate the required quantities, the reorganisation energy and the coupling, by density functional-based tight binding (DFTB) calculations.. Due to its computational efficiency as well as the opportunity to tune some calculation features, the DFTB method is well suited for this purpose. In doing so, the coupling elements have been calculated for various stacking formations. In order to derive a single quantity, which can been used for calculate the transfer rates, an energy-weighted statistical approach has been utilised.

The obtained values allow to analyse the charge carrier mobilities in dependence of isomeric effects as the orientation of the individual units, of the molecular structure as fuctionalization, or the meaning of stacking properties as parallel and anti-parallel.

15 min. break

DS 58.6 Fri 11:00 H40

Comparison of electrostatic, inductive and dispersive excitation energy shifts for the example of a molecular crystal — •Jörg Megow — University of Potsdam, Germany

The description of dispersive excitation energy shifts is necessary whenever different molecules within a supramolecular aggregate experience a different environment. A new approach that is based on an extended dipole approximation for higher transition densities in the sum over states expression [1] allowed for an appropriate description of gas-to-crystal-shifts in thin 3,4,9,10-perylenetetracarboxylic diimide (PTCDI) films [2]. It was also possible to explain the splitting of the main bands in the UV/Vis spectrum of double-walled tubular cyanine aggregates [3] as well as the line shift and broadening of the measured UV/Vis spectrum of pheophorbide *a* dendrimers [4]. For the example of a PTCDI crystal the different contributions to the overall site energy shifts are calculated while approximating the sum over states expressions for the energy shifts due to dispersion and inductive polarization, respectively. It is shown that the dispersive site energy shift dominates the site energy shifts due to electrostatic interaction and inductive polarization.

[1] A. Stone, *The theory of intermolecular forces*, Oxford University Press (2013); [2] J. Megow, T. Körzdörfer, T. Renger et al., J. Phys. Chem. C 119, 5747-5751 (2015); [3] J. Megow, M. I. S. Röhr, M. Schmidt am Busch et al., PCCP 17, 6741-6747 (2015); [4] J. Megow, ChemPhysChem 16, 3101-3107 (2015)

DS 58.7 Fri 11:15 H40

Efficient first-principles based screening for high charge carrier mobility in organic crystals — •Christoph Schober, Karsten Reuter, and Harald Oberhofer — Technische Universität München

In organic electronics, charge carrier mobility is a key performance parameter. Due to the complex manufacturing processes of e.g. organic field effect transistors (OFETs) measured mobilities are often heavily affected by the device preparation. This masks the intrinsic materials properties and therewith hampers the decision whether further device optimization for a given organic molecule is worthwhile or not. We developed a fast and efficient protocol with a descriptor based on electronic coupling values to assess the expected performance of organic materials for application in organic electronic devices. Applying this protocol to experimental structures of organic crystals obtained from the Cambridge Structural Database (CSD), we screened about 40000 structures employing only first principle methods. Out of the 28000 successfully calculated structures we selected 2000 candidates with above- average electronic couplings for additional calculations and in-depth analysis using statistical methods and automated classification based on chemical structure. This allowed us not only to identify a number of specific crystals with exceptionally high electronic coupling values and therefore promising properties, but also possible lead structures which can be the basis for in-depth theoretical and experimental studies of new classes of materials for organic electronics.

DS 58.8 Fri 11:30 H40

In-situ x-ray investigation of the structure formation of metal films on photoactive polymers — •Franziska C. Löhrer[1], Volker Körstgens[1], Matthias Schwartzkopf[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Deutsches Elektronensynchrotron DESY, 22607 Hamburg, Germany — [3]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, 24143 Kiel, Germany

Photoactive polymers have received high attention in recent years due to a large variety of different applications in molecular electronics. Although organic materials are used in the active layers of these devices, typically in many cases the electrodes are still made from metals. Thus, the polymer-metal interfaces are inherently present in all these novel devices. Our work takes a deeper look at the morphology of interfaces between photoactive layers and metal contacts deposited on top of them. We investigate morphological changes during sputter deposition of metal films (electrodes) onto photoactive films using in-situ GISAXS. Probing the sputter process in-situ allows highly time resolved insights into the deposition behavior of the metal depending on the polymer layer's properties. The deposition behaviors of gold and aluminium are compared, as both metals are frequently used as electrodes. The photoactive films consist of the low band gap polymer PTB7 as well as of PTB7:PCBM blends. The final film morphology is characterized via SEM and XRR after sputter deposition.

DS 58.9 Fri 11:45 H40

Charge-Transfer - Solvent Interaction Predefines Doping Efficiency in p-Doped P3HT-Films — •Lars Müller[1,2,6], Diana Nanova[1,2,6], Tobias Glaser[2,6], Sebastian Beck[2,6], Annemarie Pucci[2,6], Anne K. Kast[3,6], Rasmus R. Schröder[3,4,6], Eric Mankel[5,6], Robert Lovrincic[1,6], and Wolfgang Kowalsky[1,2,6] — [1]IHF, TU Braunschweig — [2]KIP, Heidelberg University — [3]BioQuant, Heidelberg University — [4]CAM, Heidelberg University — [5]Surface Science Division, TU Darmstadt — [6]InnovationLab, Heidelberg

Doping of organic semiconductors is a prerequisite for the production of efficient devices such as organic light emitting diodes. Numerous recent publications reveal new insights on doping mechanisms and charge transfer, emphasizing the need for further investigations, especially on polymer systems. In this work, we study p-type doping of poly(3-hexylthiophene) (P3HT) with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ), spin coated from the solvents chlorobenzene or chloroform. We find that films prepared from chloroform show a higher conductivity than films prepared from chlorobenzene. To clarify this unintuitive behavior, electron diffraction is used to reveal differences in the structural order within films from the two solvents. Additionally, UV-Vis and infrared spectroscopy help to expand the view to electronic properties such as vibrational or polaronic absorptions. It turns out that structural order and electronic properties in doped films are predefined by the interaction of the solvent with charge-transfer complexes already in solution.