Thin Films Division
Fachverband Dünne Schichten (DS)

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Overview of Invited Talks and Sessions

(Lecture rooms: CHE 89, CHE 91, and HSZ 02; Posters: P1)

Gaede Prize Talk

DS 26.1	Wed	12:30–13:00	HSZ 02	**Spectroscopy and microscopy of graphene on metals** — •Yuriy Dedkov

Invited Talks

DS 4.1	Mon	15:00–15:30	CHE 91	**Interfaces of archetype magnetic molecules: from interface dipoles to charge and spin transfer** — •Martin Knupfer
DS 9.1	Tue	9:30–10:00	CHE 91	**Chalcopyrite semiconductors: atomic-scale structure and band gap bowing** — •Claudia S. Schnohr, Stefanie Eckner, Helena Kämmer, Tobias Steinbach, Martin Gnauck, Andreas Johannes, Christian A. Kaufmann, Christiane Stephan, Susan Schorr
DS 9.2	Tue	10:00–10:30	CHE 91	**Polarized mid-infrared spectroscopy of split-ring resonators and metal nanoparticle-organic hybrids** — •Thomas W.H. Oates, Dimitra Gkogkou, Timur Shaykhutdinov, Tolga Wagner, Karsten Hinrichs
DS 11.1	Tue	9:30–10:00	CHE 89	**Giant magnetoelectric thin film composites** — •Andre Piorra, Robert Jahns, Enno Lage, Christine Kirchhof, Erdem Yarar, Volker Röbisch, Dirk Meyners, Reinhard Knöchel, Eckhard Quandt
DS 11.6	Tue	11:15–11:45	CHE 89	**Carbon nanotubes for piezoresistive electro-mechanical transducers incorporating a wafer-level technology** — •Sascha Hermann, Alexey Shaporin, Jens Bonitz, Steffen Hartmann, Jana Kalbacova, Raul D. Rodriguez, Dietrich R.T. Zahn, Jan Mehner, Bernhard Wunderle, Stefan E. Schulz, Thomas Gessner
DS 11.9	Tue	12:15–12:45	CHE 89	**Integration of individual SWCNTs into field-effect transistor-based sensors** — •Miroslav Haluska, Wei Liu, Kiran Chikkadi, Matthias Muoth, Tobias Suss, Stuart Truax, Cosmin Roman, Chrisofer Hierold
DS 16.1	Tue	14:00–14:30	CHE 89	**Carbon Wonderland from an Engineering Perspective** — •Franz Kreupl, Stefan Kapser, Sebastian Hübner
DS 24.1	Wed	9:30–10:00	CHE 89	**Scaling limits and future prospects of resistive switching devices: From materials to systems** — •Victor Zhirnov
DS 25.1	Wed	11:15–11:45	CHE 89	**Nanoscale redox-processes in resistive switching oxide devices** — •Regina Dittmann
DS 34.1	Wed	18:30–19:00	CHE 89	**Materials engineering for phase change memory** — •Simone Raoux, Huai-Yu Cheng
DS 37.1	Thu	9:30–10:00	CHE 91	**Photovoltaics with Copper Oxides** — •Bruno Meyer
DS 37.2	Thu	10:00–10:30	CHE 91	**Energy band alignment at interfaces of polycrystalline semiconductors for thin film solar cells** — •Andreas Klein
DS 37.3	Thu	10:30–11:00	CHE 91	**Use of doped oxides for enhanced performance solar cells** — •Judith MacManus-Driscoll

DS 37.4	Thu	11:15–11:45	CHE 91	**Nanowire device concepts for thin film photovoltaics** — •Silke Christiansen
DS 37.5	Thu	11:45–12:15	CHE 91	**Core shell ZnO nanowire heterostructures for solar cells** — •Vincent Consonni
DS 37.6	Thu	12:15–12:45	CHE 91	**Potential and challenges of kesterite-type materials for thin film solar cells** — •Thomas Unold
DS 39.1	Thu	9:30–10:00	CHE 89	**Switching kinetics in phase change materials** — •Martin Salinga
DS 49.1	Fri	9:30–10:00	CHE 91	**Synthesis, Characterization, and Application of Tunable Resistance Coatings** — •Jeffrey W. Elam

Invited talks of the joint symposium SYOM

See SYOM for the full program of the symposium.

SYOM 1.1	Fri	9:30–10:10	HSZ 02	**Atomic-scale dopant wires for quantum computer architectures** — •Michelle Y Simmons
SYOM 1.2	Fri	10:10–10:50	HSZ 02	**$1+\delta$: Tuning the Dimensionality of Organic Conductors** — •Martin Dressel
SYOM 1.3	Fri	11:10–11:50	HSZ 02	**Spectral and transport properties of one-dimensional correlated electrons** — •Volker Meden
SYOM 1.4	Fri	11:50–12:30	HSZ 02	**Atomic nanowires on surfaces: Spectroscopic reality versus theoretical fiction** — •Ralph Claessen

Invited talks of the joint symposium SYCM

See SYCM for the full program of the symposium.

SYCM 1.1	Mon	15:00–15:30	HSZ 02	**Complexity on Compression: The Crystallography of High-Density Matter** — •Malcolm McMahon
SYCM 1.2	Mon	15:30–16:00	HSZ 02	**X-Ray Microscopy with Coherent Radiation: Beyond the Spatial Resolution of Conventional X-Ray Microscopy** — •Christian G. Schroer
SYCM 1.3	Mon	16:00–16:30	HSZ 02	**Modulated martensite: A scale bridging Lego game for crystallographers and physicists** — •Sebastian Fähler
SYCM 1.4	Mon	16:45–17:15	HSZ 02	**Switching of magnetic domains reveals evidence for spatially inhomogeneous superconductivity** — •Michel Kenzelmann
SYCM 1.5	Mon	17:15–17:45	HSZ 02	**The key role of magnetic neutron diffraction in materials science** — •Laurent C. Chapon

Invited talks of the joint symposium SYSG

See SYSG for the full program of the symposium.

SYSG 1.1	Tue	9:30–10:00	HSZ 02	**Intrinsic magnetism in graphene** — •Irina Grigorieva
SYSG 1.2	Tue	10:00–10:30	HSZ 02	**Defect Induced Magnetic Moments in Graphene** — •Roland Kawakami
SYSG 1.3	Tue	10:30–11:00	HSZ 02	**Role of MgO barriers for spin and charge transport in Co/MgO/graphene spin-valve devices** — •Bernd Beschoten
SYSG 1.4	Tue	11:15–11:45	HSZ 02	**Defect-Mediated Spin Relaxation and Dephasing in Graphene** — Mark Lundeberg, Silvia Folk, •Joshua Folk
SYSG 1.5	Tue	11:45–12:15	HSZ 02	**Electron spin relaxation in graphene: resonant scattering off local magnetic moments** — •Jaroslav Fabian, Denis Kochan, Martin Gmitra

Invited talks of the joint symposium SYMO

See SYMO for the full program of the symposium.

SYMO 1.1	Mon	9:30–10:00	HSZ 02	**Molecular quantum spintronics with single-molecule magnets** — •Wolfgang Wernsdorfer

SYMO 1.2	Mon	10:00–10:30	HSZ 02	**EPR Studies of Rare-Earth Molecular Nanomagnets** — •Stephen Hill, Sanhita Ghosh, Dorsa Komijani, Salvador Cardona-Serra, Jose-Jaime Baldovi, Yan Duan, Alejandro Gaita-Arino, Eugenio Coronado
SYMO 1.3	Mon	10:45–11:15	HSZ 02	**On-surface magnetochemistry of spin-bearing metalorganic molecules** — •Peter M. Oppeneer, Kartick Tarafder, Ehesan Ali, Nirmalya Ballav, Christian Wäckerlin, Thomas A. Jung
SYMO 1.4	Mon	11:15–11:45	HSZ 02	**Interfacing single-molecule magnets with metals** — •Andrea Cornia, Valeria Lanzilotto, Luigi Malavolti, Matteo Mannini, Mauro Perfetti, Luca Rigamonti, Roberta Sessoli
SYMO 1.5	Mon	11:45–12:15	HSZ 02	**Linking magnetic molecules to themselves, to others and to surfaces** — •Richard Winpenny

Sessions

DS 1.1–1.14	Mon	9:30–13:15	CHE 91	**Application of Thin Films**
DS 2.1–2.9	Mon	9:30–12:15	ZEU 222	**Organic Electronics and Photovoltaics I (joint session with CPP, HL, O)**
DS 3.1–3.8	Mon	10:30–13:15	TRE Ma	**Focus Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale I (jointly with O)**
DS 4.1–4.10	Mon	15:00–17:45	CHE 91	**Magnetic / Organic Interfaces, Spins in Organics and Molecular Magnetism (jointly with MA)**
DS 5.1–5.10	Mon	15:00–18:00	ZEU 222	**Organic Electronics and Photovoltaics II (joint session with CPP, HL, O)**
DS 6.1–6.18	Mon	15:00–20:00	CHE 89	**Thin Film Characterization: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS,...)**
DS 7.1–7.10	Mon	16:00–18:45	TRE Ma	**Focus Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale II (jointly with O)**
DS 8.1–8.7	Mon	18:00–19:45	CHE 91	**Organic Electronics and Photovoltaics III (jointly with CPP, HL, O)**
DS 9.1–9.10	Tue	9:30–12:45	CHE 91	**Layer Properties: Electrical, Optical, and Mechanical Properties**
DS 10.1–10.12	Tue	9:30–12:45	BEY 118	**Multiferroics I (jointly with MA, DF, KR, TT)**
DS 11.1–11.11	Tue	9:30–13:15	CHE 89	**Focus Session: Sensoric Micro and Nano-systems I**
DS 12.1–12.4	Tue	10:30–11:50	GER 37	**High- and low-k-dielectrics (Joint Session with DF)**
DS 13.1–13.9	Tue	10:00–12:30	POT 081	**Organic semiconductors: Photovoltaics (Jointly with HL, CPP)**
DS 14.1–14.9	Tue	10:30–13:15	TRE Ma	**Focus Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale III (jointly with O)**
DS 15.1–15.7	Tue	14:00–15:45	POT 081	**Organic semiconductors: Transistors and OLEDs (Jointly with HL, CPP)**
DS 16.1–16.8	Tue	14:00–16:15	CHE 89	**Focus Session: Sensoric Micro and Nano-systems II**
DS 17.1–17.9	Tue	14:00–16:15	CHE 91	**Ion and Electron Beam Induced Processes**
DS 18.1–18.12	Wed	9:30–12:45	CHE 91	**Organic Thin Films I**
DS 19.1–19.13	Wed	9:30–13:00	HSZ 04	**Multiferroics II (jointly with MA, DF,KR, TT)**
DS 20.1–20.10	Wed	9:30–13:00	POT 081	**Focus Session: Emerging oxide semiconductors I (jointly with HL, DF, O)**
DS 21.1–21.12	Wed	9:30–12:45	ZEU 260	**Organic Electronics and Photovoltaics IV (joint session with CPP, HL, O)**
DS 22.1–22.10	Wed	10:30–13:15	TRE Ma	**Focus Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale IV (jointly with O)**
DS 23.1–23.1	Wed	10:30–11:15	GER 37	**Invited Talk - Stefan Förster (Joint Session with DF, O, KR, MM)**
DS 24.1–24.5	Wed	9:30–11:00	CHE 89	**Focus Session: Resistive Switching by Redox and Phase Change Phenomena I (Memristive devices and new circuit concepts)**
DS 25.1–25.5	Wed	11:15–12:45	CHE 89	**Focus Session: Resistive Switching by Redox and Phase Change Phenomena II (Valence and phase change in oxides)**
DS 26.1–26.1	Wed	12:30–13:00	HSZ 02	**Gaede Prize Talk**
DS 27.1–27.13	Wed	15:00–18:30	CHE 91	**Organic Thin Films II**

DS 28.1–28.1	Wed	15:00–15:45	GER 37	**Invited Talk - Heidemarie Schmidt (Joint Session with DF, MA, HL, KR, MM)**
DS 29.1–29.12	Wed	15:00–18:15	ZEU 260	**Organic Electronics and Photovoltaics V (joint session with CPP, HL, O)**
DS 30.1–30.12	Wed	15:00–18:45	POT 081	**Focus Session: Emerging oxide semiconductors II (jointly with HL, DF, O)**
DS 31.1–31.11	Wed	16:00–19:15	TRE Ma	**Focus Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale V (jointly with O)**
DS 32.1–32.6	Wed	15:00–16:30	CHE 89	**Focus session: Resistive Switching by Redox and Phase Change Phenomena III (Defect and material engineering in oxides)**
DS 33.1–33.6	Wed	16:45–18:15	CHE 89	**Focus session: Resistive Switching by Redox and Phase Change Phenomena IV (Kinetic in oxides and phase change)**
DS 34.1–34.5	Wed	18:30–20:00	CHE 89	**Focus Session: Resistive Switching by Redox and Phase Change Phenomena V (Structure, growth and general properties of PC materials)**
DS 35.1–35.70	Wed	17:00–20:00	P1	**Poster I: Application of thin films; Focus session: Sensoric micro and nano-systems; Focus Session: Sustainable photovoltaics with earth abundant materials; Graphen (joint session with TT; MA; HL; DY; O); Ion and electron beam induced processes; Layer properties: electrical, optical, and mechanical properties; Magnetic/organic interfaces, spins in organics and molecular magnetism; Micro- and nanopatterning (jointly with O); Organic electronics and photovoltaics (jointly with CPP, HL, O); Thermoelectric materials**
DS 36.1–36.6	Thu	9:30–12:45	BEY 118	**Focus Session: Unconventional Spin Structures (jointly with MA)**
DS 37.1–37.6	Thu	9:30–12:45	CHE 91	**Focus Session: Sustainable Photovoltaics with Earth Abundant Materials I**
DS 38.1–38.10	Thu	10:30–13:15	TRE Ma	**Focus Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale VI (jointly with O)**
DS 39.1–39.6	Thu	9:30–11:15	CHE 89	**Focus Session: Resistive Switching by Redox and Phase Change Phenomena VI (Kinetics and Transport in PC materials)**
DS 40.1–40.6	Thu	11:30–13:00	CHE 89	**Focus Session: Resistive Switching by Redox and Phase Change Phenomena VII (Optical properties and theory of PC materials)**
DS 41.1–41.10	Thu	15:00–17:30	CHE 91	**Focus Session: Sustainable Photovoltaics with Earth Abundant Materials II**
DS 42.1–42.15	Thu	15:00–19:00	CHE 89	**Thermoelectric Materials**
DS 43.1–43.31	Thu	16:00–19:00	P1	**Poster II: Organic thin films; Atomic layer deposition, Thin film characterization: Structure analysis and composition (XRD, TEM, XPS, SIMS, RBS, ...)**
DS 44.1–44.21	Thu	16:00–19:00	P1	**Poster III: Focus session: Resistive switching by redox and phase change phenomena**
DS 45.1–45.27	Thu	16:00–19:00	P1	**Poster IV: One-Dimensional Metals: Reality or Fiction**
DS 46.1–46.8	Thu	17:45–19:45	CHE 91	**Organic Electronics and Photovoltaics VI (jointly with CPP, HL, O)**
DS 47.1–47.7	Fri	9:30–11:15	CHE 89	**Micro- and Nanopatterning (jointly with O)**
DS 48.1–48.9	Fri	9:30–12:00	HSZ 04	**Topological Insulators (jointly with MA,HL,O,TT)**
DS 49.1–49.10	Fri	9:30–12:30	CHE 91	**Atomic Layer Deposition**
DS 50.1–50.9	Fri	10:15–12:30	POT 051	**Organic semiconductors: Material properties (jointly with HL, CPP)**
DS 51.1–51.7	Fri	11:30–13:15	CHE 89	**Graphene (joint session with TT, MA, HL, DY, O)**

Annual General Meeting of the Thin Films Division

Thursday 19:00–20:00 Room CHE 89

DS 1: Application of Thin Films

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

DS 1.1 Mon 9:30 CHE 91

Lattice dynamics of epitaxial EuSi2 thin films and nanostructures — •Anja Seiler[1,2], Olga Bauder[1,2], Shyjumon Ibrahimkutty[1,2], Przemyslaw Piekarz[3], Daniel Merkel[4], Rudolf Rüffer[4], Tilo Baumbach[1,2], Michael Fiederle[5], and Svetoslav Stankov[1,2] — [1]Laboratory for Applications of Synchrotron Radiation, KIT, Germany — [2]Institute for Photon Science and Synchrotron Radiation, KIT, Germany — [3]Institute of Nuclear Physics, Polish Academy of Sciences, Poland — [4]European Synchrotron Radiation Facility, France — [5]Freiburg Materials Research Center, Germany

The continuous downscaling of the CMOS devices demands a constant search for new self-organizing nanostructures. The rare earth silicides became especially attractive due to their very low Schottky barrier of 0.3-0.4 eV on n-type silicon [1-3]. It is very well known that the finite material's sizes at the nanoscale significantly modify their thermoelastic properties. Therefore it is mandatory to get comprehensive understanding of the lattice dynamics in order to even tailor the properties at the nanoscale. Here we will present experimental data on in situ nuclear inelastic scattering [4] from 151Eu for the phonon density of states of EuSi2 thin films and nanoislands. The experimental results are compared with the ab intio calculations.

[1] G.L. Molnar et al., J. Appl. Phys. 90, 503 (2001). [2] M. Ieong et al., Mater. Today 9, 26 (2006). [3] N. Reckinger et al., Appl. Phys. Lett. 94, 191913 (2009). [4] S. Stankov et al., Chapter 1 in "Mössbauer Spectroscopy: Applications in Chemistry, Biology, Industry, and Nanotechnology" (2013)

DS 1.2 Mon 9:45 CHE 91

Properties of Sol-Gel derived Ge nanocrystals embedded in thin SiO$_2$ layers — •Ansgar Dominique Donner[1], Sebastian Knebel[1], Ivana Capan[2], Harald Rösner[1], Hartmut Bracht[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, WWU Münster, Münster, Germany — [2]Ruder Bošković Institute, Zagreb, Croatia

Besides a variety of potential applications in the field of optoelectronics, germanium (Ge) nanocrystals (NCs) are a widely-discussed alternative to poly-silicon (Si) floating gates in nonvolatile memory devices such as Flash or EEPROM, because they promise to be less sensitive to charge leakage and thus information loss. We have developed a highly scalable and cost-efficient wet-chemical sol-gel process for the synthesis of Ge NCs embedded in thin Si dioxide films. Using TEM and other techniques, we have studied these Ge NCs and find that their structural properties can be varied over a wide range by different compositions of the precursor material or different annealing conditions. In an attempt to realize non-volatile memory devices based on our sol-gel derived thin films with embedded Ge NCs, we have fabricated first MOSFET devices to characterize the charge storage behavior of these thin films involving Ge NCs as floating gate.

DS 1.3 Mon 10:00 CHE 91

Electrical resistivity of high-conductivity perovskite SrMoO$_3$ at microwave frequencies — •Arzhang Mani[1], Aldin Radetinac[1], Mohammad Nikfalazar[2], Sergiy Melnyk[2], Philipp Komissinskiy[1], Yuliang Zheng[2], Rolf Jakoby[2], and Lambert Alff[1] — [1]Institute of Material Science, Technische Universität Darmstadt, Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany — [2]Institut of Microwave Engineering, Technische Universität Darmstadt, Merckstraße 25, 64283 Darmstadt, Germany

Epitaxial SrMoO$_3$ thin films were grown on single crystal GdScO$_3$ (110) substrates using pulsed laser deposition (PLD). The lithography process of SrMoO$_3$ thin films for patterning the co-planar waveguide (CPW) structures is challenging due to the high oxygen affinity of SrMoO$_3$. However, successful patterning of SrMoO$_3$ electrodes for electrical measurements by means of lithography and wet etching was achieved. Making a comparison between the electrical resistivity of SrMoO$_3$ and SrRuO$_3$ as a common oxide electrode material, we show that SrMoO$_3$ exhibits a record-low DC resistivity of 27 $\mu\Omega$cm at room-temperature. Furthermore, SrMoO$_3$ exhibits an AC resistivity of 27 $\mu\Omega$cm in the range of 1-20 GHz, making it the best candidate for integration into all-oxide electronic devices for microwave applications.

DS 1.4 Mon 10:15 CHE 91

Rolled-up nanomembranes for field effect transistors and fluidic sensing applications — •Daniel Grimm[1,2], Cesar Bufon[1,2], Paola Atkinson[1], Dominic Thurmer[1], Franziska Schäffel[1], Sandeep Gorantla[1], Alicja Bachmatiuk[1], and Oliver Schmidt[1,2] — [1]Institute for Integrative Nanosciences, IFW Dresden, Germany — [2]Technische Universität Chemnitz, Material Systems for Nanoelectronics, Germany

In this work we demonstrate for the first time a three-dimensional free-standing metal oxide field-effect-transistor based on strained hybrid nanomembranes [1]. The fabrication process combines conventional device patterning with selective etching to form the three-dimensional rolled-up transistor (RUFET). Extremely small bending radii in the range of 5um can be achieved by taking advantage of the self-rolling technique. The hollow core of the as-produced RUFETs can be further explored foruidic sensing applications with a large sensitivity when feeding polar solvents through the tubes. By standard two-dimensional lithography, the Ohmic contacts, gate electrodes and Al2O3 dielectrics are defined on the surface of single-crystalline semiconducting multilayers. Upon selective etching of an underlying sacrificial layer, the complete planar transistor curls up so that the nanomembrane based channel bonds back onto the gate electrode. This rolled-up technique yields a substantial reduction of the device footprint and the as-produced RUFET can be driven in the depletion mode regime with gate-voltage swings around 160 mV/decade and on-off ratios being several orders of magnitudes. [1] D. Grimm et al., Nano Letters 13,213(2013)

DS 1.5 Mon 10:30 CHE 91

Metal Oxides and SURMOF-Hybrid material assemblies for Photonic and Optical Applications — •Engelbert Redel — IFG (Institut fuer Funktionelle Grenzflaechen)/KIT, Eggenstein-Leopoldshafen, Karlsruhe, DE

Porous hierarchical and photonic materials assemblies will be presented from a library of different metal oxide nanomaterials and hierarchical multilayer constructions. Potential applications of such materials will be presented, reaching from optical and tune able and porous 1D photonic crystals (PCs) to transparent and conductive oxides (TCOs) porous thin films, white light broad-band bragg reflectors as well as electrochromo-photonic switches. Furthermore the optical and dielectric properties of single porous SURMOF thin films as well as multilayered photonic SURMOF-Hybrid materials will be presented in terms of optical sensing.

1 a) E. REDEL, C. HUAI, M. RENNER, G. V. FREYMANN, G. A. OZIN SMALL 2011, 7, 3465-3471. b) E. REDEL, P. MIRTCHEV, C. HUAI, S. PETROV, G. A. OZIN ACS NANO, 2011, 5, 2861-2869.

2 E. REDEL, C. HUAI, S. PETROV, D. OMER, P. O'BRIEN, M. G. HELANDER, J.MLYNARSKI, G. A. OZIN, SMALL 2012, 8, 3806-3809.

3 E. REDEL, J. MLYNARSKI, J. MOIR, A. JELLE, C. HUAI, S. PETROV, M. G. HELANDER, F. C. PEIRIS, G. V. FREYMANN, G. A. OZIN Advanced Materials 2012, 24, OP265-OP269.

4 E. REDEL, Z. WANG, S. WALHEIM, J. LIU, H. GLIEMANN, C. WOELL, Appl. Phys. Lett. 2013, 103, 091903; doi: 10.1063/1.4819836

DS 1.6 Mon 10:45 CHE 91

Phonon Blocking in Multilayers produced by Pulsed Laser Deposition — •Florian Döring[1], Christian Eberl[1], Anna Major[1], Susanne Schlenkrich[1], Felix Schlenkrich[1], Martin Lüttich[2], Maria Mansurova[2], Benjamin Lenk[2], Sarah Hoffmann[3], Markus Münzenberg[2], and Hans-Ulrich Krebs[1] — [1]Institute for Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]1st Institute of Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Institute for x-ray physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Multilayer insulations are a modern high-technology approach for minimizing thermal transport, which is important for thermoelectric materials, thermal barrier coatings, solid state refridgerators and cryogenic applications. In these multilayer structures, the thermal conductivity can be reduced by an increasing number of interfaces between two materials with a high acoustic mismatch resulting in different phonon dispersion relations. Therefore, different types of multilayers, consisting of various metals (e.g. W, Ti, or Cu), oxides (e.g. ZrO2 or MgO) and polymers (e.g. PC), were selected and pulsed laser deposited (PLD at 248 nm) with high quality and afterwards analysed by ultrafast pump-probe reflectivity measurements. Thereby we found fast phonon modes on ps time scales that indicate possible candidates for THz frequency band gap phononic metamaterials. In this contribution, the necessary steps for the fabrication of phononic metamaterials by PLD and first results of reflectivity measurements are discussed.

Coffee break (15 min)

DS 1.7 Mon 11:15 CHE 91

Multisegment-actuated micro-lenses based on ultrathin diamond membranes — •Johannes Fries[1], Verena Zuerbig[1,2], Wilfried Pletschen[1], Christoph E. Nebel[1], Oliver Ambacher[1,2], and Vadim Lebedev[1] — [1]Fraunhofer IAF, Freiburg, Germany — [2]IMTEK, University of Freiburg, Germany

The drawback of modern tunable micro-lenses based on polymers or silicon is the limitation in their mechanical and tribological properties. In order to overcome these limits, nanocrystalline diamond (NCD) elastic layers were combined with piezo-actuators made from aluminium nitride (AlN) or lead zirconate titanate (PZT). NCD thin films have excellent properties for manufacturing mechanically stable, ultrathin membranes, e.g. a high Young's modulus and an optical transparency from infrared to deep UV. In such ultrathin unimorph structures heavily boron-doped NCD layers (B:NCD) can serve as transparent front electrodes with conductivities up to 100 S/cm. Such bilayer structures were used to fabricate circular membranes. These unimorph membranes were tested towards their electrical, mechanical and optical properties. Finally, membrane-based multisegment piezo-actuated micro-lenses were fabricated. The performance of the micro-lenses was analyzed statically using white light interferometry and dynamically using laser Doppler vibrometry. Symmetric and asymmetric deflection of the lens surface was demonstrated by applying different voltages on each independent segment. These mirco-lenses can be used as focus and aberrations corrector in complex optical systems.

DS 1.8 Mon 11:30 CHE 91

Design, fabrication and performance of polymer actuators for on-chip variable focal length microlenses — •Christian Schirrmann, Boscij Pawlik, Kirstin Bornhorst, and Florenta Costache — Fraunhofer Institute for Photonic Microsystems IPMS, Dresden, Germany

We employed the finite element method (FEM) to simulate the electromecanical behavior of monolayer and multilayer bending actuators based on PVDF-TrFE-CFE (61.7%/29.8%/8.5%) terpolymer of high electrostrictive strain. The actuator geometry (i.e. radial shape), the actuator stack structure, the polymer layer thickness, as well as the electrode material were adjusted in order to improve the deflection characteristics of the actuator. For the actuator fabrication, a layer-by-layer process flow was developed, which included polymer and metallic electrode layers deposition, structuring and direct bonding. The analysis of the actuator performance by means of interferometric methods indicated that very large deflections could be obtained. Furthermore, the optimized terpolymer bending actuator was employed in the design of a microlens with electrically adjustable focal length. This microlens consisted of two microfluidic compartments sealed by an elastic lens membrane. Here, the integrated actuator played the role of a pump. The variable micro-lens chip geometry was optimized using 3D-FEM simulations and fabricated using planar microtechnology. For a microlens with 3 mm aperture diameter, we could achieve a tuning range in the refractive power between 0 and more than 20 dpt for fairly low operation voltages.

DS 1.9 Mon 11:45 CHE 91

Reduction via PLD: Growth of highly conductive $SrMoO_3$ thin films using various reducing atmospheres — •Aldin Radetinac, Arzhang Mani, Philipp Komissinskiy, and Lambert Alff — Institute for Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany

We have investigated the growth of $SrMoO_3$ by pulsed laser ablation out of a $SrMoO_4$ target. To stabilize $SrMoO_3$, one oxygen atom per formula unit has to be removed out of the material flux during the film growth. To achieve effective reduction, the atmosphere was varied from ultra high vacuum (10^{-9} torr) to Ar- and H_2+Ar mixtures. We show that laser pulse rate and gas flow have a high impact on the actual film quality for reductive film growth. Thus, thin films of metastable materials can be grown by pulsed laser deposition with their growth speed, microstructure, surface morphology and homogeneity controlled by the choice of growth parameters.

This work was supported by the DFG projects GRK 1037 (TICMO) and KO 4093/1-1.

DS 1.10 Mon 12:00 CHE 91

Work function tuning of pyrolytic carbon electrodes and integration in nanoelectronic devices. — •Andreas Krause[1], Andrew Graham[1], Thomas Mikolajick[1,2], and Walter M. Weber[1] — [1]namlab gGmbh, D-01187 Dresden — [2]Institut fuer Halbleiter- und Mikroelektronik IHM, TU Dresden

Pyrolytic carbon is an extraordinary material, which can be used as an electrode material for nanoelectronic device integration. The carbon layers have been grown by CVD below 900C. With a work function of 4.6 eV and high conformity, it poses a real alternative to standard TiN or other electrode materials. Composing of a polycrystalline mixture of graphite-like (sp^2) and amorphous (sp^3) carbon, it exhibits an metal ohmic behavior with $1.5\, m\Omega cm$. The amount of graphite-like (conductive) proportions can be changed with the annealing temperature and easily controlled with Raman spectroscopy. The work function of 4.6 eV has been tuned in our experiments with the introduction of nitrogen as dopant to the surface layer. [Aichmayr et al., 2007 IEEE Symposium on VLSI Technology] [A. Graham et al., J. Appl. Phys. 2010, 107(11)] [A. Graham et al., J. Appl. Phys. 2010, 108(10)]

DS 1.11 Mon 12:15 CHE 91

Dynamic Effects in the Power Spectral Density Determination of Multilayers with EUV Light — •Anton Haase, Victor Soltwisch, Christian Laubis, and Frank Scholze — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin

The throughput of EUV lithography systems is presently strongly limited by the available radiant power at the waver level. Besides increasing the power of EUV sources, also the quality of the optical elements plays a key role. With state of the art multilayer mirrors the main cause of diminished reflectance is surface and interface roughness as well as interface diffusion. Both properties lead to diffuse scattering reducing the intensity of specular reflected light in the relevant EUV spectral range around 13.5 nm below the theoretical limit. The intensity distribution of diffusely scattered light provides information on vertical and lateral correlations of spacial frequencies of roughness through the appearance of resonant diffuse scattering (RDS) sheets. The study of off-specular scattering thus serves as a natural tool for the investigation roughness power spectral densities (PSD) of the interfaces. We found that dynamical scattering contributions from thickness oscillations (Kiessig fringes) lead to Bragg lines which intersect the RDS sheets. This causes strong resonant enhancement in the scatter cross section. Thus for power spectral density studies of multilayer interface roughness, resonant dynamical scattering can not be neglected. We considered the scatter enhancement by applying fully dynamic distored wave Born approximation to extract the power spectral density of roughness.

DS 1.12 Mon 12:30 CHE 91

Fabrication of Multilayer Zone Plates for hard x-ray point nano focusing — •C. Eberl[1], F. Döring[1], F. Schlenkrich[1], T. Liese[1], V. Radisch[1], M. Osterhoff[2], A. Robisch[2], A. Ruhlandt[2], S. Hoffmann[2], M. Krenkel[2], M. Bartels[2], M. Sprung[3], H.U. Krebs[1], and T. Salditt[2] — [1]Institut für Materialphysik — [2]Institut für Röntgenphysik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]HASYLAB at DESY, Notkestr. 85, 22607 Hamburg, 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 thin multilayers grown on wires are promising optical elements. Different materials such as W/Si, W/ZrO_2 and Ta_2O_5/ZrO_2 were used for the growth of high quality multilayers by pulsed laser deposition (PLD). They were investigated by X-ray reflectivity, transmission electron microscopy in cross-section and in-situ rate monitoring approving high accuracy in layer thickness as well as smoothness and well defined interfaces. In contrast to sputter deposition, where mostly cumulative roughness is observed, PLD shows smoothing effects, even on wires which is due to the energetic particle deposition. Only based on the knowledge of the underlying deposition processes high quality multilayers according to the zone plate law could be deposited onto a wire. Using these coated wires, highly precise MZP optics were fabricated by focused ion beam

(FIB) showing hard x-ray point focusing with unprecedented focal sizes of less than 5 nm.

DS 1.13 Mon 12:45 CHE 91

Interface investigation of ion-beam deposited Chromium/ Scandium multilayer mirrors — •Stefan Radünz[1,2], Alexander Guggenmos[1,2], Roman Rauhut[1,2], Bert Nickel[3], Sriram Venkatesan[4], Angela Wochnik[4], Christina Scheu[4], Eric M. Gullikson[5], Ferenc Krausz[1,2], and Ulf Kleineberg[1,2] — [1]LMU München, Fakultät für Physik, Garching, Germany — [2]MPQ, Garching, Germany — [3]CeNS, LMU München, München, Germany — [4]LMU München, Fakultät für Chemie, München, Germany — [5]CXRO, Lawrence Berkeley National Lab, Berkeley, USA

Highly reflective multilayer mirrors for beam steering, spectral shaping or as focusing elements for the water window spectral range, between the K-absorption edges of carbon and oxygen (284 eV and 543 eV, respectively) are of great interest for various applications like high-resolution microscopy, time-resolved (soft) x-ray spectroscopy or x-ray astronomy. Their demand for low-photon loss optics challenges the manufacturing process to create interfaces as perfect as possible due to the huge loss in reflectivity which arises from boundary imperfections. We present our achievements in minimizing the interface roughness of ion-beam deposited Cr/Sc multilayer mirrors by optimizing the kinetic energy of the utilized Krypton ions both in the deposition and the interface polishing process. The characteristics of our ion-beam polished nanolayers can be investigated using in-situ ellipsometry. Experimental results from measurements using X-ray reflectometry, spectral ellipsometry and XUV reflectrometry as well as TEM cross section images are shown and discussed.

DS 1.14 Mon 13:00 CHE 91

Wet-chemical Synthesis of $SrTiO_3$-Ruddlesden-Popper-Phases for photoelectrochemical Watersplittingg — •Diana Karsch, Doreen Eger, Erik Mehner, Hartmut Stöcker, and Dirk Meyer — TU Freiberg - Institut für experimentelle Physik

The photoinduced watersplitting promises a considerably simplification for the hydrogen production. Therefore the energy of photons, e.g. the sunlight, is used for splitting the water into its molecular components, Oxygen and Hydrogen. This is worked out by irradiation of light with a suitable wavelength to a semiconductor.

Thin films of $SrTiO_3$-Ruddlesden-Popper-Phases are produced by sol gel synthesis and are characterized due to phase content and morphology. For comparison of phase setup additionally one sample with stoichiometric relations is produced by ion beam implantation in a $SrTiO_3$ single crystal. The setup of crystalline phases in the film was investigated with *in-situ* X-ray diffraction.

The samples show delicate, spongy structures on the surface, which are visible by electron scanning microscopy. In addition to the RP-phases all samples have a relevant part of impurity phases. Further photoelectrochemical measurements with sol gel synthesized thin layers have been executed for the first time. The results show that the thin layer working electrodes are suitable for water splitting.

DS 2: Organic Electronics and Photovoltaics I (joint session with CPP, HL, O)

small molecules, hybrid materials

Time: Monday 9:30–12:15 Location: ZEU 222

Invited Talk DS 2.1 Mon 9:30 ZEU 222

Structure-property relations in perylene bisimids: Charge mobility, exiton diffusion and singlet exciton fission — •Ferdinand Grozema — Delft University of Technology, Department of Chemical Engineering, Delft, The Netherlands

Perylene diimides (PDIs) represent a class of materials that is promising for application as the active layer in field effect transistors and as an electron accepting material in organic photovoltaic cells. The electronic properties of PDI-based materials strongly depend on the supramolecular order in the material. Therefore, a thorough understanding of the relation between the electronic properties and the organization on the molecular scale can result in design rules for the synthesis of new π-conjugated organic molecules .

To achieve this we have performed a combined experimental and theoretical study of the electronic properties of a large library of PDI derivatives that differ in the side chains, resulting in subtle differences in the crystal structure. By time-resolved microwave conductivity measurements we show a strong correlation between the supramolecular organization and the charge carrier mobility, with a maximum mobility of 0.41 cm2/Vs. Singlet exciton fission, a process in which a singlet excited state is efficiently converted into two triplets, is also found to be strongly dependent on the supramolecular organization.

This comprehensive study shows that the engineering of the supramolcular organization in PDIs and conjugated molecules in general is viable approach to tailor a variety of electronic properties of such materials over a wide range.

DS 2.2 Mon 10:00 ZEU 222

Influence of morphology on organic solar cell performance comparing crystalline diindenoperylene (DIP) and its amorphous derivative tetraphenyldibenzoperiflanthene (DBP) — •Stefan Grob, Mark Gruber, Ulrich Hörmann, Theresa Linderl, and Wolfgang Brütting — University of Augsburg, Germany

The DIP molecule, consisting of seven benzene and two cyclopentadiene rings, forms the backbone of the DBP molecule, which has two further benzene rings and four additional, rotatable phenyl groups. Compared to the planar arrangement of DIP, these phenyl groups give DBP a more three-dimensional shape, changing the growth behavior in thin films completely. While we observe crystalline domains of almost upright standing DIP, layers of DBP exhibit an amorphous character and therefore a relatively small exciton diffusion length, being about ten times shorter than that of its crystalline counterpart. However, the drawback of the upright standing arrangement of DIP molecules is the unfavorable orientation of the transition dipole moment resulting in a low absorption coefficient and thus a smaller short-circuit current density. The difference in morphology also leads to different coupling between donor and acceptor molecules at the interface. As a consequence there is an appreciable distinction in the recombination processes occurring within the solar cell. We investigate this phenomenon by temperature-dependent j-V-measurements, electroluminescence and photothermal deflection spectroscopy. Based on these results, we discuss the influence of different film structure and morphology on electrical transport and device performance.

DS 2.3 Mon 10:15 ZEU 222

Spray deposition of zinc oxide nanostructured films for applications in dye-sensitized solar cells — •Kuhu Sarkar[1], Erik V. Braden[1], Stefan Pogorzalek[1], Shun Yu[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

Zinc oxide (ZnO) has emerged as a suitable alternative to titania (TiO2) in the recent years in the field of dye-sensitized solar cells (DSSCs). The inorganic metal oxide films for DSSCs are highly desirable to have an increased surface for enhanced adsorption of a photosensitizer. Hence, nanostructured films of ZnO are synthesized from a solution based approach. Different deposition techniques are investigated to have a significant film thickness for a considerable amount of light absorption. In this respect, spray deposition is shown to be a highly efficient and scalable technique to produce films matching the above-mentioned criteria. Surface as well as bulk morphology of the films have been studied using SEM and GISAXS. These ZnO films are successfully shown to provide good performance in a dye-sensitized solar cell with the highest short circuit current density reported so far.

DS 2.4 Mon 10:30 ZEU 222

Extremely Thin Absorber Solar Cells based on Sb_2S_3 — •Eugen Zimmermann, Jonas Weickert, Thomas Pfadler, James Dorman, and Lukas Schmidt-Mende — Universität Konstanz

The introduction of nanostructured metal oxides as electron acceptor resulted in the concept of extremely thin absorber solar cells. Thus, low cost fabricated inorganic semiconductors like Sb_2S_3 can be utilized as sensitizer, which typically possess promising properties, such as a tunable band gap and high extinction coefficient. However, optimization of the fabrication process and a detailed characterization of intrinsic properties is unavoidable in order to find the best device architecture and suitable material combinations for highly efficient solar cells. For this purpose, chemical bath deposition conditions and parameters have been examined and resulted in a detailed recipe for fabrication of high quality Sb_2S_3 coatings. In combination with optimized layer thicknesses of P3HT, efficiencies of up to 3.2% could be achieved in flat heterojunction architecrue. In order to identify intrinsic limitations, comparative measurements with P3HT:PCBM cells have been, revealing monomolecular recombination processes of excitons, a potential dependency of charge separation, and long charge carrier pathways as main loss mechanisms of fabricated flat heterojunction cells. In addition, investigation of several hole transport materials (HTM) revealed a disadvantageous influence on charge generation due to the parasitic absorption of light by the HTM. Based on these results, the use of nanostructured metal oxides in combination with transparent HTMs is proposed to possibly overcome some of the found limitations.

DS 2.5 Mon 10:45 ZEU 222

Towards low-temperature synthesis of polymer/titania hybrid films for application in photovoltaics — Martin A. Niedermeier[1], Monika Rawolle[1], Erik V. Braden[1], Kuhu Sarkar[1], Eva M. Herzig[2], Volker Körstgens[1], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]TU München, Munich School of Engineering, James-Franck-Str. 1, 85748 Garching

In a hybrid solar cell an inorganic matrix, such as titania, is combined with a hole-conducting polymer to form a so-called bulk heterojunction. The functionality of such a system depends strongly on the quality of the polymer/semiconductor interface. A very common approach to fabricate that interface is the so-called backfilling of the existing inorganic matrix with the conducting polymer. This approach is generally a two-step process, as the fabrication of the inorganic matrix usually involves high temperatures, which destroy all organic material present in the system. To date the subsequent backfilling of that matrix remains challenging, since a lot of problems have to be overcome. A workaround to these problems is promised by a low-temperature sol-gel process, in which the polymer and the inorganic semiconductor network are fabricated simultaneously. Approaches towards such low-temperature synthesis of polymer/titania hybrid films for application in photovoltaics are presented. These novel routes make use of special tailored block copolymers as structure directing agent. Film morphology and device function are investigated.

15 min break

DS 2.6 Mon 11:15 ZEU 222

Photoinduced charge transfer in $CuInS_2$ nanocrystal/polymer composites — •Rany Miranti[1], Yuliar Firdaus[2], Christopher Krause[1], Mark van der Auweraer[2], Holger Borchert[1], and Jürgen Parisi[1] — [1]Univ. of Oldenburg, Dept. of Physics, Energy and Semiconductor Research Laboratory, 26129 Oldenburg, Germany — [2]Lab. for Photochemistry & Spectroscopy, Div. of Mol. Imaging & Photonics, Chemistry Dept., Katholieke Universiteit Leuven, Celestijnenlaan 200 F B-3001 Heverlee, Belgium.

The photoinduced excited states and the effects properties of charge transfer in $CuInS_2$ (CIS) nanocrystal/polymer composites were studied by applying quasi steady-state photoinduced absorption (PIA) and steady state photoluminescense as well as time-resolved photoluminescense. The time-resolved properties and excited state dynamics of our systems were studied using the time-correlated single photon counting (TCSPC) technique. We used two different systems of composites with two different kind of polymer, i.e. poly(3-hexylthiophene) (P3HT) and poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)] (PCPDTBT). Optical absorption and emission spectra of thin films of CIS nanocrystal/polymer composites exhibit several interesting features such as luminescence quenching and polaronic photoinduced absorption (PIA) indicating photoinduced charge transfer. The effect of different organic ligands surrounding the CIS nanocrystals on the charge separation process in CIS nanocrystal/ polymer composites will be presented as well.

DS 2.7 Mon 11:30 ZEU 222

Structured growth of ZnO for light trapping enhancement in organic solar cells — •Nivedita Yumnam and Veit Wagner — Jacobs University, 28759 Bremen, Germany

Organic photovoltaic cells are promising candidates for large-area and low-cost production of solar cells. However, their performance is limited due to the short diffusion length of excitons and low absorption in the active semiconductor layer. The absorption of light can be enhanced by incorporating ZnO nanostructures, which act as scattering centres and hence, they increase the optical path length of light. Our work focuses on the investigation of light trapping mechanism of solar cells based on electrochemically grown ZnO nanorod and active layer of conjugated polymer P3HT and PCBM. The size and the structure of the ZnO nanorods are varied by changing the parameters of electrochemical deposition. Angle resolved scattering measurements are employed to investigate the amount of light scattered by the nanorods. These results are correlated to the performance of the solar cell determined from electrical measurements.

DS 2.8 Mon 11:45 ZEU 222

Temperature-dependent molecular orientation of the organic semiconductor PTCDI-C_8: Optical and structural properties — •Sebastian Bommel[1,2], Linus Pithan[2], Christopher Weber[2], Anton Zykov[2], Gonzalo Santoro[1], Stephan V. Roth[1], Jörg Megow[2], and Stefan Kowarik[2] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

Optical and structural properties of molecular materials are not only essential for the rational design of opto-electrical devices, but also for the understanding of intermolecular interactions. Here, we report on the structural and optical properties of the organic semiconductor PTCDI-C_8 investigated by temperature-dependent Grazing Incidence X-ray Diffraction (GIXD) and photoluminescence (PL) measurements. Our *in situ* studies yield a large impact of temperature on unit cell parameters and optical transitions. The energy of the optical transition E_{10}-E_{01} in the PL spectra shifts from 1.80 eV for 273 K to 1.85 eV for 413 K. Furthermore, a rearrangement of the molecular ensemble was found, indicated by a large change of the beta-angle of the PTCDI-C8 unit cell from 107° (273 K) to 102° (413 K). The influence of these structural changes, which are an indication for a change of molecular orientation with temperature, on the optical properties will be discussed in detail. Additionally, the structural and optical properties are supported by temperature-dependent molecular dynamics (MD) simulation based calculations.

DS 2.9 Mon 12:00 ZEU 222

Highly Efficient Silicon/Polythiophene Hybrid Solar Cell Devices — •Matthias Zellmeier[1], Johannes Frisch[2], Silvia Janietz[3], Norbert Koch[2], Jörg Rappich[1], and Norbert Nickel[1] — [1]Helmholtz-Zentrum Berlin, Institut für Silizium Photovoltaik, Kekulèstr. 5, D-12489 Berlin — [2]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6,D-12489 Berlin — [3]Fraunhofer-Institut für Angewandte Polymerforschung IAP, Abteilung Polymere und Elektronik, Geiselbergstr. 9, D-14476 Potsdam

Highly efficient hybrid solar cell devices based on crystalline silicon with three different solution processed polymer emitter layers are realized. The inorganic part of the device is optimized with a hole-selective back contact (BSF) and a low defect density hot water oxide ($D_{it}=2\times10^{-12}$ eV^{-1}cm^{-2}), which provides the necessary wetting properties for the solution processed emitter layers. The applied polymer materials, e.g. poly(3-hexylthiophene-2,5-diyl) (P3HT), poly(3-[3,6-dioxaheptyl]-thiophene) (P3DOT), and poly(3-[2,5,8-trioxanonyl]-thiophene) (P3TOT), differ mainly in the oxygen content in the side groups. Substituting the alkyl chains attached to the thiophene rings with ether groups leads to a modified layer formation during spin coating. The results of the optical, electrical and structural characterization of the polymer layers is correlated to the key figures in the final devices. The open circuit voltage V_{OC} increases from 0.3 V to 0.5 V and the short circuit current j_{SC} increases from 15.2 mA cm^{-2} up to 28.3 mA cm^{-2} in the sequence P3HT, P3DOT, P3TOT and results in a power conversion efficiency close to 10 % for a planar Si/P3TOT device.

DS 3: Focus Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale I (jointly with O)

Non-equilibrium processes such as charge and heat transport are central to electronic and thermoelectric applications. Understanding these phenomena at the nanoscale challenges both theory and experiment. Basic theoretical issues are related to the role of quantum mechanics, the interplay of ballistic, diffusion and hopping processes, the importance of dissipation, the effect of electronic correlation, and the signatures of unusual quantum states. On the experimental side devising measurements to unravel these phenomena in a controlled way poses severe difficulties. In this regard, optical lattices of cold atoms are emerging as a powerful laboratory to test theoretical models and discover unforeseen phenomena.

This symposium will cover current issues in the field by bringing together scientists working in different specific areas with the aim of fostering interdisciplinary discussion, assessing current theoretical understanding, and indicating future goals with emphasis on electronic structure theory.

Organizers: Roberto Car (Princeton), Kristian S. Thygesen (Lyngby) and Matthias Scheffler (Berlin)

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

Topical Talk DS 3.1 Mon 10:30 TRE Ma

Molecular junction transport: some theoretical and computational considerations — •Mark Ratner[1] and Matthew Reuter[2] — [1]Chemistry, Northwestern University, Evanston Illinois 60208 USA — [2]Chemistry, Northwestern University, Evanston Illinois 60208 USA

Following the development of break junction techniques, and very elegant measurements by many labs worldwide, the understanding of the community for single molecule transport junctions on the experimental side has been very nicely unified. While there are still challenges, interpretations of the transport (and indeed of some second-order response properties) is now quite sophisticated.

There have been major advances in the computational approaches also, and in many cases, computations and measurements can be compared quantitatively. But there are some remaining difficulties in the computational and theoretical approaches, and this talk will discuss a few of them.

The topics addressed will be: single molecule aspects, histograms and their usage, time-dependence of the transport, and ghost transmission and computational accuracy.

DS 3.2 Mon 11:00 TRE Ma

On the description of biased nanocontacts from ab initio — •Steven Achilles[1], Jürgen Henk[1], Michael Czerner[2], Christian Heiliger[2], and Ingrid Mertig[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany — [2]I. Physikalisches Institut, Justus Liebig University, D-35392 Giessen, Germany

A suitable description of arbitrary shaped and biased nanocontacts is very important for investigating and predicting physical effects of materials on the nanometer scale. In particular, the electronic transport properties under finite bias voltages are of great interest.

To account for systems under finite bias we extended our Korringa-Kohn-Rostoker Green's function method [1] to the Keldysh formalism [2]. The method was developed for different types of geometries, i.e. planar junctions [3] and embedded real-space clusters [4]. Both implementations include a self-consistent treatment of the electronic structure under external bias using the nonequilibrium density.

We present ab initio results of voltage drops, the charge relaxation under finite bias voltage and current-voltage characteristics for different types of geometries.

[1] R. Zeller, P.H. Dederichs, B. Ujfalussy, L. Szunyogh, and P. Weinberger, Phys. Rev. B 52, 8807 (1995).; P. Zahn, I. Mertig, R. Zeller, and P.H. Dederichs, Mat. Res. Soc. Symp. Proc. 475, 525 (1997).
[2] L.V. Keldysh, Sov. Phys. JETP 20 (4), 1018-1026 (1965).
[3] S. Achilles et al., Phys. Rev. B 88 (12), 125411 (2013).
[4] S. Achilles et al., to be published

DS 3.3 Mon 11:15 TRE Ma

Elasticity changes in molecular junctions under bias: an ab-initio study — •Clotilde S. Cucinotta[1], Meilin Bai[1,2], Ivan Rungger[1], Shmin Hou[2], and Stefano Sanvito[1] — [1]School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2, Ireland — [2]2Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China

Non-conservative current induced forces are at the origin of a rich variety of dynamical processes, including vibrations, rotations, phonon energy flow, desorption and reactions. The ability to simulate these phenomena paves the way for crucial advances in interface physics and in molecular electronics. New insights into how the presence of non-conservative forces can affect the vibrational spectrum of prototypic Au-H2-Au nano-junctions are obtained by the Non Equilibrium Green Functions approach combined with Density Functional Theory as implemented in the Smeagol code [1]. The modification of the phonon spectrum of the junction in the presence of an external bias is for the first time analysed, in terms of charge redistribution caused by the electron flow, potential drop and differences in an average distance collective variable. Phonon modes changes are related to a change in bias of some of the elastic constants.The importance of electric field vs. current effects is compared. The elasticity changes of the molecular junction with bias are interpreted in terms of the current flowing through the system. [1] http://www.smeagol.tcd.ie/SmeagolDownloads.htm.

DS 3.4 Mon 11:30 TRE Ma

Carbon nanotubes decorated with magnetic clusters: magnetism, electron transport and gas sensing — •Zeila Zanolli[1] and Jean-Christophe Charlier[2] — [1]Forschungszentrum Juelich, PGI and IAS, Juelich, Germany — [2]IMCN, Université catholique de Louvain (UCL), Belgium

In this work, first-principles techniques and non-equilibrium Green's function approaches are used to investigate magnetism and spin-polarized quantum transport in carbon nanotubes (CNTs) decorated with transition metal magnetic nanoclusters (NC).

For small cluster sizes (< 1 nm), *ab initio* calculations predict a considerable local magnetic moment that induces spin polarization in the host CNT due to a strong mutual interaction with the magnetic NC. Such a huge local magnetic perturbation can be tailored by molecular adsorption on the metallic NC, thus modifying both the magnetization and the spin-dependent conductance of the hybrid CNT-NC system. The adsorption of benzene on Ni- or Pt-decorated metallic CNTs has been investigated as a test case. The ab initio simulations demonstrate that the magnetization change due to the absorption of a single C_6H_6 molecule should be large enough to be detected experimentally using either magnetic-AFM or SQUID magnetometer. Consequently, the present research suggests a novel approach for single molecule gas detection, based on local magnetic moment measurements in CNT-NC hybrid systems [1].

[1] Z. Zanolli, J.-C. Charlier, ACSnano **6** (2012) 10786-10791.

15 min. break

Topical Talk DS 3.5 Mon 12:00 TRE Ma

Insight into Charge Transport in Molecular Junctions from Ab Initio Theories of Level Alignment — •Jeffrey B. Neaton — Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — Department of Physics, University of California, Berkeley, Berkeley, CA — Kavli Energy Nanosciences Institute, Berkeley, CA

Recent scanning tunneling microscope-based break-junction experiments of molecular junctions – devices formed by trapping organic molecules between macroscopic metallic electrodes – have reported robust conductance, thermopower, switching behavior, quantum interference effects, spin-filtering phenomena, and even nonlinear effects such as rectification, establishing such junctions as unique and revealing windows into the physics of charge transport at the molecular scale. In this talk, I will summarize a predictive approach to compute and understand the transport properties of molecular junctions with good accuracy. Our approach includes important exchange and correlation effects missing in standard DFT Kohn-Sham junction level alignment, building on self-energy corrections within a GW approximation. Advantages and limitations of our approach will be discussed quantitatively in the context of a direct comparison with recent photoemission and transport measurements. I will also describe applications of this approach to select junctions exhibiting novel trends in conductance, thermopower, and nonlinear IV characteristics, where new physical insight is obtained by relating computed transport phenomena to junction structure and chemistry.

DS 3.6 Mon 12:30 TRE Ma

Towards First-Principles Modeling of Solvent Effects in Photo-Catalytic Water Splitting — •Stefan Ringe, Harald Oberhofer, Sebastian Matera, and Karsten Reuter — Technische Universität München, Germany

In the context of solar energy conversion the search for new materials for photo-catalytic water splitting has received new impetus. While in general powerful, computational screening approaches are struggling with the complexity of the underlying physical processes at the solid-liquid interface. Recent work points in particular at the necessity to include at least an efficient description of solvent screening effects to compute meaningful descriptors even in simple computational hydrogen electrode approaches. To this end, we present an implementation of the modified Poisson-Boltzmann (MPB) implicit solvation model in the highly parallel and numerically efficient all-electron DFT code FHI-aims. Optimally integrating into this code environment, we solve the MPB equation in a novel approach based on an expansion of the electrostatic potential in the localized basis functions of FHI-aims. In contrast to common numerical multi-grid solvers this approach can directly make use of the optimized integration schemes used to reach self-consistency and removes the need for numerical interpolation between different grids. We demonstrate the approach and its efficiency for a range of molecular test systems, and show first results for catalytic water splitting on gold nano-clusters.

DS 3.7 Mon 12:45 TRE Ma

Towards a combined QM/MM and implicit solvent description of photoelectrochemical processes — •Markus Sinstein[1], Daniel Berger[1], Ran Jia[2], Volker Blum[3], Harald Oberhofer[1], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Jilin University, P.R. China — [3]Duke University, USA

Photoelectrochemical systems are widely explored to drive energy-relevant redox reactions like water splitting or CO_2 reduction. The detailed analysis of the involved elementary processes via first-principles calculations is challenged by the necessity to simultaneously account for the extended semiconductor photocatalyst and the liquid electrolyte. Especially for charge (proton and/or electron) transfer steps traditionally employed periodic boundary condition approaches involve charged supercells with difficult to control finite size errors. To this end, we present a solid state QM/MM embedding approach, in which only a finite cluster model of the photocatalyst surface is treated quantum mechanically and the correct Madelung potential of the periodic system is obtained by embedding into a charge field. For the efficient modeling of photoelectrochemical processes we combine this approach with an implicit solvation scheme within the DFT package FHI-aims. Finally, we also show early test results of the combined QM/MM implicit solvent model.

DS 3.8 Mon 13:00 TRE Ma

Ab-initio Simulation of Molecular Networks on the Surface of Water — •Ralph Koitz, Marcella Iannuzzi, Ari P Seitsonen, and Jürg Hutter — University of Zurich, Zurich, Switzerland

Molecules adsorbed on surfaces play an important role in catalysis, surface science, and nanotechnology. Traditionally, research has focused on various adsorbates atop metals and metal oxides using computational and surface-science techniques. More recently, however, it was demonstrated that ordered monolayer networks can also be formed on the surface of liquid water by using metal ions to bind together multidentate precursor molecules. As these assemblies are difficult to characterize, computational methods can provide valuable insight into their formation and structure.

In this contribution we present large-scale DFT-based molecular dynamics simulations of the formation of a network of *tris*-terpyridine-derived molecules (TTPB) on a water slab. In particular, we focus on the structure of the molecule on the surface, the mechanism of Zn^{2+} ion insertion from the solution and the subsequent linking of molecules into aggregates. We employ the metadynamics method to quantify the free energy surface of the involved processes. Our results provide detailed insight into on-surface and subsurface diffusion in this system and chemical reactions of TTPB on the surface of water.

DS 4: Magnetic / Organic Interfaces, Spins in Organics and Molecular Magnetism (jointly with MA)

Time: Monday 15:00–17:45 Location: CHE 91

Invited Talk DS 4.1 Mon 15:00 CHE 91

Interfaces of archetype magnetic molecules: from interface dipoles to charge and spin transfer — •Martin Knupfer — IFW Dresden and TU Dresden, Germany

The active control and the manipulation of spin degrees of freedom in organic electronic devices - often called organic spintronics - is anticipated to enable the fabrication of future electronic systems. One way to incorporate the spin degree of freedom is the use of magnetic molecules. For the understanding and development of devices, detailed knowledge on the interaction of such molecules at various interfaces, that are present in devices, is required. We have studied archetype magnetic molecules, the transition metal phthalocyanines, at a number of interfaces to e.g. simple metals, ferromagnetic materials or other organic compounds using spectroscopic methods. These studies provided detailed insight into interactions at such interfaces ranging from interface dipoles to charge and even spin transfer.

The work presented in this contribution has been carried out within the DFG research unit 1154 (Towards molecular spintronics).

DS 4.2 Mon 15:30 CHE 91

Interface and thin film properties of metal-free organic magnets — •Reza Kakavandi, Sabine-Antonia Savu, Thomas Chassé, and Maria Benedetta Casu — Institute of Physical and Theoretical Chemistry, Tübingen, Germany

Metal-free organic-based magnets are relatively new materials with open-shell structure that offer tremendous opportunity in information storage and processing technology, based on the presence of spatially delocalized unpaired electrons. Essential tools such as X-ray Photoelectron Spectroscopy (XPS) and Near Edge X-ray Absorption Fine structure (NEXAFS) Spectroscopy are utilized to study the electronic structure and the paramagnetic character of nitronyl nitroxide radicals deposited on well-defined metal-oxide surfaces. The molecule-substrate interface and the thin film properties are investigated, focusing on their impact on the magnetic character of the systems. In particular, the transitions related to the singly occupied molecular orbitals, expected for this class of materials, are investigated using NEXAFS spectroscopy.

DS 4.3 Mon 15:45 CHE 91

Investigation of the magnetic exchange coupling between MnTPPCl molecules and a ferromagnetic cobalt substrate by X-ray photo-emission electron microscopy — •Jan Girovsky[1], Michele Buzzi[1], Christian Waeckerlin[1], Dorota Siewert[2], Jan Nowakowski[1], Peter M. Oppeneer[3], Frithjof Nolting[1], Thomas A. Jung[1], Nirmalya Ballav[4], and Armin Kleibert[1] — [1]Paul Scherrer Institut, Switzerland — [2]University of Basel, Switzerland — [3]Uppsala University, Sweden — [4]Indian Institute of Science Education and Research, Pune, India

Adsorption of spin bearing metallo-porphyrins and -phthalocyanines on ferromagnetic substrates leads to an exchange induced magnetic moment on the molecules [1]. The magnetic coupling across the magneto-organic interface can be further modified by the introduction of a non-magnetic spacer layer [2]. In this contribution we use X-ray photo-emission electron microscopy combined with X-ray magnetic circular dichroism to study the magnetic exchange coupling between Mn-porphyrin molecules and a ferromagnetic cobalt substrate through a Cr spacer layer with increasing thickness. Our spectro-microscopic correlation enables us not only to study the local magnetic coupling of the molecules, but also their chemical state and the spatial distribution of the respective elements on the sample [3].

[1] A. Scheybal et al., Chem. Phys. Lett. 411, 214 (2005).
[2] C. F. Hermanns et al., Adv. Mater. 25, 3473 (2013).
[3] J. Girovsky et al., Chem. Commun., accepted (2013).

DS 4.4 Mon 16:00 CHE 91

Determination of spin polarized hybridization states of C60 on a ferromagnetic Co(001) surface and its importance for spintronic applications — •Stefan Lach[1], Oliver Ruden[1], Anna Altenhof[1], Shenwei Shi[2], Mats Fahlman[2], and Christiane Ziegler[1] — [1]Technical University of Kaiserslautern and state research centre OPTIMAS — [2]Linköping University, SE-58183 Linköping, Sweden

It is both the high electron affinity resulting in small energy barriers for electron injection at the interfaces with 3d transition metal ferromagnets and its lack of hydrogen and hence no spin dephasing by hyperfine coupling, which makes C60 an important candidate for organic spintronic devices. We present the identification of spin polarized hybrid interface states (sp-HIS) for the C60/Co(001) organic-inorganic interface. Supported by IPES measurements for the unoccupied states and XPS core level spectroscopy, we will show that the also observed Interface dipoles and the spin-split can be explained by covalent bond formation associated with a p-d hybridization between the Co atoms and the C60. Our results provide further insight into the rehybridization reactions of C60 on ferromagnetic substrates beyond a simple charge transfer.This explains the observed interface dipoles and determines the spin-split behavior. The latter is of high importance for spin filtering effects at the C60/Co(001) interface and thus for spintronic devices.

DS 4.5 Mon 16:15 CHE 91

Vertical organic spin-valves with sub-micrometer lateral dimensions — •Robert Göckeritz[1], Bodo Fuhrmann[2], Nico Homonnay[1], Tim Richter[1], Alexander Müller[1], and Georg Schmidt[1,2] — [1]Inst. f. Physik, FG Nanostrukturierte Materialien, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale) — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale)

To get a deeper insight to the underlying physics of spin transport in vertical organic spin-valve devices a promising approach is to go to smaller active device areas. A new fabrication process is presented which offers the possibility to achieve active device areas less than 100nm and which is flexible in terms of material choice for the active layers. As proof of principle magnetoresistance measurements of devices are shown with a large active area of 200x100 micrometer as well as scaled-down device with dimensions of about 500 nm using the organic semiconductor AlQ3 and LSMO and cobalt as ferromagnetic electrodes.

DS 4.6 Mon 16:30 CHE 91

Resistive switching in organic TAMR devices — •Matthias Grünewald, Nico Homonnay, Johannes Kleinlein, and Georg Schmidt — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle

Resistive switching (RS), i.e. the remanent (reversible) change of a device's resistance, is a widely investigated phenomenon as it holds the prospect for realizing high density memory devices. A lot of reports are available in the literature showing results for metal-insulator-metal structures where the insulating layer (often an oxide, rarely an organic semiconductor) is modified and hence the resistance changed. Especially for the oxide based devices a lot of models exist explaining the physics behind the effect. They are prevalently emphasizing the role of oxygen stoichiometry in these materials for their physical properties.

Here we present results showing RS in organic tunneling anisotropic magnetoresistance (TAMR) devices, in which one electrode is a complex oxide ($La_{0.7}Sr_{0.3}MnO_3$) and the organic semiconductor tris-(8-hydroxyquinoline) aluminium (AlQ_3) is used. In contrast to similar studies that demonstrate an interplay of RS and a magnetoresistance effect (MR), the latter is unambiguously identifiable as TAMR in the present devices and allows for probing the tunnel barrier between the oxide electrode and the AlQ_3 layer. This barrier is found to be changed during RS. In order to analyze the RS dynamics the barrier's modification is determined by employing I/V characterization and appropriate fitting procedures in several experiments.

DS 4.7 Mon 16:45 CHE 91

Tailoring the energy level alignment at the Co/Alq$_3$ interface by controlled cobalt oxidation — •Norman Haag, Sabine Steil, Nicolas Grossmann, Roman Fetzer, Mirko Cinchetti, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

We have studied the influence of oxygen exposure at the prototypical interface between cobalt and the organic semiconductor tris(8-hydroxyquinoline)aluminum (III) (Alq_3) by photoemission spectroscopy. We find that oxidation of the cobalt leads to a gradual suppression of hybrid interface states, to a progressive change in the work function and to a continuous energetic shift of the molecular orbitals towards higher binding energies. Based on these observations, we propose controlled oxidation of the ferromagnetic electrode as an easy and effective possibility to tune the performance of organic spintronics devices. Besides this method yields insight into possible origin of the interfacial dipole.

DS 4.8 Mon 17:00 CHE 91

Detailed analysis of sharp nonreactive interface formation in soft-landing conditions: ferromagnetic metallic top contacts onto model wide-gap organic semiconductor using rare-gas condensed at 30K. — •Sergey Babenkov[1], Olga Molodtsova[1], Jens Viefhaus[1], Matthias Kalläne[2], Eric Kröger[2], Arndt Quer[2], Cristoph Seibel[4], Frank Scholz[1], Jörn Seltmann[1], Leif Glaser[1], and Victor Aristov[1,3] — [1]DESY, Hamburg, Germany — [2]CAU, Kiel, Germany — [3]ISSP RAS, Chernogolovka, Russia — [4]UW, Würzburg, Germany

The present work studies the formation of sharp non-reactive metal-organic interfaces at soft landing conditions. In previous work it has been shown that at low coverage of Fe on copper-phthalocyanine (CuPc) there is a strong chemical reaction under room temperature (RT) conditions. In contrast, the results of investigation of size selected clusters in condensed rare gas matrices show almost no diffusion or agglomeration of metal atoms into the organic substrate. In our present investigation by XPS using the PETRA III synchrotron radiation facility at DESY, the formation of interfaces between well-ordered thin film of CuPc with iron and nickel at room and low temperatures (LT) and in condensed Xe matrix were studied. The observed XPS spectra show a strong chemical reaction of the metal with the organic film at RT conditions both for iron and for nickel while at LT with Xe a sharp non-reactive interface formation is observed. This sharp metal-organic interface formation obtained at soft landing conditions can be used for spin injection in spintronic devices.

DS 4.9 Mon 17:15 CHE 91

Fermi level engineering in organic semiconductors for controlled manufacturing of charge and spin transfer materials — •Rico Friedrich[1,2], Berthold Kersting[3], and Jens Kortus[1] — [1]Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Str. 23, D-09596 Freiberg, Germany — [2]Present address: Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [3]Institut für Anorganische Chemie, Universität Leipzig, Johannisallee 29, D-04103 Leipzig, Germany

The rational design of materials for organic electronics and spintronics has been a long-standing challenge. In this presentation it will be demonstrated by theoretical means how to achieve Fermi level engineering in an organic semiconductor like for instance a metal phthalocyanine. It turns out that substitution of the peripheral hydrogen atoms by either fluorine atoms or methoxy groups allows to tune the Fermi level by about 1.5 eV [1]. Finally, we show how such tuning could be exploited to achieve a systematic way to manufacture charge and spin transfer materials by studying the system $(MeO)_8CoPc/F_{16}CoPc$ and compare its electronic and magnetic properties to the first representative of this materials class namely $MnPc/F_{16}CoPc$ [2].

[1] R. Friedrich, B. Kersting, and J. Kortus, Physical Review B **88**, 155327 (2013).
[2] S. Lindner, M. Knupfer, R. Friedrich, T. Hahn, and J. Kortus,

Physical Review Letters **109**, 027601 (2012).

DS 4.10 Mon 17:30 CHE 91

Magnetic Exchange Coupling of Iron-Porphyrin to c(2x2) Oxygen-reconstructed Co(100) Surfaces: Insights from Ab initio Theory — •Md. Ehesan Ali and Peter Oppeneer — Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden

The spin-interface magnetic properties of Fe-porphyrins adsorbed on c(2x2) oxygen-reconstructed Co(100) surfaces have been studied applying density functional theory.[1,2] The electrostatic interaction between electronegative oxygen atoms and the pi-electron cloud of the porphyrin plays a vital role in the binding mechanism of porphyrins to the oxygen-reconstructed surfaces. We have investigated this using various dispersion interactions included functionals in combination with the on-site Coulomb correlation corrected DFT+U method. The surface diffusion of porphyrin molecules is determined from finite-temperature ab initio molecular dynamics simulations, which reveal a promising possibility of controlling the interface magnetic properties upon controlling the molecule-surface dynamics.[3]

References: [1] M. Bernien, J. Miguel, C. Weis, Md. E. Ali et al., Phys. Rev. Lett. 102, 047202 (2009). [2] A. P. Weber, A. N. Caruso, E. Vescovo, Md. E. Ali et al., Phys. Rev. B 87, 184411 (2013). [3] Md. E. Ali and P. M. Oppeneer, Submitted.

DS 5: Organic Electronics and Photovoltaics II (joint session with CPP, HL, O)

Simulations, Polymers, Solar Cells

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

DS 5.1 Mon 15:00 ZEU 222

Quantumchemical Calculation of Zn-Porphyrine-Indolocarbazole-Conjugates — •Ksenia Korshunova and Wichard J. D. Beenken — Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

We have investigated the structure of Zn-porphyrin-indolocarbazole conjugates with a different number of indolocarbazol meso-substituents without and with THF and DMF axial ligands by quantumchemical methods in order to interpret experimental data such as Absorption spectra, fluorescence lifetime and quantum yields in different solutions. Contrarily to our expectations, we found very weak deformation the Zn-porphyrin macrocycle under the influence of axial THF and DMF ligands, which only tend to pull the central Zn-atom out of its equilibrium position in the macrocycle plane. This means that the very different fluorescence yields for Zn-porphyrin-indolocarbazoles in toluole, THF, and DMF cannot be explained by a conformational change.

DS 5.2 Mon 15:15 ZEU 222

Estimating Coulomb model parameters in organic molecules from first principles — •Irina Petreska[1,2], Ljupco Pejov[2], Ljupco Kocarev[3,4], and Gertrud Zwicknagl[1] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, 38 106 Braunschweig, Germany — [2]Faculty of Natural Sciences and Mathematics, Ss. Cyril and Methodius University, 1 000 Skopje, Republic of Macedonia — [3]Macedonian Academy of Sciences and Arts, Skopje, Republic of Macedonia — [4]Faculty of Computer Science and Engineering, Ss. Cyril and Methodius University, 1 000 Skopje, Republic of Macedonia

The Coulomb parameters are estimated from electronic structure calculations based on Density Functional Theory (DFT). Of particular interest are phenylene ethynylene oligomers exhibiting electric-field controlled conductance switching. The charge transport properties are analyzed adopting a simplified two-site model accounting for Coulomb correlation effects. The Coulomb parameters are deduced from a population analysis. The DFT calculations employ a combination of the Becke's three parameter adiabatic connection exchange functional (B3) with the Lee-Yang-Parr correlation one (LYP). The Kohn-Sham SCF equations are iteratively solved using the LANL2DZ basis set, for orbital expansion, on an "ultrafine" grid for numerical integration.

DS 5.3 Mon 15:30 ZEU 222

Theoretical Study of Simultaneous Electron- and Excitation Energy Transfer in a Fullerene-Chromophore Complex — •Thomas Plehn, Jörg Megow, and Volkhard May — Humboldt-Universität zu Berlin, Germany

Mainly during the last decade fullerene based molecular systems have been of increasing interest with regard to future components in dye sensitized solar cells and artificial photosynthetic systems. This theoretical study focuses on the characteristic photoinduced charge separation process in a supramolecular complex containing a single fullerene and six pyropheophorbide-a molecules. For this purpose the excitation energy transfer processes are treated among the six chromophores. Simultaneously electron transfer takes place from the excited chromophores to the fullerene. The whole investigation uses molecular dynamics simulations of the highly flexible complex in explicit solvent environment. The transfer phenomena are described in terms of a special mixed quantum-classical version of the Förster- [1] and the well-known classical Marcus rate. Finally the charge separation process is computed concerning an ensemble of complexes. The resulting dynamics are in very good agreement with appropriate experimental data [2].

[1] J. Megow et al., ChemPhysChem 2011, 12 645-656

[2] M. Regehly et al., J. Phys. Chem. B 2007, 111, 998

Invited Talk DS 5.4 Mon 15:45 ZEU 222

Controlled crystallization of semiconducting polymer thin films — •Sabine Ludwigs — Institute for Polymer Chemistry, University of Stuttgart, Germany

The talk will give an overview over current activities in my team on the morphological control of semiconducting polymers for applications in polymer electronics. Different methods to induce and control crystalline order over large areas in thin films will be presented. These include swelling and deswelling in defined solvent vapour atmospheres of good solvents and crystallization under confinement and with external fields. Regarding polymer materials we are currently extending our studies from conventional p-type semiconductors based on pure thiophenes like P3HT[1] to high performance p-type low bandgap polymers such as PCPDTBT[2] and n-type polymers such as PNDI2OD-2T[3]. The control of molecular orientation over macroscopic distances allows us to study the relationship between the polymer microstructure and the resulting charge transport properties along specific crystallographic directions.

[1] E. Crossland, K. Tremel, F.S.U. Fischer, K. Rahimi, G. Reiter, U. Steiner, S. Ludwigs, Adv. Mater. 2012, 24, 838. [2] F.S.U. Fischer, K. Tremel, A.-K. Saur, S. Link, N. Kayunkid, M. Brinkmann, D. Herrero-Carvajal, J. T. López Navarrete, M. C. Ruiz Delgado, S. Ludwigs, Macromolecules 2013, 46, 4924. [3] K. Tremel, F.S.U. Fischer, N. Kayunkid, R. DiPietro, R. Tkachov, A. Kiriy, D. Neher, S. Ludwigs, M. Brinkmann, Charge Transport Anisotropy in Highly Oriented Thin Films of the Acceptor Polymer P(NDI2OD-T2), submitted.

15 min break

DS 5.5 Mon 16:30 ZEU 222

Conjugated oligomers near surfaces with different physical and chemical nature: MD simulation of adsorption layers — •Olga Guskova[1] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, D-01069 Dresden — [2]Techische Universität Dresden, Institut für Theoretische Physik, Zellescher Weg 17, D-01062 Dresden

Atomistic molecular dynamics simulations are used to explore some general principles of 2D supramolecular organization of conjugated oligomers on adsorbing substrates. Two systems are studied: (i) terminally substituted dicyanovinyl quaterthiophenes, prototypic absorbers for small molecule organic solar cells on a silica surface [1] and (ii) 2,5-dialkoxy-phenylene-thienylene-based oligomers on epitaxial monolayer graphene [2]. We demonstrate that the driving force of molecular orientation on substrate is embodied by the chemical nature of the surface and the character and position of functional groups the conjugated molecule bearing, i.e. the underlying balance of forces defines the spatial orientation - standing upright or lying-down molecules on

substrates. This force balance clearly allows isolated molecules to explore flat, bent or twisted molecular conformations and to exploit force anisotropies to maximize their interactions when crystals are growing.
[1] O.A. Guskova et al. // J. Phys. Chem. C 2013. V. 117. P. 17285.
[2] R. Shokri et al. // J. Am. Chem. Soc. 2013. V. 135. P. 5693.

DS 5.6 Mon 16:45 ZEU 222

Frank elastic constants in nematic mesophases of polymeric semiconductors — •Patrick Gemünden, Kurt Kremer, and Kostas Ch. Daoulas — Max Planck Institute for Polymer Research, Mainz

Liquid crystalline (LC) mesophases of polymeric semiconductors[1] can facilitate material processing. We develop a particle-based modeling approach considering poly(alkylthiophenes) as a test system for studying nematic mesophases. The method uses “soft tube” representations of chains where non-bonded potentials are defined by soft, directional interactions.[2,3] Here, we focus on Frank elastic constants (FC). Calculating FCs is important for comparing material properties from the soft model with experiments, studying theoretical questions related to FCs in polymer nematics and linking particle-based and continuum descriptions of LCs. We calculate FCs related to bend, splay and twist deformations from the fluctuations of the local nematic director. Indeed, the magnitudes of the FCs from our simulations agree with experiments on polymer nematics. We study the dependence on system parameters, e.g. chain length, and compare with predictions by analytical field theory.[4] Eventually we study local density fluctuations in the nematic samples, which, as predicted by theory, lead to an anisotropic scattering pattern and can be related to the elastic properties.

[1] Ho et al., Macromolecules 43, 7895 (2010) [2] Gemünden et al., Macromolecules 46, 5762 (2013) [3] Daoulas et al., J. Phys.: Condens. Matter 24, 284121 (2012) [4] Le Doussal & Nelson, Europhys. Lett. 15, 161 (1991)

DS 5.7 Mon 17:00 ZEU 222

Modeling LC mesophases in polymeric semiconductors with soft directional interactions — Patrick Gemünden, Carl Poelking, Kurt Kremer, Denis Andrienko, and •Kostas Daoulas — Max Planck Institute for Polymer Research, Mainz

Often in Soft Matter mesoscale behavior couples across a hierarchy of scales to details of molecular architecture and interactions. When modeling such materials, features accounting for the latter must be included even in drastically coarse-grained (CG) representations. Focusing on liquid crystalline (LC) mesophases of polymeric semiconductors, we highlight a top-down strategy for developing such models, projecting classical density functionals on particle-based representations. Poly(3-alkylthiophenes) (P3AT) are considered as an example. Two different CG models are developed, representing: a) the polymer chain with a ”soft” flexible tube [1] and b) each alkylthiophene as a plate-like object [2]. The first describes uniaxial nematics and the second captures biaxial nematic ordering, mimicking effects of anisotropy in microscopic interactions and chain architecture. We demonstrate that the model reproduces realistic material properties in nematic mesophases. In biaxial morphologies we discuss how collective orientation and planarization of molecules affects the lengths of conjugated segments, defined via conjugation-breaking torsional defects [3]. First results on the interplay between nematic ordering and phase separation in blends of P3AT with nanoparticles are presented.[1] Daoulas et al, J. Phys.: Condens. Matter (2012) 24, 284121 [2] Gemünden et al, Macromolecules (2013) 46, 5762 [3] Rühle et al, J. Chem. Phys. (2010) 32, 134103.

DS 5.8 Mon 17:15 ZEU 222

Correlating structural order and morphology with transport properties in donor-acceptor block copolymers for organic photovoltaics — •Gaurav Gupta[1], Chetan Raj Singh[2], Ruth Lohwasser[3], Peter Muller Buschbaum[4], Mukundan Thelekkat[3], Harald Hoppe[2], and Thomas-Thurn Albrecht[1] — [1]Martin-Luther-Universität Halle-Wittenberg,Germany — [2]Technische Universität Ilmenau, Germany — [3]University of Bayreuth,Germany — [4]Technische Universität München,Germany

Microphase separated donor-acceptor block copolymers are promising systems for morphology control in OPV’s. A nanostructure on exciton diffusion length scale, crystalline order and percolating pathways for charge transport are pre-requisites for obtaining good device properties. We here present a systematic study of the correlation between structure and charge transport in thin films of P3HT-b-PPerAcr after different thermal treatments. Combining AFM, microscopy and GISAXS we show that films annealed in the melt state above the melting temperatures of both components form typical microphase separated structures oriented parallel to the substrate, while films crystallized from the disordered state as obtained from spin coating show no well-defined microphase separated structures. GIWAXS measurements reveal that crystallization from the ordered state leads to strongly textured samples. Charge carrier mobilities as measured by SCLC were improved by 2 orders of magnitude in films crystallized from the disordered state, the unfavorable orientation of the microphase morphology in melt annealed films resulted in poor device performance.

DS 5.9 Mon 17:30 ZEU 222

Origins of Reduced Nongeminate Recombination in P3HT:PCBM Organic Solar Cells — •Michael C. Heiber[1], Julien Gorenflot[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Understanding the nongeminate recombination processes that are the dominant loss mechanisms in organic solar cells is critical to improving device performance. In P3HT:PCBM blends, nongeminate recombination has been found to be significantly slower than expected from Langevin theory and also exhibits super-second order kinetics. Several theories for this behavior have been proposed, but a complete model has not yet been reached. To shed light on this problem, we have used a combination of transient absorption spectroscopy experiments and kinetic Monte Carlo simulations. By modeling the temperature dependence of the polaron transients measured in both neat P3HT films and annealed P3HT:PCBM blend films, we demonstrate the effects of phase separation, carrier trapping, and charge transfer states on the magnitude of the recombination rate. Furthermore, we show that while neat P3HT films exhibit second order recombination and mobility behavior indicating a Gaussian density of states (DOS), P3HT:PCBM blends are complicated by super-second order recombination that is indicative of an exponential DOS and mobility measurements that are consistent with a Gaussian DOS. To unify these observations, we show that a separate distribution of charge transfer states must be included.

DS 5.10 Mon 17:45 ZEU 222

Model systems for interchromophoric interactions in conjugated polymer materials — •Thomas Stangl[1], Daniela Schmitz[2], Klaas Remmerssen[2], Dominik Würsch[1], Florian Steiner[1], Sigurd Höger[2], Jan Vogelsang[1], and John Lupton[1] — [1]Universität Regensburg, Regensburg, Deutschland — [2]Universität Bonn, Bonn, Deutschland

A set of pi-conjugated oligomer dimers templated in molecular scaffolds is presented as a model system of the interactions between chromophores in conjugated polymers. Single-molecule spectroscopy was used to reveal electronic aggregation between two oligomers with different well-defined distances and single polymer chains. It is concluded that the model systems can be used to investigate the impact of H-aggregation as a function of interchromophoric distance by simultaneous measurement of lifetime and single-molecule spectra. This reveals a strong heterogeneity in coupling strengths even for identical single molecules. Further, it is shown that the coupling strength varies over time on a single molecule, leading to the conclusion that electronic aggregation has to be understood as a dynamic property. In bulk polymer films, such interchromophoric coupling impacts the functionality, e.g. the emission color and the migration of excitation energy to quenching sites. Realizing the presence and dynamics of such interactions is crucial for understanding limitations in quantum efficiency of larger conjugated polymer materials.

DS 6: Thin Film Characterization: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS,...)

Time: Monday 15:00–20:00 Location: CHE 89

DS 6.1 Mon 15:00 CHE 89

Lattice Dynamics and Hyperfine Interactions in fcc Europium Islands — •Olga Bauder[1,2], Przemyslaw Piekarz[3], Anja Seiler[1,2], Shyjumon Ibrahimkutty[1,2], Daniel G. Merkel[4], Marcin Zajac[4], Rudolf Rüffer[4], Tilo Baumbach[1,2], Krzysztof Parlinski[3], and Svetoslav Stankov[1,2] — [1]Laboratory for Applications of Synchrotron Radiation, Karlsruhe Institute of Technology, Germany — [2]Institute for Photon Science and Synchrotron Radiation, Karlsruhe Institute of Technology, Germany — [3]Institute of Nuclear Physics, Polish Academy of Sciences, Poland — [4]European Synchrotron Radiation Facility, France

Employing in-situ nuclear inelastic scattering on 151Eu we investigated the phonon DOS of fcc europium islands with a nominal coverage of 2, 3, 5, 10, and 24 monolayers (ML) grown on the Nb(110)/Al2O3 and compared the results with that of the bulk bcc Eu. The experimental results reveal a systematic shift of the phonon spectrum to high energies and significant suppression of the low-energy phonon modes as the nominal Eu coverage is reduced. The observed phenomenon is attributed to the notable lattice compression of about 9 % in the fcc Eu islands, as well as to the naturally formed monolayer of EuO on the oxygen-induced (6x2) reconstructed Nb(110) surface. These findings are supported by the in-situ nuclear forward scattering spectra that reveal the presence of quantum beats attributed to the difference between the isomer shift of the EuO interface layer and the metallic Eu.

DS 6.2 Mon 15:15 CHE 89

In situ PLD synchrotron characterization for the detection of domain formation during Ba0.5Sr0.5TiO3 growth on MgO — Sondes Bauer[1], •Alan Molinari[2], Sergey Lazarev[1], Andreas Breitenstein[1], Philipp Leufke[2], Robert Kruk[2], Horst Hahn[2], and Tilo Baumbach[1] — [1]Karlsruhe Institute of Technology (KIT), Synchrotron Facility ANKA, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology (INT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

A highly sophisticated pulsed laser deposition (PLD) chamber has recently been installed at the Nano beamline of the synchrotron facility ANKA (Karlsruhe, Germany), which allows for comprehensive studies on the PLD growth process of thin films by combining in situ reflection high energy electron diffraction (RHEED) with the in situ synchrotron high resolution X-ray diffraction and surface diffraction methods.

Ba0.5Sr0.5TiO3(BST) grown on MgO is the first system studied in this in situ PLD chamber being analyzed by in situ X-ray reflectivity, in situ two-dimensional reciprocal space maps (2D-RSMs) and acquisition of time resolved diffraction profiles during the ablation process. The stability of morphology during the PLD growth is demonstrated to be seriously affected by the film thickness: after a critical thickness of hc = 107 nm, BST on MgO reveals a splitting of the diffraction peak into two distinguishable peaks proving the formation of a new kind of domain.

DS 6.3 Mon 15:30 CHE 89

RF-sputtering deposition of Ag: in-situ time-resolved GISAXS investigation — •Gonzalo Santoro[1], Shun Yu[1], Sarathlal K. Vayalil[1], Ralph Döhrmann[1], Daniel Mosegui-González[2], Peter Müller-Buschbaum[2], Margarita Hernández[3], Concepción Domingo[3], and Stephan V. Roth[1] — [1]DESY, Notkestr. 85, D-22607, Hamburg, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, D-85748, Garching, Germany — [3]Institute of Structure of Matter, IEM-CSIC, Serrano 121-123, E-28006, Madrid, Spain

Ag nanocoatings have shown to exhibit excellent properties that can be exploited for applications such as antibacterial coatings, plasmonic devices or sensors [1-3]. However, in order to fully control the desired final properties of the nanocoatings, that are very sensitive to the morphology developed during the deposition, it is mandatory to achieve a profound understanding of the growth kinetics of Ag.

This work presents in-situ time-resolved Grazing Incidence Small Angle X-ray Scattering (GISAXS) results concerning the time evolution of the nanostructures developed during the RF-sputtering of Ag. The Surface Enhanced Raman Spectroscopy (SERS) activity of the prepared Ag coatings for different film thicknesses is also presented and correlated to their nanostructure.

[1] F. Faupel, et al., Adv.Eng. Mat. 12, 1177 (2010); [2] M. Rycenga, et al., Chemical Reviews 111, 3669 (2011); [3] J. Chen, et al., Biosens. Bioelectron. 44, 191 (2013).

DS 6.4 Mon 15:45 CHE 89

metal layer growth on Alq3: towards OLEDs — •Shun Yu[1], Yuan Yao[2], Gonzalo Santoro[1], Peng Zhang[1], Sarathlal Koyiloth Vayalil[1], Matthisas Schwartzkopf[1], Ezzeldin Metwalli[2], Peter Müller-Buschbaum[2], and Stephan V. Roth[1] — [1]Photon Science, DESY, Notkestraße 85, 22607, Hamburg — [2]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic light emitting diodes have entered the market as the next generation digital displays and solid-state lighting devices. Its typical multilayer device structure emphasizes the significance of understanding the interfacial structure and properties. Comparing to evaporate the metal contact, Here we used sputter deposition to prepare Al, Ag and Au electrical contact onto Tris(8-hydroxyquinolinato)aluminium (Alq3), the activating layer. The interaction between metals and Alq3 has been studied by different spectroscopic techniques and theoretical methods at atomic level. The growth of metallic thin film demands deep understanding concerning the dynamic process. In this work, we have exploited in situ grazing incidence small angle X-ray scattering technique to monitor the growth of metallic thin film on top of Alq3 layer during the sputtering process in real time. We elucidate interesting results that the highly reactive Al manifest completely different growth mode compared to the Ag and Au, showing three-stage growth mode, nano-pillar structure and great roughness correlation to the substrate. Whereas, Ag and Au grow in a continuous way involving clustering and coarsening.

DS 6.5 Mon 16:00 CHE 89

Epitaxial MgO/GaAs(001) studied by in-situ X-ray diffraction — •Thomas Hentschel, Michael Hanke, Oliver Bierwagen, Andre Proessdorf, and Jens Herfort — Paul-Drude-Institut Berlin, Hausvogteiplatz 5-7, 10117 Berlin, Germany

The integration of Magnesiumoxide MgO into magnetic tunnel junctions or ferromagnet/semiconductur-hybrid structures acting as a potential tunnel and diffusion barrier has drawn much attention in the last years. Although the growth of MgO by different procedures is well established and used in various applications, its structural properties and growth mechanisms apparently have not been of much interest yet.

This contribution presents *in-situ* X-ray diffraction measurements carried out during molecular beam epitaxy of 5 to 30 nm thick MgO films on GaAs(001). All samples were grown at a substrate temperature of $T_S = 350$ °C by evaporating metallic Mg from an effusion cell with a sapphire crucible and providing additional molecular oxygen at a partial pressure of 10^{-6} mbar. It is observed that the in-plane orientation of MgO depends on the growth rate, while the ouf-of-plane orientation remains unchanged with $\mathrm{MgO}_{[001]}\|\mathrm{GaAs}_{[001]}$. For a growth rate of 1 Å/min the cubic rocksalt structure-like MgO with a misfit of about 25% to GaAs grows directly cube-on-cube on top of the substrate with an in-plane orientation of $\mathrm{MgO}_{[110]}\|\mathrm{GaAs}_{[110]}$. If the growth rate is increased by a factor of 4 the in-plane orientation rotates by 45°. The resulting orientation is $\mathrm{MgO}_{[100]}\|\mathrm{GaAs}_{[110]}$. We attribute this in-plane rotation to unoxidized Mg clusters formed at the GaAs interface.

DS 6.6 Mon 16:15 CHE 89

Optimization of crystal and morphological Parameters wetchemical synthesized $LiNbO_3$-Films — •Doreen Eger, Diana Karsch, Erik Mehner, Hartmut Stöcker, and Dirk Meyer — TU Freiberg - Institut für experimentelle Physik

Lithium niobate is a versatile applicable material. Some applications require thin films on substrates, which can be produced only with high effort until now. The wet-chemical synthesis is an environment friendly alternative for coating. In this contribution the influence of processing parameters of annealing on substrates made of silicium are investigated.

Samples dip-coated with three different sols or solutions are annealed at different high temperatures. For morphology analysis of the films mainly confocal and scanning electron microscopy are used. The portions of crystalline lithium niobate and other phases are investigated by grazing incidence X-ray diffraction.

The coating based on $NbCl_5$ shows the best results. The annealing at about 800 °C for 4 h yields the maximum amount of crystalline Lithium niobate with in parallel minimal impurity phases.

Coffee break (15 min)

DS 6.7 Mon 16:45 CHE 89

Spray pyrolysis of Mo-based nanostructures and thin films — •Marlis Ortel and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen

The high potential of Transition Metal Dichalgonides (TMD) in 2D electrical thin film devices was shown recently. A major bottle neck of the material system is the lack of suitable deposition methods for large-area applications. Up to now mainly electrical devices applying mechanical exfoliation have been reported.

In this work we report on spray pyrolysis of Mo-based nanostructures. Therefore concentration dependent ageing tests of the precursor solution (e.g. H2O, DMSO) were conducted in order to find an optimized starting solution. The layers were grown on silicon dioxide and mica substrates. The solvents utilized were altered with respect to Leidenfrost temperature, surface energy and solubility of the precursor material. Finally the material parameters were correlated with measurements conducted by AFM (atomic force microscopy) and SEM (scanning electron microscope) in order to investigate the physical mechanisms causing the growth of different types of nanostructures, i.e. layers or rods. A fluid mechanics based growth model was developed assuming colloidal growth of the nanostructures in the precursor.

DS 6.8 Mon 17:00 CHE 89

Chemical composition of Mo-based layers deposited by spray pyrolysis — Marlis Ortel, •Torsten Balster, and Veit Wagner — Research Center for Functional Materials and Nanomolecular Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Mechanical and liquid exfoliation are well known techniques to produce nano flakes for high performance transition metal dichalcogenide (TMD) thin film transistors (TFTs). However, up to now there is a lack of deposition processes for large area processing.

In this work, the focus is on spray pyrolysis which is a suitable deposition technology for large area thin film growth. Understanding of decomposition processes during growth is essential to deposite high quality thin films. The chemical composition in the deposited layer results from those decomposition processes and can be monitored by X-ray photoelectron spectroscopy (XPS). The investigated MoS_2 thin films were deposited from non-toxic precursor solutions, e. g. ammonium tetrathiomolybdate (ATTM) dissolved in dimethyl sulfoxide (DMSO). The chemical composition of the thin films was analyzed with respect to the decomposition temperature of the precursor and whether Mo and S can be provided from a single source. Generally, it was found that Mo-based thin films deposited far above the decomposition temperature (e.g. at 360°C) require an additional sulfur source to successfully grow MoS_2.

DS 6.9 Mon 17:15 CHE 89

Combinatorial epitaxial strained film growth: a new tool to adjust functional properties — •Sandra Kauffmann-Weiss[1,2,3], Sven Hamann[4], Ludwig Reichel[1,2], Alexander Siegel[4], Vasilis Alexandrakis[4], Rene Heller[5], Alfred Ludwig[4], Ludwig Schultz[1,2], and Sebastian Fähler[1,3] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Dresden University of Technology, Institute for Materials Science, 01062 Dresden, Germany — [3]Technische Universität Chemnitz, Faculty of Natural Science, Institute of Physics, 09107 Chemnitz, Germany — [4]Ruhr-University Bochum, Faculty of Mechanical Engineering, Institute of Materials, 44801 Bochum, Germany — [5]Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany

Whereas in bulk lattice parameters can only be changed by composition or temperature, coherent epitaxial growth of thin films allows adjusting the lattice parameters independently. Up to now only discrete values were accessible by using different buffer layers or substrate materials. As a new tool for an efficient search for optimum parameter we present a continuous variation of lattice parameters of an alloy buffer layer by combinatorial film deposition of a Cu-Au layer on wafer level. These libraries are versatile as they allow tuning functional properties of various types of materials, ranging from (magnetic) shape memory alloys over multiferroics to permanent magnets.

Work was funded by DFG through SPP 1239 and EU through REFREEPERMAG.

DS 6.10 Mon 17:30 CHE 89

Investigating the oxidation process of the $Pt_3Ti(111)$ alloy surface on the atomic scale — •Marco Moors[1,2], Maria Buchholz[2,3], Séverine Le Moal[2,4], Klaus Wandelt[2,5], and Rainer Waser[1] — [1]Forschungszentrum Jülich — [2]Universität Bonn — [3]Karlsruher Institut für Technologie — [4]Université Paris Sud — [5]University of Wroclaw

The oxidation of reactive bimetallic alloys like the $Pt_3Ti(111)$ surface is a promising approach to grow atomically thin titanium oxide films with a high degree of surface order on a metallic conducting substrate. Depending on the used preparation conditions several ordered oxide phases with both rectangular and hexagonal symmetry have been observed. The morphology of these phases is dominated by the surface strain caused by the interplay of the hexagonal substrate symmetry and the favoured rectangular oxide symmetry.

In this presentation the focus is set on the investigation of the first steps of the complex oxidation process on the atomic scale. At low oxygen pressures a titanium oxide phase with a characteristic zigzag structure is formed by a temperature induced segregation process of titanium atoms from the bulk to the outermost surface layer. By variation of the oxygen dosage and temperature the oxide coverage can be controlled ranging from small single islands up to the complete coverage of the entire surface. Due to the surface strain in all cases a regular arrangement of surface defects along the trenches between the zigzag lines can be observed, which may be important for the catalytic activity as well as for self assembly processes.

DS 6.11 Mon 17:45 CHE 89

Isolating free-standing diamond-like carbon membranes from coated biodegradable plastic materials — •Christian B. Fischer, Bastian Pause, Lukas Hoffmann, Alberto Catena, and Stefan Wehner — Department of Physics, University Koblenz-Landau, 56070 Koblenz, Germany

Diamond-like carbon (DLC) as an isolated single free-standing thin film is a very exciting material since it exhibits outstanding properties like high hardness, chemical inertness, selective barrier characteristics etc. The preparation of a 100 nm thick single free-standing DLC-film follows the route of depositing carbonaceous precursors on selected supporting materials first. The isolation of single DLC-pieces is very challenging and comprises several single steps in general. In the present work we report an easy access for stable isolated amorphous carbon (a-C:H) films via delamination from a coated biodegradable polymer. DLC contains a mixture of sp3- and sp2-centers determining its intrinsic hardness. By enhancing the proportion of sp2-carbons a more flexible carbon layer on the pure bioplastic polyhydroxybutyrat (PHB) foil as support is realized by PECVD. Delamination is performed using several organic solvents. The surface structures of uncovered materials and isolated thin films have been analyzed by SEM and AFM spectroscopy. Significant differences of the contact side depending on the used solvent are found. This provides further insights into the interaction of hard DLC coating and soft plastic material.

DS 6.12 Mon 18:00 CHE 89

Strontium segregation in LaAlO3/SrTiO3 and NdGaO3/SrTiO3 oxide heterostructures investigated by XPS — •Uwe Treske[1], Nadine Heming[1], Martin Knupfer[1], Bernd Büchner[1], Emiliano Di Gennaro[2], Umberto Scotti di Uccio[2], Fabio Miletto Granozio[2], and Andreas Koitzsch[1] — [1]Institute for Solid State Research, IFW-Dresden, P.O. Box 270116, DE-01171 Dresden, Germany — [2]CNR-SPIN and Dipartimento di Fisica, Complesso Universitario di Monte S.Angelo, Via Cintia, 80126 Naples, Italy

Pulsed laser deposition grown $LaAlO_3$ and $NdGaO_3$ on TiO_2-terminated $SrTiO_3$ with different film thicknesses were investigated by soft X-ray photoemission spectroscopy. The surface sensitivity of the measurements has been tuned by varying photon energy $h\nu$ and emission angle Θ. In contrast to the core levels of the other elements, the

Sr 3*d* line shows an unexpected splitting for higher surface sensitivity, signaling the presence of a second unexpected strontium component. From our quantitative analysis we conclude that during the growth process Sr atoms diffuse away from the substrate and segregate at the surface of the heterostructure, possibly forming strontium oxide.

Coffee break (15 min)

DS 6.13 Mon 18:30 CHE 89

Structural characterization of CeO2 thin films grown on Yttria-Stabilized Zirconia — •Björn Arndt[1,2], Patrick Müller[1,2], Heshmat Noei[1], Thomas Keller[1], Vedran Vonk[1], Andreas Nenning[3], Jürgen Fleig[3], and Andreas Stierle[1,2] — [1]Deutsches Elektron-Synchrotron (Desy), D-22607 Hamburg, Germany — [2]Fachbereich Physik, Universität Hamburg, D-20355 Hamburg, Germany — [3]Institute of Chemical Technologies and Analytics, Vienna University of Technology, 1060 Vienna, Austria

Apart from its use in catalytic converters, CeO2 offers a variety of possible applications: for hydrogen production via photon induced water-splitting, as a support for metal nanoparticles, or as an electrolyte or anode material for Solid-Oxide Fuel Cells. The reason for this lies in the ability of CeO2 to form oxygen vacancies in the bulk and at the surface, thus being able to store, conduct and release oxygen. Doping with a trivalent oxide (in this case Gadolinia) induces oxygen vacancies, making them available under non-reducing conditions. For a better understanding of the above mentioned properties of Ceria, it is important to study its structure under oxygen-deficient conditions. Therefore, 10% Gd-doped CeO2 thin films were grown on Yttria-Stabilized Zirconia (110) and (111) by pulsed laser deposition, inducing a nominally 5% oxygen vacancy concentration in the films. The films were studied by grazing incidence x-ray diffraction, x-ray reflectivity and atomic force microscopy. XRD-Measurements were performed at the ID03-Beamline at the ESRF as well as using a conventional lab source. The films are shown to be atomically smooth and epitaxial to the YSZ substrates.

DS 6.14 Mon 18:45 CHE 89

Partial Crystallinity in Alkylsilanes Monolayers — •Hans-Georg Steinrück[1], Moshe Deutsch[2], Ben Ocko[3], and Andreas Magerl[1] — [1]1Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen Nürnberg, Germany — [2]Bar-Ilan University, Ramat- Gan, Israel — [3]Brookhaven National Laboratory, Upton NY, USA

Alkylsilane (denoted as Cn, n = 12, 14, 18, 22, 30) self-assembled monolayers (SAMs) on the amorphous oxide of silicon are vertically aligned and densely packed as shown by X-ray reflectivity. A new 3-slab model simulating the electron density profile was developed yielding only four free fit parameters (roughnesses of each interface and the density of one slab). All other parameters for the alkyl chain were fixed to the values in the rotator phase [1] and to the chemical bond length in the linker group region. For all Cn, expect C12, a hexagonal ordering with a lattice constant of $a = 4.82\ \AA$ is revealed by X-ray grazing incidence diffraction. Interestingly, the analysis of the intensity distribution along q_z (Bragg rod) reveals that crystalline phase is less than the length of the molecule. We argue that this reflects gauche defects at the chain ends [2] as well as steric hindrance in the linker group region [3]. The percentage of the surface normal crystalline part of the alkyl chain increases up to 60% for C18 and linearly drops down to 40% for C30.

[1] Ocko, B.M. et al., PRE 1997, 55, 3164-3182.
[2] Allara, D.L. et al., Langmuir 1995, 2357-2360.
[3] Prasad, S. et al., A. PRL 2008, 101, 065505-065505.

DS 6.15 Mon 19:00 CHE 89

Non-destructive and non-preparative chemical nanometrology of interfaces at tunable high information depths — •Beatrix Pollakowski[1], Peter Hoffmann[2], Marina Kosinova[3], Olaf Baake[2], Valentina Trunova[3], Rainer Unterumsberger[1], Wolfgang Ensinger[2], and Burkhard Beckhoff[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany — [2]Technische Universität Darmstadt, Materials Sciences, Darmstadt, Germany — [3]Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia

The development of improved characteristics of functional nanoscaled devices involves novel materials, more complex structures and advanced technological processes, requiring analytical methods to be well adapted to the nanoscale. Thus, non-destructive and non-preparative techniques for chemical nanometrology providing sufficient sensitivity, reliable quantification and high information depths to reveal interfacial properties. Appropriate measurement strategies adapted to a nanoscaled stratified sample enables the combined technique NEXAFS and GIXRF to provide interfacial species information. The validation of this method for interface speciation has been performed at nanolayered model structures consisting of a Si substrate, a physically vapor deposited Ni metal layer and, on top, a chemically vapor deposited $B_xC_yN_z$ light element layer. The chemical bonds in the interfaces were to be determined by the GIXRF-NEXAFS technique. B. Pollakowski et al., Anal. Chem. 85,193 (2013)

DS 6.16 Mon 19:15 CHE 89

Quantitative grazing incidence X-ray fluorescence analysis for reference-free elemental depth profiling of thin films — •Cornelia Streeck[1], Beatrix Pollakowski[1], Christian Herzog[2], Janin Lubeck[1], Martin Gerlach[1], Philipp Hönicke[1], Rainer Unterumsberger[1], Stephan Brunken[3], Christian Kaufmann[3], Burkhard Beckhoff[1], Birgit Kanngiesser[2], and Roland Mainz[3] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin — [2]Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 12109 Berlin

Synchrotron-radiation based X-ray fluorescence analysis under grazing incidence (GIXRF) conditions provides a non-destructive access to the compositional depth profile of thin films in the nano and micro meter range. Using reference-free GIXRF measurements and a fundamental parameter based quantification no well-characterized standards for calibration purposes are required. As an example, thin films of Cu(In,Ga)Se2 (CIGSe) have been were investigated, which are used as absorber layer of thin film solar cells. In the case of CIGSe, a graded band gap is created by a depth-dependent variation of the absorber matrix elements. To correlate the device functionality with the respective material properties, both the absolute composition and the in-depth gradient in CIGSe thin films require reliable determination. Due to the lack of appropriate reference materials, non-destructive GIXRF is used to address this analytical challenge.

DS 6.17 Mon 19:30 CHE 89

Resonant Soft X-Ray Reflectometry on strained $LaSrMnO_4$ thin films — •Martin Zwiebler[1], Jorge-Enrique Hamann-Borrero[1], Mehran Vafaee[2], Ronny Sutarto[3], Feizhou He[3], Lambert Alff[2], Bernd Büchner[1], and Jochen Geck[1] — [1]IFW Dresden, Helmholtzstraße 20, 01097 Dresden, Germany — [2]Institute of Material Sciences, Technische Universität Darmstadt, 64287 Darmstadt, Germany — [3]Canadian Light Source Inc., 44 Innovation Boulevard, Saskatoon SK S7N 2V3, Canada

The strong electron-lattice coupling in the perovskite manganites provides a unique opportunity to tune the electronic properties of these materials via lattice strain. $LaSrMnO_4$ is a good model material with well-known orbital occupation in the bulk material. We present a study of the depth-resolved electronic properties in a tensile strained $LaSrMnO_4$ film by the means of resonant X-ray reflectometry (RXR) and XAS. We find evidence for Mn^{2+} on the surface and we extract the depth profile of the Mn valence throughout the film.

DS 6.18 Mon 19:45 CHE 89

Resonant X-ray reflectometry study of $YBa_2Cu_3O_{7-\delta}$ thin films: An atomic approach to reflectivity — •Jorge E. Hamann-Borrero[1], Sven Partzsch[1], Benjamin Gray[2], Sebastian Macke[3], Enrico Schierle[4], Martin Zwiebler[1], John W. Freeland[5], Jak Chakhalian[2], Bernd Buechner[1], and Jochen Geck[1] — [1]IFW-Dresden — [2]Department of Physics University of Arkansas, USA — [3]Max Planck-UBC Centre for Quantum Materials, Vancouver, Canada — [4]Helmholtz-Zentrum Berlin für Materialien und Energie — [5]Advanced Photon Source, Argonne National Laboratory, Illinois, USA

We present a Cu $L_{2,3}$ Resonant X-ray Reflectometry study of a (001)-YBCO thin film grown on $SrTiO_3$. The reflectivities measured using σ and π polarized light show a strong dichroism due to the local anisotropy of the different copper sites at the plane and chain layers of this compound. Within the scanned **q**-range also the (001) Bragg reflection appears highlighting the importance of the interference between the different scattering centers in the sample.

In order to describe the observed intensities, traditional models such as the Parrat's formalism fail, since they neglect the interference between the atomic scatterers. Therefore, we employed a new atomistic approach to model reflectivity where the most important structural, finite size, surface and interface effects, are considered by explicitly defining the atom positions together with their anisotropic scattering form factors. First calculations will be presented and discussed.

DS 7: Focus Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale II (jointly with O)

Time: Monday 16:00–18:45 Location: TRE Ma

Topical Talk DS 7.1 Mon 16:00 TRE Ma

Simulating heat transport: from large scale molecular dynamics to first-principles calculations — •Davide Donadio — Max Planck Institute for Polymer Research, Mainz, Germany

The necessity to design materials and devices able to harness thermal energy, and possibly convert it into more amenable energy forms, has stimulated a major effort in the scientific community to understand heat transport at the mesoscale and the nanoscale. In this talk I will discuss different atomistic approaches to simulate nanoscale heat transport, ranging from large scale molecular dynamics simulations with classical empirical potentials at equilibrium and non-equilibrium conditions, to lattice dynamics calculations with force-constants computed by first principles. Applications will include silicon and carbon nanostructures, phase-change materials and molecular junctions.

DS 7.2 Mon 16:30 TRE Ma

First principles study of thermal conductivity cross-over in nano-structured Zinc-Chalcogenides — •Ankita Katre[1], Atsushi Togo[2], Ralf Drautz[1], and Georg K. H. Madsen[1] — [1]ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]ESISM, Kyoto University, Sakyo, Kyoto 606-8501, Japan

Nano-structured Zinc-Chalcogenides are interesting for thermoelectric applications due to their low thermal conductivity.[1] A simple model study has reported how the thermal conductivity of ZnS, ZnSe and ZnTe can potentially show a cross-over as a function of the maximal mean free path of the phonons.[2] We have applied the Boltzmann transport equation in the relaxation time approximation to verify this. We find that thermal conductivity of ZnS crosses ZnSe and ZnTe and explain this in terms of the different contributions of phonon modes in these materials. Furthermore, the cross-over is found to be strongly influenced by isotope scattering. The calculated thermal conductivity is found to be strongly dependent on the volume and we explain the observed differences between LDA and GGA calculations. We compare further calculated thermal properties, such as the thermal expansion coefficient, to experiment to validate our approach.

[1] L.Zhen, S.Qiao, D.Y.Xiang, H.Z.Zhong, and Q.L.Gao, J. Mater. Chem. 22, 22821 (2012). [2] N.Mingo and D.Broido, Phys. Rev. Lett. 93, 246106 (2004).

DS 7.3 Mon 16:45 TRE Ma

Density-functional perturbation theory for lattice dynamics with numeric atom-centered orbitals — •Honghui Shang, Christian Carbogno, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin

The response of the electronic structure to atomic displacements gives rise to a variety of interesting physical phenomena, which can be probed by experimental techniques such as infrared or Raman spectroscopy or neutron diffraction. The response can be conveniently computed from first principles by means of density-functional perturbation theory (DFPT). Here we present our implementation in the all-electron atom-centered numeric orbital code FHI-aims [1]. Our approach combines the accuracy of an all-electron full-potential treatment with the computationally efficiency of localised atom-centered basis sets that is necessary to study large and complex systems. We verified the accuracy of our DFPT implementation by comparing the vibrational frequencies to finite-difference reference calculations and literature values. Due to the atom-centered nature of the integration grids in FHI-aims, the portion of the grid that belongs to a certain atom also moves when this atom is displaced. Here we demonstrate that, unlike for first derivatives (i.e. forces) [2], this moving-grid-effect plays an important role for second derivatives (i.e. vibrational frequencies). Further analysis reveals that predominantly diagonal force constant terms are affected, which can be bypassed efficiently by invoking translational symmetry.

[1] V. Blum et al. Comp. Phys. Comm. 180, 2175 (2009)

[2] B. Delley, J. Chem. Phys. 94, 7245 (1991).

DS 7.4 Mon 17:00 TRE Ma

Breakdown of Fourier law in layered materials — •Andrea Cepellotti[1], Giorgia Fugallo[2], Francesco Mauri[3], and Nicola Marzari[1] — [1]THEOS, École Polytechnique Fédérale, Lausanne — [2]IMPMC, Universite Pierre et Marie Curie, Paris — [3]LSI, École Polytechnique, Paris

We compute the thermal conductivity in crystalline layered materials by solving the Boltzmann Transport Equation (BTE) for phonons [1], with the phonon-phonon collision rates obtained from density-functional perturbation theory. We find that in 2D materials, such as graphene and related compounds, and even in 3D layered materials, like bulk graphite, the single-mode relaxation time approximation (SMRTA) cannot describe heat transport correctly, underestimating by one order of magnitude or more thermal conductivities and phonons' mean free paths. Instead, we show that the exact self-consistent solution of the BTE provides results in excellent agreement with experimental measurements [2]. The shortcomings of the SMRTA lie in the assumption that heat flow is transferred only by individual phonon excitations, whereas in layered materials the transport can only be explained in terms of collective phonon excitations. The characteristic length of these collective excitations is often comparable with that of the experimental sample - as a result, Fourier's law become questionable, since its statistical nature makes it applicable only to systems larger than a few mean free paths.

[1] G. Fugallo et al., Phys. Rev. B, **88**, 045430 (2013).

[2] A. A. Balandin, Nat. Mater. **10**, 569 (2011).

DS 7.5 Mon 17:15 TRE Ma

High Temperature Thermal Conductivity from First Principles — •Christian Carbogno[1], Rampi Ramprasad[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Chemical, Materials & Biomolecular Engineering, University of Connecticut, Storrs, USA

In spite of significant research efforts, a first principles determination of the thermal conductivity at high temperatures has remained elusive. Under such conditions, Boltzmann transport techniques [1] that include anharmonic effects only perturbatively become inaccurate or even inapplicable. In this work, we overcome this limitation by performing first-principles Green-Kubo simulations [2], in which all orders of anharmonicity are incorporated by the means of *ab initio* molecular dynamics. The thermal conductivity is then assessed from the autocorrelation function of the heat flux in thermodynamic equilibrium. We discuss the details of our implementation and the definition of our heat flux that is based on the virial theorem. We validate our approach by presenting calculations for ZrO_2 that also showcase the importance of higher order anharmonic effects in materials with low thermal conductivities. Eventually, we discuss how our technique can be coupled to multi-scale models to achieve a computationally efficient and accurate description of the thermal conductivity at the nanoscale.

[1] D. A. Broido *et al.*, *Appl. Phys. Lett.* **91**, 231922 (2007).

[2] R. Kubo, M. Yokota, S. Nakajima, *J. Phys. Soc. Jpn.* **12**, 1203 (1957).

DS 7.6 Mon 17:30 TRE Ma

Accurate Modelling of the Polymorphism and Elastic Response of Molecular Materials from First Principles — •Anthony Reilly and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Molecular materials are of great fundamental and applied importance in science and industry, with numerous applications in pharmaceuticals, electronics, sensing, and catalysis. A key challenge for theory has been the prediction of their stability, polymorphism and response to perturbations. While pairwise models of van der Waals (vdW) interactions have improved the ability of density functional theory (DFT) to model these systems, quantitative and even qualitative failures often remain. Here, we show how a many-body description of vdW interactions can dramatically improve the accuracy of DFT for molecular materials, yielding quantitative description of stabilities and polymorphism for these challenging systems. Moreover, the role of many-body vdW interactions goes beyond stabilities to response properties. In particular, we have studied the elastic properties of a series of molecular crystals, finding that many-body vdW interactions can account for up to 30% of the elastic response, leading to quantitative and qualitative changes in elastic behavior. We will illustrate these crucial effects with the challenging case of the polymorphs of aspirin, leading to a better understanding of the conflicting experimental and theoretical studies of this system.

DS 7.7 Mon 17:45 TRE Ma

Surface chemistry on nanostructured oxides: do we have to go beyond hybrid DFT? — •Daniel Berger, Harald Oberhofer, and Karsten Reuter — Technische Universität München, Germany

Nanostructured oxide surfaces are promising candidates for a wide range of energy and catalysis applications. For first-principles modeling of corresponding surface chemical reactions the current state-of-the-art is generally defined by hybrid-level density-functional theory (DFT). Systematic work assessing the achieved accuracy at this level is nevertheless scarce, also owing to the fact that higher-level reference methods are often not available for standard periodic boundary condition supercell calculations. To this end, we present a study benchmarking semi-local and hybrid DFT against (renormalized) second-order perturbation theory (MP2,rPT2) as recently implemented in the FHI-aims package [1]. We make the efficient usage of the latter theories for oxide surfaces possible through a solid-state embedding framework, in which a central cluster region is described quantum mechanically, the long-range electrostatic interactions in the oxide are accounted for through a polarizable monopole field, and a shell of norm-conserving pseudopotentials correctly connects the two regions. We illustrate the performance of the various levels of theories using the water-splitting reaction at ideal and defected $TiO_2(110)$ surfaces as showcase. [1] X. Ren *et al.*, Phys. Rev. B **88**, 035120 (2013)

DS 7.8 Mon 18:00 TRE Ma

Atoms-in-solids perspective on polarizabilities and van der Waals coefficients in semiconductors — •Guo-Xu Zhang, Anthony M. Reilly, Alexandre Tkatchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

The calculation of response properties of solids including their polarizabilities and van der Waals (vdW) coefficients usually requires the knowledge of the full electronic bandstructure. For non-covalently bound solids, such as noble-gas and ionic crystals, atoms-in-solids model can be successfully utilized to define their polarizabilities. Here we critically assess the atoms-in-solids model for covalently-bound solids, ranging from wide-gap (10 eV) to narrow-gap (below 1 eV) semiconductors. We model their response by assigning a single quantum harmonic oscillator to every atom, where the parameters of the oscillators are defined as functionals of the electron density, following the Tkatchenko-Scheffler method [1]. The response function is then calculated by solving self-consistent screening equations of classical electrodynamics, without any explicit information about the electronic bandstructure [2]. The calculated polarizabilities and vdW coefficients for 23 semiconductors are compared with TDDFT and experimental benchmark data, revealing an overall agreement within 10%. The efficiency of our method and the accuracy of the calculated vdW parameters allows us to demonstrate the crucial role of vdW interactions in the cohesive properties of the 23 semiconductors. [1] Tkatchenko and Scheffler, PRL (2009); [2] Tkatchenko, DiStasio, Car, Scheffler, PRL (2012).

DS 7.9 Mon 18:15 TRE Ma

Adsorption at semiconductor surfaces - an energy analysis method — •Ralf Tonner and Marc Raupach — Fachbereich Chemie & Materials Sciences Centre, Philipps-Universität Marburg, Germany

The chemical bond is one of the most fundamental concepts in chemistry. Classifications such as covalent, ionic or metallic bonding are central in discussing trends in different compounds and predicting new reactivity. Several very helpful concepts and methods were developed to understand the chemical bond at surfaces.[1] The question about energetic contributions to surface chemical bonds on the other hand did not receive great attention although energy changes are the ultimate driving force in bond formation.

Starting from preliminary work by Philippsen and Baerends,[2] we implemented all terms of an Energy Decomposition Analysis (EDA) to obtain quantitative data about energetic contributions to chemical bonding in periodic systems. This periodic EDA method was applied to questions of chemisorption of organic molecules at semiconductor surfaces where it can shed light on the nature of the surface-adsorbate bonds.

[1] a) A. Nilsson, L. G. M. Pettersson, J. Nørskov, Chemical Bonding at Surfaces and Interfaces, Elsevier, Amsterdam, 2007; b) A. Groß, Theoretical Surface Science, Springer, Berlin, Heidelberg, 2009. [2] P. H. T. Philipsen, E. J. Baerends J. Phys. Chem. B 2006, 110, 12470.

DS 7.10 Mon 18:30 TRE Ma

Non-local density functionals meet many-body dispersion: A hybrid approach for van der Waals interactions — •Jan Hermann, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Different approaches to treating van der Waals (vdW) interactions in density-functional theory can be loosely divided into the atom-based and the ones based on non-local functionals. The first type comprises a range of methods from atom-pairwise additive schemes by Grimme to many-body dispersion (MBD) approach of Tkatchenko et al. Usually, these methods require precalculated atomic parameters and thus rely on information not explicitly contained in the electron density. The other category consists of nonlocal functionals either of the Langreth and Lundquist or the Vydrov and van Voorhis (VV) type. In these approaches, the vdW interaction is obtained as a functional of the electron density and at most a few tuning parameters are needed.

Here, we show that these two contrasting approaches can be synergistically combined. We use the polarizability from the nonlocal functional of VV within the MBD method of Tkatchenko et al. Such a combination is worthy for several reasons. First, it is an atom-centered approach with no atomic parameters. Second, it puts aside the problem of partitioning electron density between atoms, which can be problematic in some cases. Third, it enables more direct comparison of so far unrelated methods. Fourth, it highlights the idea of combining working elements from different approaches.

DS 8: Organic Electronics and Photovoltaics III (jointly with CPP, HL, O)

Time: Monday 18:00–19:45 Location: CHE 91

DS 8.1 Mon 18:00 CHE 91

Studying the electric potential of organic solar cells — •Michael Scherer[1,2,3], Tobias Jenne[1,2,3], Rebecca Saive[1,2,3], Felix Schell[1,2,3], Robert Lovrincic[1,2,3], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab GmbH, Heidelberg — [2]TU Braunschweig — [3]Universität Heidelberg

Despite steadily increasing efforts in the research on organic semiconductors, many of the models applied in the field are restricted to small clusters of molecules or model systems only, thus lacking prediction when it comes to full devices. With scanning Kelvin probe microscopy (SKPM) accompanied by device simulations we try to access the physics of entire OSC devices and bridge the gap between the molecular and the macroscopic understanding.

Our scanning probe station is placed within the vacuum of a scanning electron microscopy (SEM)/focused ion beam (FIB) cross beam system. We prepare OSC cross sections with the FIB and place the cantilever under SEM observation right at the cross section. Thus we are able to investigate the potential distribution of OSCs in situ with SKPM.

The SKPM measurements are backed by IV characterization and device simulations. Varying the parameter of the active layer/contact interface, we investigate their impact on the potential distribution and the device characteristics of the OSC. In IV measurements and cross sectional SKPM measurements we check the validity of the applied models and identify loss mechanisms and their localization in the solar cell device.

DS 8.2 Mon 18:15 CHE 91

Correlation of electric properties and interface band alignment in organic light-emitting diodes — •Maybritt Kühn[1,2], Eric Mankel[1,2], Christof Pflumm[3], Thomas Mayer[1,2], and Wolfram Jaegermann[1,2] — [1]Technische Universität Darmstadt, Institute of Materials Science, Surface Science Division — [2]InnovationLab GmbH, Heidelberg — [3]Merck KGaA, Darmstadt

Organic light-emitting diodes consist of several functional organic layers sandwiched between two electrodes with different work functions. At the current onset voltage the applied electric field is high enough that charge carrier injection and transport begins. In some device structures the onset voltage increases with increasing thickness of the emission layer. We present a detailed study on this up to now unpredictable phenomenon by combining IV-measurements and interface investigations using photoelectron spectroscopy (XPS/UPS). We focus on two isomers synthesized by Merck that serve as matrix material in the emission layer-one showing the changes in onset voltage the other not. The complex device architecture was reduced to a model device system using NPB as hole-transport layer and the undoped isomers as emission layer. The shift in onset voltage can still be observed in the model devices as well in hole-only devices derived from the model system. By stepwise evaporation of the respective isomer onto NPB we performed PES-interface experiments and analyzed the band alignment between NPB and the isomers in an integrated UHV system. It was found that the hole injection barrier is larger by about 200 meV in case of the isomer showing the observed shift in onset voltage.

DS 8.3 Mon 18:30 CHE 91

Temperature dependent exciton diffusion length in ZnPc — •Bernhard Siegmund[1], Johannes Widmer[1], Simone Hofmann[1], Moritz Riede[2], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Dresden, Germany — [2]Current address: Clarendon Laboratory, Oxford, England

The photo-current of organic solar cells is the result of a multi-step process. It includes the generation and diffusion of excitons as well as their separation into free charge carriers, the transport to the electrodes, and their final extraction. One bottleneck for highly efficient devices is the short exciton diffusion length in organic materials.

In this work, the singlet exciton diffusion length ℓ_{diff} in the absorber material ZnPc is studied. For this purpose, the photo-current of organic solar cells, incorporating ZnPc and C$_{60}$ in a flat heterojunction architecture, is measured and modelled as a multi-step process. ℓ_{diff} is extracted from a thickness variation of the absorber layer, as not yet encountered in the context of modelling the photo-current to determine ℓ_{diff} before. Measurements at varying temperature between 200 K and 370 K reveal a thermal activation of the diffusion length above 310 K. This is interpreted as promotion of the excitons to higher energies with a density of states allowing for enhanced hopping transport. The activation energy is considered as a measure for the energetic disorder of the excitonic states. These investigations aim for a better understanding of exciton migration in order to design materials with longer exciton diffusion lengths for highly efficient organic solar cells.

DS 8.4 Mon 18:45 CHE 91

The effect of gradual fluorination on the opto-electronic properties of F$_n$ZnPc/C$_{60}$ bilayer cells — •M. Brendel[1], A. Steindamm[1], A. Topczak[1], and J. Pflaum[1,2] — [1]Exp. Phys. VI, JMU Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

The respective position of energy levels at the donor/acceptor heterojunction is crucial for the resulting parameters of an organic solar cell. For instance the open circuit voltage (V$_{oc}$) is correlated to the energy difference between the highest occupied molecular orbital (HOMO) of the donor and the lowest unoccupied molecular orbital (LUMO) of the acceptor, the so-called effective band gap (E$_{g,eff}$). To gain insights into this correlation, tailoring of energy levels by chemical modification is a powerful approach. In this contribution, we investigate the impact of gradual fluorination of zinc phthalocyanine on the opto-electronic properties of F$_n$ZnPc/C$_{60}$ (n=0,4,8,16) bilayer cells. Upon fluorination, HOMO and LUMO levels are shifted towards lower energies. The gain in V$_{oc}$ for F$_4$ZnPc/C$_{60}$ and F$_8$ZnPc/C$_{60}$ by 11% and 23% respectively, compared to ZnPc/C$_{60}$, confirms qualitatively the expected energy level scheme. Besides, the differences between $e \cdot \Delta$ V$_{oc}$ and ΔE$_{g,eff}$ hint at the occurrence of dipoles and their gain in strength with increasing degree of fluorination. As will be shown, this dipol can be correctly accounted for in a plate capacitor geometry, considering image charges at the interface induced by electronegative fluorine in the immediate vicinity of C$_{60}$ molecules. We thank S. Sundarray and P. Erk from BASF for providing F$_4$ZnPc. Financial support by the DFG (program SPP1355) and the BMBF (GREKOS program).

DS 8.5 Mon 19:00 CHE 91

Effect of Counter-Anions During Electrodeposition on the Charge Transport Dynamics in Sensitized *ZnO* Solar Cells — •Christoph Richter, Max Beu, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Thin porous *ZnO*/*EosinY* films have been electrochemically deposited from oxygen-saturated aqueous solution. During the electrochemical deposition chloride or perchlorate as different counter-anions have been used. After the removal of *EosinY* with *KOH* the films have been sensitized with the indoline dye D149. These electrodes were used in dye-sensitized solar cells (DSCs) and the charge transport dynamics were studied with electrochemical impedance spectroscopy (EIS), intensity modulated current/voltage spectroscopy (IMPS/IMVS) and IV-curves. Doping of the *ZnO* films by *Cl* alters the charge transfer dynamics by filling of otherwise unoccupied states in *ZnO* and changing the concentration of available trap states. By changing the counter-anion to perchlorate well-reproducible results could be obtained which open the way to further improvements in DSCs.

DS 8.6 Mon 19:15 CHE 91

Efficiency roll-off in organic light-emitting diodes: influence of emitter position and orientation — •Caroline Murawski[1], Philipp Liehm[1,2], Simone Hofmann[1], Karl Leo[1], and Malte C. Gather[1,2] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]present address: SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS (UK)

In this contribution, we study the efficiency decrease of organic light-emitting diodes (OLEDs) at high brightness (so-called roll-off).[1] We find a strong influence of the emitter-cathode distance and the transition dipole orientation of the emitter molecules on the roll-off by comparing two phosphorescent emitters (Ir(MDQ)2(acac) and Ir(ppy)3).[2] The measurements are modeled using triplet-triplet-annihilation (TTA) theory. A comparison of experiment and theory reveals the critical current density and the TTA rate constant and shows that the differences in roll-off behavior are predominantly caused by a change of the decay rates inside the OLED cavity. In order to provide guidelines for designing OLEDs with optimal high-brightness efficiency, we model the roll-off as a function of the emitter-cathode distance, emitter dipole orientation, and radiative efficiency.

[1] C. Murawski, K. Leo, and M.C. Gather, Adv. Mater. 10.1002/adma.201301603 (2013).

[2] C. Murawski, P. Liehm, K. Leo, and M.C. Gather, Adv. Funct. Mater. 10.1002/adfm.201302173 (2013).

DS 8.7 Mon 19:30 CHE 91

Solution-based planarization layers for organic solar cells on flexible silver nanowire transparent electrodes — •Jan Ludwig Bormann[1], Franz Selzer[1], Nelli Weiss[2], Lars Müller-Meskamp[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, TU Dresden — [2]Physikalische Chemie, TU Dresden

Flexible transparent electrodes made of silver nanowires (AgNWs) are an emerging research field for different optoelectronic devices such as organic transistors, organic light emitting diodes (OLED) and organic photovoltaics (OPV). They exhibit excellent electrical and optical properties (sheet resistance of 11 Ohm/sq at 85% transmittance) and are suitable for the application on flexible substrates. These transparent electrodes show high roughness and therefore require a planarization layer for fabricating efficient small molecule devices.

In this work, solution-based organic materials are processed with spin coating to planarize the AgNW electrode. A solution processed small molecule layer acts as planarizing layer and as hole transport layer in organic solar cells with a bulkheterojunction comprising the fullerene C60 as acceptor and different small molecule donor layers (oligothiophenes and phtalocyanines) . The efficiency of these devices is comparable or even better to reference devices with indium tin oxide (ITO) as transparent electrode.

DS 9: Layer Properties: Electrical, Optical, and Mechanical Properties

Time: Tuesday 9:30–12:45 Location: CHE 91

Invited Talk DS 9.1 Tue 9:30 CHE 91

Chalcopyrite semiconductors: atomic-scale structure and band gap bowing — •Claudia S. Schnohr[1], Stefanie Eckner[1], Helena Kämmer[1], Tobias Steinbach[1], Martin Gnauck[1], Andreas Johannes[1], Christian A. Kaufmann[2], Christiane Stephan[2], and Susan Schorr[2] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Cu(In,Ga)Se_2 is one of the most promising material systems for thin film photovoltaics with record efficiencies above 20% on laboratory scale. The material crystallizes in the chalcopyrite type crystal structure where the anion is typically displaced from its ideal lattice site due to the different properties of the neighbouring cations. This subtle structural variation has a strong influence on the energy band gap. Therefore, we have studied the atomic-scale structure of Cu(In,Ga)Se_2 as a function of composition using extended X-ray absorption fine structure spectroscopy and valence force field simulations. The local atomic arrangements are found to deviate significantly from the long-range crystallographic structure and the material is characterised by structural inhomogeneity on the atomic scale. Regarding the anion position, two different displacement mechanisms have to be distinguished both of which influence the nonlinear change of the band gap with material composition. Similar results were also obtained for Cu(In,Ga)S_2 indicating that our findings represent general features of these highly relevant yet complex chalcopyrite semiconductors.

Invited Talk DS 9.2 Tue 10:00 CHE 91

Polarized mid-infrared spectroscopy of split-ring resonators and metal nanoparticle-organic hybrids — •Thomas W.H. Oates, Dimitra Gkogkou, Timur Shaykhutdinov, Tolga Wagner, and Karsten Hinrichs — Leibniz-Institut für Analytische Wissenschaften - ISAS- e.V., Albert-Einstein Str. 9, 12489, Berlin, Germany

Metal nano-antennas are increasingly utilized to focus the electric far-field, with the goal of enhancing and manipulating interactions with organic resonators in the near-field. In the infrared spectral fingerprint region, the use of polarized infrared spectroscopy provides unique information concerning the 3D orientation of the resonant structures. We present the results of ellipsometry and polarized infrared microscopy investigations of an array of split-ring resonators (SRR) and metal nanoparticle (NP) films with adsorbed self-assembled monolayers. The SRRs show an extrinsic chiral response directly related to the combined symmetry of the metallic structures and the electric field of the incident radiation. Rigorous coupled wave analysis simulations give excellent agreement with the experimental results. The polarized reflection spectra of the metal NP-organic hybrids display surface-enhanced infrared absorption (SEIRA). Using a combinatorial fabrication method we produce an array of nanoparticle sizes, shapes and fill-factors on a single substrate. This allows us to precisely identify the optimal conditions for maximal SEIRA enhancement. The additional information provided by polarized spectroscopy allows us to discuss the origins of the SEIRA effect.

DS 9.3 Tue 10:30 CHE 91

Investigations of the dependency of the infrared-optical and electrical properties of ITO coatings on the dip coating parameters and the coating thickness — •Nadine Wolf, Thomas Weis, and Jochen Manara — Bavarian Center for Applied Energy Research (ZAE Bayern)

Tin doped indium oxide (ITO) coatings were prepared with ITO nanoparticle suspensions via dip coating technique. The coatings have been prepared with different withdrawal speeds so that the coatings exhibit different thicknesses. If the thickness of the ITO coatings increases, the amount of free charge carriers within these coatings also increases and therefore the infrared-optical and electrical properties of the ITO coatings alter up to a certain extent, too. The change of the thickness and the optical constants of the ITO coatings with the withdrawal speed are measured with ellipsometry measurements. The infrared-optical and electrical properties are measured with Fourier transform infrared (FTIR) spectroscopy and four point probe measurements respectively. In this work the dependency of these properties is discussed as a function of the thickness and therefore withdrawal speed.

DS 9.4 Tue 10:45 CHE 91

Sputter yield amplification upon reactive serial co-sputtering of doped TiO2 — •Rüdiger M. Schmidt[1], Tomas Kubart[2], Andreas Pflug[3], and Matthias Wuttig[1,4] — [1]I. Institute of Physics, RWTH Aachen University, Germany — [2]Solid State Electronics, The Ångström Laboratory, Uppsala University, Sweden — [3]Fraunhofer IST, Braunschweig, Germany — [4]JARA - Fundamentals of Future Information Technologies

TiO_2 plays a prominent role in several applications such as anti-reflective coatings and self-cleaning surfaces, mainly because of its high refractive index. Most frequently this material is deposited by reactive magnetron sputtering. Unfortunately TiO_2 suffers from a comparatively low deposition rate. To increase the deposition rate, Sputter Yield Amplification (SYA) can be used through recoil of the sputtering species at implanted heavy dopants below the target surface. Here we present experimental results for different heavy dopants using a dedicated sputter deposition tool. By use of serial co-sputtering in situ variations of the target stoichiometry can be facilitated, which enable systematic studies of SYA. To quantify the amplification, film thicknesses have been deduced by x-ray reflectometry measurements and subsequent simulations. Ellipsometry as well as reflectance and transmission data have been taken to model the dielectric function of the resulting films giving access to the refractive index.

DS 9.5 Tue 11:00 CHE 91

Sponge-like Si-SiO2 nanocomposite as photovoltaic absorber * influence of composition of the SiOx precursor — •Erik Schumann[1], Karl-Heinz Heinig[1], René Hübner[1], Jose Luis Endrino[2], and Gintautas Abrasonis[1] — [1]Helmholtz-Zentrum Dresden, Rossendorf, Dresden, Germany — [2]Abengoa Research, Sevilla, Spain

Absorber layers consisting of nanostructured Si are candidates to improve the efficiency of thin film Si solar cells. Si-SiO2 nanocomposites with sponge-like Si embedded in SiO2 are promising materials as they exhibit a widened band gap and maintain the electrical interconnectivity. These structures can be formed upon annealing of SiOx films (x<1), which leads to spinodal phase separation into a percolacated network of Si nanowires embedded in SiO2. This can be accompanied by crystallization of the silicon. The influence of the composition of the precursor SiO2 on the evolving sponge-like nanostructure is investigated. SiOx layers have been grown by reactive sputter deposition. SiOx layers with compositions between x=0 and x=1.2 have been studied. The transformation of SiOx into Si-SiO2 nanocomposites has been performed by scanning a diode laser line source. Dwell times in the ms range and power densities of the red laser light of about 103 W/cm2 have been investigated. While thin a-Si films show crystallization under our annealing conditions, oxygen-rich films with Si structures smaller than 2 nm do not crystallize. Our results demonstrate that the composition of the precursor material is of crucial importance to obtain a Si-SiO2 nano sponge-like material suitable as photovoltaic absorber.

Coffee break (15 min)

DS 9.6 Tue 11:30 CHE 91

The Origin of the Radial Distribution of the Electronic and Structural Properties of Magnetron Sputtered ZnO:Al Thin Films — •André Bikowski[1], Thomas Welzel[2], and Klaus Ellmer[1] — [1]Helmholtz-Zentrum Berlin, D-14109 Berlin — [2]Technische Hochschule Mittelhessen, D-35390 Gießen

We investigated the electronic and structural properties of magnetron sputtered ZnO:Al films by means of radially resolved X-ray diffraction, resistivity, and plasma process monitor measurements.

It is known for a long time now that films sputtered onto stationary substrates exhibit a pronounced radial distribution of their electronic and structural properties. Mainly there exist two explanations for this effect: (i) The inhomogeneities are caused by excess oxygen reaching the substrate surface or (ii) they are due to a bombardment of the growing films by high energetic oxygen.

We were able to clearly correlate the radially resolved ion energy distribution spectra of high energetic negative oxygen ions to the electronic and structural properties of the films, and hence found model (ii) to be more appropriate. Since these high energetic negative ions exhibit energies in the range of several hundred eV in the case of DC sputtering, and the formation energies of defects in ZnO are some 10 eV only, a strong impact of the high energetic ions on the structural and the related electronic properties is to be expected. Generally, the results show a decisive role of high energetic oxygen for magnetron sputtering, which has to be taken into account also for other TCO materials such as $\mathrm{In_2O_3}$:Sn or $\mathrm{SnO_2}$:F.

DS 9.7 Tue 11:45 CHE 91

Structural and Electrical Characterization of the Ferecrystals $[(\mathrm{PbSe})_{1.14}]_m(\mathrm{NbSe}_2)_n$ — •Corinna Grosse[1], Matti Alemayehu[2], Olivio Chiatti[1], Anna Mogilatenko[1], David C. Johnson[2], and Saskia F. Fischer[1] — [1]Novel Materials, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Chemistry, University of Oregon, Eugene, OR, 97401, USA

Ferecrystals are layered intergrowth compounds consisting of alternating few-atomic-layers thin sheets of transition metal dichalcogenide (TMD) and metal chalcogenide layers. TMDs exhibit interesting electrical properties such as charge density waves, superconductivity or an ultralow thermal conductivity [1]. In contrast to conventional misfit layer compounds, ferecrystals exhibit a turbostratically disordered structure and their layer thickness and stacking sequence are tunable.

In this study, we synthesized the ferecrystals $[(\mathrm{PbSe})_{1.14}]_m(\mathrm{NbSe}_2)_n$ and measured their in-plane electrical properties as a function of layer sequence (m and n) and temperature (down to $T = 300$ mK). The crystal structure was analyzed using X-ray- and electron diffraction, scanning transmission electron microscopy and energy-dispersive X-ray spectroscopy. The structure of the PbSe and $\mathrm{NbSe_2}$ constituents was resolved down to the atomic scale. The influence of the ferecrystal structure on the electrical properties is discussed. [1] C. Chiritescu, D. G. Cahill, N. Nguyen, D. C. Johnson *et al.*, Science **315**, 351 (2007).

DS 9.8 Tue 12:00 CHE 91

Effect of temperature on the electrical and mechanical performance of Al-Li thin films deposited on viscoelastic substrates — •Alla S. Sologubenko, Diana Courty, and Ralph Spolenak — Laboratory for Nanometallurgy (LNM), ETH Zurich, Wolfgang-Pauli-Strasse 10, CH-8093 Zurich, Switzerland

Grain boundary cohesion and adhesion of the metallic thin film to a polyimide substrate are two factors crucially affecting the structural integrity of Al-Li alloys upon tensile loading. Al-Li thin film alloys of different compositions and microstructures were subjected to mechanical loading experiments accompanied by electrical resistance measurements in a tensile stage equipped with an in-situ heating module. The experiments performed at 100°C show drastic change in both, mechanical and electrical responses of the thin films of all compositions in comparison to room temperature measurements. This behavior evidences a large enhancement of adhesion in the thin film-substrate system due to the temperature increase. The exceptionally good performance of the equisize-grained Al-5 at.%Li alloy at both temperatures is attributed to an effect of the small intermetallic phase particles on the film plasticity and grain boundary cohesion.

DS 9.9 Tue 12:15 CHE 91

Thick LCMO manganite films grown by MAD — •F. Fischgrabe[1], E.S. Zhukova[2,3], B. Gorshunov[2,3], M. Dressel[3], and V. Moshnyaga[1] — [1]I. Physikalisches Institut, Universität Göttingen, Germany — [2]Prokhorov General Physics Institute, Russian Academy of Sciences,Moscow, Russia — [3]I. Physikalisches Institut, Universität Stuttgart, Germany

We report preparation and characterization of $La_{1-x}Ca_xMnO_3$ (LCMO) x=0,5-0,96 films with thickness $0,5\mu m$. Thick epitaxial manganite films could be interesting for THz as well as for far IR Fourier spectroscopy measurements, aimed to study low-energy excitations, like CDW and folding phonons, important for the manganite physics. The samples were grown using metalorganic aerosol deposition (MAD) technique. To verify the film quality XRD, DC and AC resistivity (f=0,1Hz-40MHz; T=5-300K), STM, REM, Squid, Raman, and THz measurements were carried out. $0,5\mu m$-thick LCMO films with $x \geq 0,5$ show charge-order transitions and residual resistivity, $\rho(300K) \approx 10^{-4}\Omega cm$. The films show crossover from insulating to semiconductor-like behaviour at high temperatures. We further demonstrate drastic changes of all measured properties with increasing doping level, aswell as dependance on comensurate dopinglevels. Furthermore we present results on freestanding films also prepared by MAD technique. Preparationprocedure and first results aswell as comparison with films on MgO will be shown.

DS 9.10 Tue 12:30 CHE 91

Investigating Few Layer Gallium Selenide (GaSe) with Advanced Atomic Force Microscopy and Optical Techniques — •Matthias A. Fenner[1], Raul D. Rodriguez[2], Alexander Villabona[2,3], Santos A. Lopez-Rivera[3], and Dietrich R.T. Zahn[2] — [1]Agilent Technologies, 60528 Frankfurt, Germany — [2]Semiconductor Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [3]Universidad de Los Andes, Applied Physics Lab, Merida 05101, Venezuela

Gallium selenide (GaSe) nanosheets have been reported to exhibit superior properties in field effect transistors and photo detectors as compared to other two-dimensional, layered materials [1-3]. We prepared few layer GaSe flakes by mechanical transfer to a graphite substrate. Individual flakes of several tens micrometer size are obtained and can readily be detected by optical microscopy. We used atomic force microscopy to investigate the nanoscale mechanical and electrical properties of the flakes. We will discuss the remarkable differences observed in the same area investigated by Raman spectroscopy and imaging, in particular, the correlation between the first order Raman modes of GaSe and the selective enhancement of the underlying graphite substrate.

[1] P. Hu, Z. Wen, L. Wang, P. Tan, K. Xiao, Acs Nano, 6 (2012) 5988. [2] S. Lei, L. Ge, Z. Liu, S. Najmaei, G. Shi, G. You, J. Lou, R. Vajtai, P.M. Ajayan, Nano Lett., 13 (2013) 2777. [3] D.J. Late, B. Liu, J. Luo, A. Yan, H.S.S.R. Matte, M. Grayson, C.N.R. Rao, V.P. Dravid, Adv. Mat., 24 (2012) 3549.

DS 10: Multiferroics I (jointly with MA, DF, KR, TT)

Time: Tuesday 9:30–12:45 Location: BEY 118

DS 10.1 Tue 9:30 BEY 118

***Ab initio* study of electronic transport in the Co/PZT-based tunnel junctions** — •Vladislav Borisov[1], Sergey Ostanin[1], Igor Maznichenko[2], Arthur Ernst[1], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Magnetoelectric coupling at the multiferroic interfaces FM/FE (FM=Co,Fe, FE=PbTiO$_3$,PZT) was studied from first principles. The magnetic interfacial effect, which is controlled by the FE polarization, originates from the charge transfer and *d*-orbital redistribution of Co/Fe and Ti mediated by the *p*-states of interfacial oxygens. In PZT, the presence of Zr dopants may locally enhance the effect. We analysed also the spin polarization of tunneling electrons in Co/PTO/Co and Fe/PTO/Co junctions, in which the calculated four-state conductance can account for the ferroelectrically switchable TMR signal observed recently in LSMO/PZT/Co [1].

[1] D. Pantel *et al.*, *NATURE MATERIALS* **11**, 289 (2012).

DS 10.2 Tue 9:45 BEY 118

Tunneling transport and memristive effects in PbTiO3- based multiferroic tunnel junctions — •Andy Quindeau, Marin Alexe, and Dietrich Hesse — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

A gradually tunable resistance effect based on the tunnel electroresistance (TER) of multiferroic tunnel junctions is investigated. The ferroelectric tunnel barrier comprises, a PbTiO3 layer of a few nm thickness, is embedded between two different ferromagnetic layers, viz. La0.7Sr0.3MnO3 and cobalt. In this capacitor geometry an electric bias, applied perpendicularly to the films, results in a direct tunneling current flowing between the two electrodes. The tunnel resistance is dependent on the polarization of the ferroelectric, which is switchable via relatively high voltage pulses. Due to the variation of the pulse parameters a variety of non-volatile resistance states can easily be achieved. These gradually tunable resistance states, characteristic for a memristor device, can be explained by a ferroelectric domain distribution inside the ferroelectric film: Domains with different polarities can coexist inside one capacitor after partial polarization switching and act as parallel connected tunnel barriers with different tunnel resistances. Temperature dependent measurements show the influence of different electron transport mechanisms, which will be discussed. The impact of the memristive states on the tunnel magnetoresistance (TMR) can be shown.

DS 10.3 Tue 10:00 BEY 118

Lattice and polarizability mediated spin activity in EuTiO3 — •Annette Bussmann-Holder[1], Kevin Caslin[1,2], Patrick Reuvenkamp[1], Zurab Guguchia[3], Hugo Keller[3], Reinhard Kremer[1], and Jürgen Köhler[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstr.1, D-70569 Stuttgart, Germany — [2]Brock University, 500 Glenridge Ave., St. Catharines L2S-3A1, Ontario, Canada — [3]Physik-Institut der Universität Zürich, Winterthurerstr. 190, CH-8057 Zürich, Switzerland

EuTiO3 is shown to exhibit novel strong spin-charge-lattice coupling deep in the paramagnetic phase. Its existence is evidenced by an, until now, unknown response of the paramagnetic susceptibility at temperatures exceeding the structural phase transition temperature TS=282K. The extra features in the susceptibility follow the rotational soft zone boundary mode temperature dependence above and below TS. In addition, novel magnetostriction experiments and dielectric constant measurements have been performed which both reveal giant anomalies related to the antiferromagnetic phase transition at TN=5.7K and the structural phase transition at TS. The theoretical modeling consistently reproduces these anomalies and provides evidence that EuTiO3 has considerable analogies to SrTiO3 but also substantial differences stemming from the Eu 4f spins which are lattice activated at high temperatures far above TN.

DS 10.4 Tue 10:15 BEY 118

Magnetoelectric coupling in a composite multiferroic structure revealed by Ferromagnetic Resonance — •Alexander Sukhov[1], Paul P. Horley[2], Chenglong Jia[3], and Jamal Berakdar[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle/Saale, GERMANY — [2]Centro de Investigacion Materiales Avazados, S.C. (CIMAV), Chihuahua/Monterrey, MEXICO — [3]Lanzhou University, Lanzhou, CHINA

We theoretically study [1] a thin multiferroic junction related to a barium titanate (tetragonal or rhombohedral phase) layer in contact with an iron layer. Depending on the type of the magnetoelectric coupling at the interface - either due to screening charge or due to an epitaxial strain resulting in a strong magnetoelastic coupling - we present a detailed analysis of the response of the multiferroic structure to magnetic radio-frequency fields by means of ferromagnetic resonance as a function of the applied electric field.

[1] A. Sukhov, P.P. Horley, C.-L. Jia, J. Berakdar, J. Appl. Phys. **113**, 013908 (2013).

DS 10.5 Tue 10:30 BEY 118

Magnetoelectric monopoles in bulk periodic solids — •Michael Fechner[1], Eric Bousquet[1], Alexander Balatsky[2], Nicoal A. Spaldin[1], and Lars Nordström[3] — [1]ETH Zürich, Department for Materials Theory, Zürich, Switzerland — [2]NORDITA, KTH Royal Institute of Technology and Stockholm University, Stockholm, Sweden — [3]Department of Physics and Astronomy, Uppsala University, Sweden

The magnetoelectric (ME) response is described by a second rank tensor that can be decomposed into irreducible isotropic diagonal, antisymmetric and trace-free part. Here we show that the former component can be identified with a ferroic ordering of magnetoelectric monopoles[1]. We further develop a scheme to calculate the ME monopole in bulk periodic solids, by exploiting similarities to the ferroelectric polarization. Finally, as an example we present results for the series of lithium transition metal phosphate compounds (LiMPO$_4$, with M = Co, Fe and Ni), which include both ferromonopolar and antiferromonopolar ordered cases. We predict for the latter case a q-dependent diagonal ME effect.

[1] N . A. Spaldin et al., PRB 88, 094429 (2013)

DS 10.6 Tue 10:45 BEY 118

Different routes for enhanced control of ferroelectric polarization by magnetic field — •I. Fina[1,2], V. Skumryev[3,4], D. O'Flynn[5], G. Balakrishnan[5], N. Dix[2], J. M. Rebled[2,6], P. Gemeiner[7], X. Marti[8], F. Peiró[6], B. Dkhil[7], F. Sánchez[2], L. Fàbrega[2], and J. Fontcuberta[2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Institut de Ciència de Materials de Barcelona, Catalonia, Spain — [3]Institució Catalana de Recerca i Estudis Avançats (ICREA), Catalonia, Spain — [4]Universitat Autònoma de Barcelona, Barcelona, Spain — [5]University of Warwick, Coventry, United Kingdom — [6]LENS - MIND/IN2UB, Barcelona, Spain — [7]Propriétés et Modélisation des Solides, Paris, France — [8]Faculty of Mathematics and Physics, Praha, The Czech Republic

I will focus on the direct magnetoelectric effect, control of polarization vector by magnetic field, in single-phase and composite multiferroic materials in thin film form.

In single-phase multiferroic materials, cycloidal magnet, we will see that strong coexistence of polar and non-polar regions allow large susceptibilities leading to a full control of the polarization vector by means of magnetic field [1]. In composite materials, ferromagnetic-ferroelectric heterostructures, the limiting factor is the substrate clamping effect. We will show that we can overcome this undesired effect, enhancing the presence of some small quantity of defects. These defects store the needed elastic energy, enhancing the magnetoelectric coupling, which result in huge effects near room temperature [2].

[1] I. Fina, et al., Phys. Rev. B 88, 100403(R) (2013). [2] I. Fina, et al., Nanoscale 5, 8037 (2013).

15 min. break

DS 10.7 Tue 11:15 BEY 118

Investigation of A-site Bismuth based double perovskites as potential room-temperature multiferroics — •Vikas Shabadi, Mehran VafaeeKhanjani, Mehrdad BaghaieYazdi, Aldin Radetinac, Philipp Komissinskiy, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt, Germany

A-site Bismuth based double perovskites ($Bi_2BB'O_6$), where ferroelectricity arises from the stereochemically active $6s^2$ lone pair of electrons on the Bi^{3+} cations, provide a vital test bed to engineer room temperature multiferroicity. Here, different combinations of 3d-3d or 3d-5d cations may be introduced at the B-site in order to obtain an effective ferri/ferromagnetic moment. The 3d-3d compound Bi_2FeCrO_6 (BFCO) has drawn a heightened interest due to its large experimentally reported ferroelectricity and divergent observations of its magnetic properties. We report epitaxial BFCO thin films grown by pulsed laser deposition on single crystal $SrTiO_3(100)$ substrates. Detailed structural characterization was performed by X-ray Diffraction and the magnetic properties were studied with a SQUID magnetometer. We show that BFCO adopts a superstructure with the same unit cell as the chemically ordered double perovskite. The magnetization is a function of chemical but not of structural order.

DS 10.8 Tue 11:30 BEY 118

Room temperature magnetism and ferroelectricity in eps-Fe2O3 thin films — •I. Fina[1], M. Gich[2], A. Morelli[1], F. Sánchez[2], M. Alexe[1], J. Fontcuberta[2], and A. Roig[2] — [1]Max Planck Institute of Microstructure Physics D-06120 Hallle/Salle, Germany — [2]Institut de Ciència de Materials de Barcelona ICMAB, Consejo Superior de Investigaciones Científicas CSIC, Campus UAB 08193 Bellaterra, Catalonia, Spain

The quest for magnetoelectric multiferroics is driven by the promise of a novel generation of devices combining the best characteristics of ferromagnetic and ferroelectric materials. These cherished applications require materials displaying a substantial magnetization and electric polarization which are coupled and coexist well above room temperature. These properties are not commonly fulfilled by single phase materials and firm candidates for the development of these technologies are still sought.

In this contribution, we will report on epitaxial eps-Fe2O3 thin films grown by Pulsed Laser Deposition on (111) SrTiO3 and present recent data on its structural, magnetic and dielectric characterization. The films are ferromagnetic and ferroelectric at room temperature and display magnetization and polarization values at remanence of about 50 emu/cm3 and 1 uC/cm2 with a long retention. A magnetocapacitive response has also been detected indicating that the films present coupling between both ferroic orders.

DS 10.9 Tue 11:45 BEY 118

Time-resolved analysis of switching in spiral multiferroics — •Jonas Stein[1], Tobias Cronert[1], Jeannis Leist[2], Karin Schmalzl[3], A Agung Nugroho[4], Alexander C Komarek[5], Götz Eckold[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Physikalische Chemie, Universität Göttingen — [3]JCNS at ILL, France — [4]Institut Teknologi Bandung, Indonesia — [5]MPI für chemische Physik fester Stoffe

Multiferroic crystals are promising materials for future memory devices with extremely low power consumption. The rise time between two states is a crucial parameter for a possible application and was investigated in the spiral spin multiferroic $TbMnO_3$. Polarized neutron diffraction is able to determine the ratio of chiral domains, which can be controlled by an external electric field. Using the stroboscopic technique we can follow the reversion of chiral domains in the timescale of a few 100 microseconds to hours. In $TbMnO_3$ we find a clear logarithmic relation between the rise time and temperature that is fulfilled over 5 decades.

DS 10.10 Tue 12:00 BEY 118

Thermodynamic properties of the new multiferroic material $(NH_4)_2[FeCl_5(H_2O)]$ — •Matthias Ackermann[1], Daniel Brüning[2], Thomas Lorenz[2], Petra Becker[1], and Ladislav Bohatý[1] — [1]Institut für Kristallographie, Universität zu Köln, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany

Multiferroic materials with coupled ferroelectric and (anti-)ferromagnetic order in the same phase have attracted considerable interest during the last decade. The search for new multiferroic materials is an important issue to further improve the understanding of the underlying coupling mechanisms. Here, we present a detailed investigation of the new multiferroic compound $(NH_4)_2[FeCl_5(H_2O)]$ [1]. Our measurements of pyroelectric currents reveal, that the electric polarization occuring in the antiferromagnetically ordered phase can drastically be influenced by applying magnetic fields. Based on the results of these dielectric investigations, together with measurements of thermal expansion, magnetostriction and specific heat, detailed magnetic field versus temperature phase diagrams are derived. Depending on the direction of the magnetic field up to three different multiferroic phases are identified, which are separated from the paramagnetic phase by a magnetically ordered, but non-ferroelectric phase.

This work was supported through the Institutional Strategy of the University of Cologne within the German Excellence Initiative.

[1] Ackermann M et al. 2013 *New J. Phys.* (in press, arXiv:1308.0285)

DS 10.11 Tue 12:15 BEY 118

Stoichiometric Effects on Crystal Quality in $LuFe_2O_4$ and $YbFe_2O_4$ — •Hailey Williamson[1,2], Geetha Balakrisnan[2], and Manuel Angst[1] — [1]Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institut PGI-4, Forschungszentrum Jülich GmbH, Jülich, Germany. — [2]Department of Physics, The University of Warwick, CV4 7AL, Coventry, UK

The multiferroic rhombohedral $LnFe_2O_4$ (Ln=Lu, Y, Yb, Tm, Ho and Er) system, which can be described as stacked hexagonal Fe bilayers separated by Lu monolayers, has been in focus since the discovery of interesting magnetic and electrical characteristics in $LuFe_2O_4$. The specific CO configuration within the Fe bilayers was initially thought to produce a ferroelectricity through cross polarization of the two layers of the bilayer. However our recent investigations indicate that the CO configuration is actually non-polar. Extensive research highlighted a large sensitivity to oxygen stoichiometry, where crystals grown in an excess/deficient oxygen partial pressure environment exhibit smeared glassy magnetic transitions and diffuse CO. Through fine tuning of the atmospheric conditions, crystals exhibiting 3D CO and magnetism were produced. Interest then spread to isostructural $YbFe_2O_4$, which has currently few detailed investigations. Single crystals of $YbFe_2O_4$ were grown in four different partial pressure atmospheres to view the effects of oxygen stoichiometry on the magnetism and CO. A series of macroscopic and microscopic measurements provided a detailed look into the effects of oxygen stoichiometry on the intrinsic characteristics as well as a comparison to that of its predecessor $LuFe_2O_4$.

DS 10.12 Tue 12:30 BEY 118

Multiferroicity in Cu_2OSeO_3? — •Eugen Ruff[1], Stephan Krohns[1], Helmuth Berger[2], Peter Lunkenheimer[1], and Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg — [2]Institute of Physics of Complex Matter, École Polytechnique Fédérale de Lausanne

Skyrmions are topologically stable vortex-like objects, for the first time detected in the B20 alloy MnSi [1]. Their electrical controllability via small currents qualifies skyrmions for applications in high-density magnetic storage devices. The recent discovery of magnetoelectric skyrmions in the insulating chiral magnet Cu_2OSeO_3 leads to another promising route to electrical control [2]. This system is suggested to carry a local electrical dipole, which implies that the skyrmions should be controllable by an external electrical field without losses due to Joule heating. Here we provide a thorough analysis of the magnetic and polar phases of this material, using SQUID and pyrocurrent measurements. In order to investigate the possible ferroelectric properties of Cu_2OSeO_3, we have performed dielectric spectroscopy in various magnetic fields in a broad frequency range below 70 K. Combining all these different techniques, we address the question whether Cu_2OSeO_3 is magnetoelectric or multiferroic. [1] S.Mühlbauer *et al.*, Science **323**, 915 (2009). [2] S.Seki *et al.*, Science **336**, 198 (2012).

DS 11: Focus Session: Sensoric Micro and Nano-systems I

One major trend in semiconductor research which was identified by the international technology roadmap for semiconductors (ITRS) is called "More than Moore". This concept explores the variety of physical phenomena which can be obtained by the integration of different technologies and functionalities to basic semiconductor research. Current focus areas comprise signal and information processing as well as the interaction with the environment in a miniaturized system. Such smart systems contain digital and analog electronics, sensors and actuators, radio frequency and high voltage modules or biotechnology. The miniaturization of the components and the utilization of nanotechnology enable new or enhanced functionalities. The topical session aims at presenting recent trendsetting micro- and nano technological concepts which are related to nano electro mechanical sensor systems. Special emphasis will be given to the integration of nanostructures and novel materials as well as the spatial and functional integration of heterogeneous components in micro and nano systems. (Organizers: Dietrich Zahn, TU Chemnitz, Thomas Gessner, Fraunhofer ENAS, Oliver Schmidt, IFW Dresden)

Time: Tuesday 9:30–13:15 Location: CHE 89

Invited Talk DS 11.1 Tue 9:30 CHE 89

Giant magnetoelectric thin film composites — •Andre Piorra, Robert Jahns, Enno Lage, Christine Kirchhof, Erdem Yarar, Volker Röbisch, Dirk Meyners, Reinhard Knöchel, and Eckhard Quandt — Faculty of Engineering, University of Kiel, Kaiserstr. 2, 24143 Kiel, Germany

Magnetoelectric (ME) composite materials show ME coefficients that are larger than that of natural multiferroics by several orders of magnitude. These ME composites have high potential for applications, e.g. as very sensitive ac magnetic field sensors. Special features are their passive nature, their high sensitivity, and their large dynamic range with linear response.

The thin film ME 2-2 composites of this work consist of either AlN or ferroelectric piezoelectrics and different magnetostrictive layers that show extremely high ME coefficient of up to 20 kV/cmOe at mechanical resonance in vacuum (1). However, these composites require in general the presence of an external d.c. magnetic bias field, which is detrimental to their use as sensitive magnetic-field sensors. Composites using exchange biased magnetstrictive layers are used to adjust the shift of the magnetostriction curve in such a way that the maximum magnetoelectric coefficient occurs at zero magnetic bias field (2). In this presentation different thin film composites will be discussed in view of their use as very sensitive magnetic field sensors .

(1) Appl. Phys. Lett. 102, (2013), 232905. (2) Nature Materials 11 (6) (2012), 523-529.

Funding via the DFG SFB 855 is gratefully acknowledged.

DS 11.2 Tue 10:00 CHE 89

Rolled-up magnetic nanomembranes: Towards 3D magnetic sensorics — •Denys Makarov[1], Christian Müller[2], Ingolf Mönch[1], and Oliver G. Schmidt[1] — [1]Institute for Integrative Nanosciences, IFW Dresden, 01069 Dresden, Germany — [2]Measurement and Sensor Technology, TU Chemnitz, 09126 Chemnitz, Germany

Rolled-up nanotechnology relies on the deterministic release of a strained nanomembrane from a sacrificial layer resulting in formation of a tube of predetermined size and geometry. The approach potentially allows to implement multiple functionalities on diagnostics e.g. electro-chemical, magnetic, optical into a single tubular architecture, thus realizing the Lab-in-a-Tube concept [1].

Here, we report on the realization of the rolled-up magnetic sensor element revealing giant magnetoresistance (GMR), which can be integrated into existing fluidic architectures as a component for the Lab-in-a-Tube [2-4]. The rolled-up tube acts as the fluidic channel guiding the magnetic objects, which can be detected with the integrated magnetic sensor. The performance of the rolled-up sensor was optimized for high sensitivity to weak magnetic fields, as required in biomedical applications, and demonstrated for the in-flow detection of CrO2 nanoparticles embedded in a biocompatible hydrogel shell [2].

[1] E. J. Smith et al., Lab Chip 12, 1917 (2012).
[2] I. Mönch et al., ACS Nano 5, 7436 (2011).
[3] C. Müller et al., Nanoscale 4, 7155 (2012).
[4] C. Müller et al., Appl. Phys. Lett. 100, 022409 (2012).

DS 11.3 Tue 10:15 CHE 89

Integrated MEMS magnetic field sensor based on ΔE-effect — •Sebastian Zabel[1], Robert Jahns[2], Stephan Marauska[3], Björn Gojdka[2], Bernhard Wagner[3], Rainhard Knöchel[1], Rainer Adelung[4], and Franz Faupel[2] — [1]Institute for Materials Science, Multicomponent Materials, Kiel University, Kiel, Germany — [2]Institute of Electrical and Information Engineering , Kiel University — [3]Fraunhofer Institute for Silicon Technology ISIT, Itzehoe, Germany — [4]Institute for Materials Science, Functional Nanomaterials, Kiel University

We present an integrated MEMS magnetic field sensor based on ΔE-effect, which extends our previous approach [Gojdka et al., Appl. Phys. Lett. 99, 223502 (2011); Nature 480, 155 (2011)]. The ΔE-effect describes a change of elastic modulus in magnetostictive materials upon application of a magnetic field. The change of elastic modulus can be measured by the change of resonance frequency of a one side clamped cantilever. The 0.2 x 1 mm SiO2 cantilever is 650 nm thick and coated with a 500 nm thick piezoelectric AlN layer on the bottom and a 2 um thick magnetostrictive FeCoSiB amorphous film on top. The piezoelectric layer is used for excitation of the first resonant bending mode as well as the readout of amplitude and phase. The sensor resonates at 6700 Hz and is encapsulated in a vacuum packing to reduce damping. Using amplitude modulation it is possible to detect small signals of 10 nT at 10 Hz. In order to use the maximal ΔE-effect a bias field of around 1.5 mT has to be applied. The advantage of the sensor concept is the possibility to measure in a broad frequency range down to DC.

DS 11.4 Tue 10:30 CHE 89

Magnetic Domains in Rolled-Up Ferromagnetic Single-Layer Nanomembranes and Magnetically Capped Tubular Architectures — •Robert Streubel[1], Denys Makarov[1], Peter Fischer[2], Rudolf Schäfer[3], and Oliver G. Schmidt[1] — [1]Institute for Integrative Nanosciences, IFW Dresden, 01069 Dresden, Germany — [2]CXRO, LBNL, Berkeley CA 94720, USA — [3]Institute for Metallic Materials, IFW Dresden, 01069 Dresden, Germany

Rolled-up magnetic nanomembranes have recently enabled novel sensoric devices and spin-wave filters. Their application potential relies on understanding the modification of magnetic configurations under external stimuli. Due to difficulties in visualizing magnetic domain patterns in these truly 3D structures, the magnetization configuration in cylindrical architectures is usually derived from integral measurements, such as magnetoresistance techniques. Here, we directly visualize magnetic domain patterns in magnetically capped tubes [1] and rolled-up single layer magnetic nanomembranes [2]. By Photoelectron emission and Kerr microscopies magnetic signals from the top part of the tube were recorded whereas magnetic soft X-ray microscopy allowed to probe internal parts of the tube. We demonstrate the possibility to tailor the magnetization orientation from longitudinal for positive magnetostrictive materials over spiral-like to azimuthal for negative ones [2]. These patterns cause distinct magnetoelectronic responses, which is relevant to know for sensoric applications.

[1] R. Streubel et al. Nano Lett. 12, 3961 (2012)
[2] R. Streubel et al., Adv. Mater. 10.1002/adma.201303003

DS 11.5 Tue 10:45 CHE 89

Giant magnetoelectric effect at low frequencies in polymer-based thin film composites — Amit Kulkarni[1], Kerstin Meurisch[1], Robert Jahns[2], Iulian Teliban[2], Andre Piorra[3], •Thomas Strunskus[1], Reinhard Knöchel[2], and Franz Faupel[1] — [1]Chair for Multicomponent Materials, Institute for Materials Science, Christian-Albrechts-University at Kiel, Kaiserstr. 2, 24143 Kiel, Germany — [2]Microwave Laboratory, Institute of Electrical and Information Engineering, Christian-Albrechts-University at Kiel, Kaiserstr. 2, 24143 Kiel, Germany — [3]Chair for Inorganic Functional Materials Institute for Materials Science, Christian-Albrechts-University at Kiel, Kaiserstr. 2, 24143 Kiel, Germany

A new approach for the preparation of polymer based magnetoelectric sensors by spin-coating is presented. Poly(vinylidene fluoride trifluoroethylene)-copolymer 70/30 mol % (PVDF-TrEF) was used as piezo and metallic glass foils as magnetostrictive phase, respectively. The piezoelectric β phase fraction of the polymer layers were optimized by annealing and the films were polarized by contact poling. These films show a saturation polarization of 10 μC/cm^2 and remanent polarization of 8 μC/cm^2. For a prototype single-sided clamped cantilever, a magnetoelectric coefficient as high as 850 V/cmOe is observed at its fundamental bending mode resonance frequency at 27.8 Hz and a detection limit of 10 pT/Hz$^{1/2}$ at its second bending mode resonance frequency at 169.5 Hz. Moreover, this technique allows easy variation of the thickness of the piezoelectric layer and much easier integration into devices.

Coffee break (15 min)

Invited Talk DS 11.6 Tue 11:15 CHE 89

Carbon nanotubes for piezoresistive electro-mechanical transducers incorporating a wafer-level technology — •Sascha Hermann[1], Alexey Shaporin[1], Jens Bonitz[2], Steffen Hartmann[1], Jana Kalbacova[3], Raul D. Rodriguez[3], Dietrich R.T. Zahn[3], Jan Mehner[1], Bernhard Wunderle[1], Stefan E. Schulz[1,2], and Thomas Gessner[1,2] — [1]Technische Universität Chemnitz, Center for Microtechnologies (ZfM), 09126 Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems (ENAS), 09126 Chemnitz, Germany — [3]Technische Universität Chemnitz, Institute of Physics, Semiconductor Physics, 09126 Chemnitz, Germany

Single-walled carbon nanotubes (SWCNTs) can exhibit a distinctive intrinsic piezoresistivity exploitable in ultra sensitive displacement and force sensors. Driven by this potential, we present our progress on the integration of suspended SWCNT arrays into microelectromechanical systems (MEMS). Thereby we focus on application oriented wafer-level technologies. Aspects like a reliable electrical/mechanical contact, chirality distribution of SWCNTs, as well defect density and impurities are addressed in this work. Therefore a MEMS test stage is going to be presented which enables an extended electrical and structural characterization of suspended SWCNTs and other 1D nanomaterials under strain, as well as a mechanical reliability test. Furthermore, we investigate the local chiral distribution of SWCNTs as well as the structural and electrical properties of SWCNTs under strain.

DS 11.7 Tue 11:45 CHE 89

Carbon nanotubes under strain: Ab-initio investigations and compact models — •Christian Wagner[1], Vladimir Kolchuzhin[2], Erik Markert[2], Jörg Schuster[3], Jan Mehner[2], and Thomas Gessner[1,3] — [1]Center for Microtechnologies, TU Chemnitz, Germany — [2]Faculty of Electrical Engineering and Information Technology, TU Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Carbon nanotubes (CNTs) are not only attracting high interest in research, but also from the application point of view. Their mechanical strength and their outstanding piezoresistive response is one example that makes them suitable for novel sensors. These properties are well-explored for pristine Single-walled CNTs. But there is a lack of quantitative description of realistic CNTs in sensor environments.

Thus, this talk focuses on one hand on ab-initio-results of the electronic structure and transport properties of defective and functionalized CNTs under strain. And on the other hand we want to condense these results in compact models that can be incorporated in large-scale sensor simulations.

The first part concerns the comparison of simplified models to DFT results of strained CNTs [1] and shows its limits. Further, the electronic transport with different simplifications including scattering is elucidated. In the second part, these effective models for all available CNT chiralities will then be used to define compact models for sensor simulations by parametrization of electronic structure results.

[1] Wagner, C. et al., Phys. Stat. Sol. B, 249, 2450 (2012)

DS 11.8 Tue 12:00 CHE 89

Adjustment of carbon nanotube properties for sensor applications using Pd adatoms: An ab-initio study — •Florian Fuchs[1], Christian Wagner[1], Andreas Zienert[1], and Jörg Schuster[2] — [1]Center for Microtechnologies, Technische Universität Chemnitz, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Carbon nanotubes (CNTs) are, thanks to their extraordinary electromechanical properties, suitable for novel sensing devices such as acceleration sensors. For such applications, CNTs with small band gaps are favored. Since type selection of CNTs is still a challenge, methods are required to tune the band gaps in situ. We suggest submonolayer metal coating as a promising approach.

By using density functional theory, we investigate the influence of Pd adatoms on the surface of a semiconducting (8,4) CNT. We show that the adatoms strongly influence the electronic properties and that the band gap can be reduced. This effect can be increased further by using higher amounts of Pd adatoms. When the adatoms finally create a closed chain along the CNT, the band gap is reduced to the desired working range of possible sensor devices. Straining the system in uniaxial direction shows that the sensibility of the band gap and therefore the suitability for strain sensors is conserved. We also vary the position of a single adatom on the CNT surface in order to judge the stability of the adsorption. The resulting energy landscape shows a valley along the tube. Within that valley, energy barriers are small enough to permit thermally activated motion of the adatom.

Invited Talk DS 11.9 Tue 12:15 CHE 89

Integration of individual SWCNTs into field-effect transistor-based sensors — •Miroslav Haluska, Wei Liu, Kiran Chikkadi, Matthias Muoth, Tobias Suss, Stuart Truax, Cosmin Roman, and Chrisofer Hierold — Micro- and Nanosystems, ETH Zurich, Tannenstrasse 3, 8092 Zurich, Switzerland

Sensor demonstrators based on single-walled carbon nanotubes (SWCNTs) have shown very promising performance, including high sensitivity, low detection limits, and ultra-low power consumption. In this presentation, we focus on sensors integrating individual SWCNTs in a field effect transistor (FET). Such carbon nanotube FETs (CNFETs) may be used for different sensor applications, e.g. NO2 gas sensors, pressure sensors, or mechanically resonating transducers. The electrical characteristics of these devices exhibit unpredictable device-to-device variations that cannot be explained solely by the different properties of the incorporated SWCNTs. The device fabrication processes and a choice of materials coming into contact with the SWCNTs can also affect the CNFET characteristics by altering the nanotube and/or the interface properties. To identify and optimize the most critical device fabrication steps, we performed a series of monitoring measurements at different stages of the fabrication process. The results we have obtained from improved nanotube integration processes, including the utilization of a temporary nanotube protection layer, give us optimistic expectations for the utilization of SWCNTs in future sensor devices. The improvements in particular include the decrease of electrical contact resistances and narrowing of Ids-Vg hysteresis widths.

DS 11.10 Tue 12:45 CHE 89

Limitations of signal to noise ratio in Schottky barrier FET based biosensors — •Sebastian Pregl[1,2,3], Larysa Baraban[1], Walter Weber[2], Thomas Mikolajick[4,2,3], and Giovanni Cuniberti[1,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials TU Dresden 01062 Dresden, Germany — [2]Namlab GmbH 01187 Dresden, Germany — [3]Center for Advancing Electronics Dresden (cfaed) TU Dresden 01062 Dresden, Germany — [4]Institute of Semiconductor and Microsystems TU Dresden 01187 Dresden, Germany

In field effect transistor (FET) based biological sensors the presence of the specimen is detected via determination of changes of the electrical potential on the sensor surface. The resolution is limited by the accuracy of the transistor source to drain current measurement. Therefore a high ratio of transconductance to current noise is desired to maximize the signal to noise ratio (SNR). Schottky barrier FETs suffer from a high serial resistance which increases the noise level in transistor regimes beyond the subthreshold. Here, a study is presented reflecting the scaling of important device parameters like threshold voltage, transconductance, current noise and subthreshold slope with respect to the nanowire length. Regarding these dependancies a compromise of transistor size to SNR can be found matching the demands of the particular measurement.

DS 11.11 Tue 13:00 CHE 89

Silicon nanowire based detection of blood proteins — •Andreas Gang[1], Sebastian Pregl[1], Felix Zörgiebel[1], Lotta Römhildt[1], Claudia Pahlke[1], Walter Weber[2,3], Larysa Baraban[1], Lars David Renner[1], Thomas Mikolajick[2,3], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]NaMLab GmbH, 01187 Dresden, Germany — [3]Center for Advancing Electronics Dresden (CfAED), TU Dresden, 01062 Dresden, Germany

A fast and reliable detection of viruses and bacteria is crucial for improving our health care system. Compared to the commonly applied enzyme-linked immunosorbent assay (ELISA) method silicon nanowire (SiNW) based bio sensors are able to provide analytical results much quicker and with lower detection limits.

Here, we present our approach towards the assembly of SiNW based sensory devices made from bottom-up grown SiNWs. Introducing well-defined Schottky barrier contacts between electrodes and SiNWs allows on/off current ratios of up to 106 and using parallel arrays of SiNWs enables on currents of over 500 A at a source drain voltage of 0.5 V.

Furthermore, we present the implementation of the SiNW device into a biocompatible micro fluidic setup as well as the immobilization of aptamer bio receptor molecules on the sensor surface to obtain a bio sensor specific for the blood coagulation protein thrombin with a detection limit in the picomolar range.

DS 12: High- and low-k-dielectrics (Joint Session with DF)

Time: Tuesday 10:30–11:50 Location: GER 37

DS 12.1 Tue 10:30 GER 37

Magnetoelectric effect in $FeCr_2S_4$ — •Martin Wohlauer, Stephan Krohns, Joachim Deisenhofer, Vladimir Tsurkan, and Alois Loidl — Universität Augsburg, Lehrstuhl für Experimentalphysik V, Universitätsstraße 1, 86150 Augsburg

The substance $FeCr_2S_4$ is a well investigated ferrimagnetic[1] spinel-type halfmetal[2]. Despite many publications describing effects in this compound over the last 50 years, the complex interactions of its many physical features leave many unanswered questions until today. Especially its magnetic and dielectric properties still show unreported effects. In this talk I'll present new measurements of dielectric constants under the influence of magnetic fields up to 7 Tesla, showing a magneto-electric coupling below 10 K. Kalvius *et al.*[3] presented evidence for a noncollinear spin structure below 40 K. The change of ϵ' by a magnetic field indicates a lowered crystal symmetry which may be caused by a helical spin configuration.

[1] G. Haacke *et al.*. *J. Phys. Chem. Solids*, **28**:1699 – 1704 (1967).
[2] M. S. Park *et al.*. *Phys. Rev. B*, **59**:10018 – 10024 (1999).
[3] G. M. Kalvius *et al.*. *J. Phys.: Condens. Matter*, **22**:052205(2010).

DS 12.2 Tue 10:50 GER 37

Barium silicate (Ba_2SiO_4) as high-k dielectric material — •Shariful Islam[1], Karl Hofmann[2], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik (ATMOS), leibniz universität hannover — [2]Inst. f. Bauelemente der Mikroelektronik, leibniz universität hannover

In search of an alternative gate oxide, the structural and electronic properties of mixed Ba/Sr silicates on Si(001) were investigated. In order to specify the stoichiometry and band gap of these oxides we used X-ray Photoelectron Spectroscopy (XPS) and Electron Energy Loss Spectroscopy (EELS) respectively. Crystal structures were investigated by Spot Profile Analysis-Low Energy Electron Diffraction (SPA-LEED). Electrical characterization was done by CV and IV measurements.

Characteristics of high-k dielectric $(Ba_{0.8}Sr_{0.2})_2SiO_4$ and Ba_2SiO_4 were studied both on structured and unstructured samples. Both oxides are stable at high temperature and at ambient atmosphere. Crystalline $(Ba_{0.8}Sr_{0.2})_2SiO4$ has dielectric constant, $\varepsilon = 18 \pm 2$. The band gap was found to be 6.0 eV, with band offsets > 2eV both for valence and conduction band. The thick crystalline layers of pure $(Ba_{0.8}Sr_{0.2})_2SiO_4$ were also grown. An $\varepsilon = 19.6 \pm 0.4$, a small reduction of bandgap to 5.7 ± 0.1 eV and band offsets comparable to $(Ba_{0.8}Sr_{0.2})_2SiO_4$ were found. Due to our growth procedure (diffusion of Si into oxide) leakage currents are still comparatively high (0.1 A/cm^2 at 1V). Further electrical and structural properties of Ba_2SiO_4 will also be presented.

DS 12.3 Tue 11:10 GER 37

Comparison of different gate dielectrics for GaN based high electron mobility transistors — •Annett Freese[1], Stefan Schmult[2], Andre Wachowiak[1], and Thomas Mikolajick[1,2] — [1]NaMLab gGmbH, Nöthnitzer Str. 64, D-01187 Dresden — [2]TU Dresden, Institute of Semiconductor and Microsystems (IHM), Nöthnitzer Str. 64, D-01187 Dresden

The wide-bandgap and high electron mobility make gallium nitride (GaN) based heterostructures particularly interesting for future high-power switching applications. However, conventional GaN heterostructure field effect transistors (HFET) use a simple Schottky gate contact. Thus, they suffer from undesired high gate leakage currents and current collapse. To eliminate these challenges, a dielectric material can be placed between the gate electrode and the semiconductor. Aluminium oxide (Al2O3), hafnium oxide (HfO2), and zirconium dioxide (ZrO2) are potential candidates for such a gate dielectric material due to their high dielectric constant as well as their high conduction band offset to GaN. Learning from silicon processing technology, a successful integration of a suitable dielectric does not only depend on its material properties, but also relies heavily on the nature of the interfaces to the top and bottom electrodes. In this work we investigated Al2O3, HfO2 and ZrO2 with respects to their structural and electrical properties on GaN. The influence of the deposition methods, Molecular Beam Deposition (MBD) and Atomic Layer Deposition (ALD), on the film quality was studied.

DS 12.4 Tue 11:30 GER 37

Effect of different precursor for Atomic Layer growth of Ga2O3 using H2O as the oxygen source — •Sakeb Hasan Choudhury, Massimo Tallarida, Chittaranjan Das, and Dieter Schmeisser — Brandenburg University of Technology, Applied Physics-Sensors technology, Konrad-Wacshmann-Allee, 17, 03046 Cottbus, Germany

Atomic Layer deposition as a technique provides appropriate thickness control, conformality and Homogeneity. However, the contribution of Precursor and Substrate in the growth process is worth exploring and cannot be avoided as previously seen in case of Trimethyl Gallium. Ga2O3 is a member of group *Transparent Conducting Oxides*, hence possess immense potential in numerous applications. In this work, we would like to report about the growth of Ga2O3 using Tris-(dimethylamino)-gallium dimer and H2O as metal and oxygen precursors, respectively. Unlike Trimethylgallium, Ga2O3 films can be produced between temperature 200-300°C using Tris-(dimethylamino)-gallium dimer and it seems to be well compatible with H2O. These films were characterized by Synchrotron X-ray photoemission spectroscopy at BESSY/HZB, Berlin and subsequent analysis reveals stable film growth and absence of growth terminating phenomenon*s.

DS 13: Organic semiconductors: Photovoltaics (Jointly with HL, CPP)

Time: Tuesday 10:00–12:30 Location: POT 081

DS 13.1 Tue 10:00 POT 081

Analytical transmission electron microscopy on hybrid solar cells based on perovskites — •Diana Nanova[1,2,4], Anne Katrin Kast[1,3,4], Christian Müller[1,4], Rasmus R. Schröder[3,4], Robert Lovrincic[1,4], and Wolfgang Kowalsky[1,4] — [1]Institut für Hochfrequenztechnik, TU Braunschweig — [2]Kirchhoff Insitut für Physik, Universität Heidelberg — [3]Cryo-EM, CellNetworks, Bioquant, Universität Heidelberg — [4]InnovationLab GmbH, Heidelberg

Hybrid solar cells based on metal-organic perovskite absorbers are of major interest due to their remarkable power conversion efficiencies of up to 15%. Recently, it has been shown that the morphology of the perovskite itself as well as the interplay between the absorber and the mesostructured electron acceptor strongly affects the electrical properties of the device. We present a combined study of the structure-function relationship of solution processed solar cells based on mesostructured perovskites. The morphology of the solar cells was studied by analytical transmission electron microscopy (ATEM). In ATEM electron energy loss spectroscopy (EELS) and electron spectroscopic imaging (ESI) are applied in order to obtain material contrast. To be able to classify the TiO2 and the perovskite rich areas in the corss-section of the device a series of monochromatic images in the low-loss regime was acquired. We observed significant changes in pore size, pore filling and pore distribution of the mesostructured layer depending on the annealing conditions of the perovskite. Furthermore, we correlated our results to the I-V characteristics of the solar cells.

DS 13.2 Tue 10:15 POT 081

Alloyed zinc sulfide - copper indium disulfide nanocrystals for application in hybrid photovoltaics — •Björn Kempken, Nikolay Radychev, Christopher Krause, Jie Li, Holger Borchert, Joanna Kolny-Olesiak, and Jürgen Parisi — Carl von Ossietzky University of Oldenburg, 26111 Oldenburg

Semiconductor nanocrystals (NCs) continue to attract immense attention because of their size-dependent optical, physical, and chemical properties which causes them to be a favourable material for hybrid solar cell applications. A promising candidate for the inorganic/organic active layer is alloys of ZnS and CuInS2 (ZCIS NCs), which on the one hand strongly absorb in the visible range up to 800 nm, and, on the other hand, belongs to the "green" type of semiconductor NCs. In the present work, high quality ZCIS NCs were synthesized and subjected to hexanethiol ligand exchange procedures. Laboratory solar cells based on blends of treated ZCIS NCs and poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)-alt-4,7(2,1,3-benzothiadiazole)] (PCPDTBT) as active layer were prepared and investigated by current-voltage and electron spin resonance measurements. Hybrid ZCIS/PCPDTBT laboratory solar cells demonstrate well pronounced diode behavior with outstanding characteristics of the open-circuit voltage which reached up to 1.2 V.

DS 13.3 Tue 10:30 POT 081

Improving efficiency of solar power generation by combination of a sensitized mesoscopic solar cell with a thermoelectric generator — •Hans-Fridtjof Pernau, Jana Heuer, Karina Tarantik, Alexandre Jacquot, Jan D. König, Martin Jägle, and Kilian Bartholomé — Fraunhofer IPM, Freiburg, Germany

Standard photovoltaic(PV) solar cells use only about half of the light spectrum provided by the sun. The infrared part is not used for producuction of electrical energy. Even further, the infrared light heats up the pv cell and decreases thereby its efficiency. The basic idea for a combined pv and thermoelectric solar cell has been published in 2008 [1]. The improvements in thermoelectric materials and scientific work on thermoelectrics lead to new ideas for those systems [2] which will be investigated in the EU-FP7-Projekt Globasol. Within the project, a hybrid solar cell made of a sensitized mesoscopic solar cell and a thermoelectric generator (TEG) will being developed. The light of the sun is split at about 800nm. The visible and ultra violet part is transfered to the sensitized mesoscopic solar cell, the infrared part illuminates the TEG cell. With the hybrid solar cell, the full solar spectrum is exploited. We present the first modeling results of the project and the first evaluation version of the hybrid cell.

[1] T.M. Tritt, H. Böttner and L. Chen, *Thermoelectric: Direct Solar Thermal Energy Conversion*, MRS Bulletin, vol.33 (2008) pp. 366-368; [2] D. Kraemer et al., *High-performance flat panel solar thermoelectric generator with high thermal concentration*, Nature materials vol.10 (2011) pp. 532-538.

DS 13.4 Tue 10:45 POT 081

Spin dynamics in organic solar cells measured by pulsed electrically detected magnetic resonance — •Alexander J. Kupijai, Konstantin M. Behringer, Martin Stutzmann, and Martin S. Brandt — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching

Organic photovoltaics are of great interest in the development of sustainable energy sources. To investigate the recombination and transport processes in organic solar cells we use the technique of pulsed electrically detected magnetic resonance (EDMR) where we measure the change of the photocurrent caused by resonant X-band microwave pulses in the presence of an external magnetic field. As test devices, we use bulk heterojunction P3HT/PCBM (poly(3-hexylthiophene-2,5-diyl) / [6,6]-phenyl C_{61} butyric acid methyl ester) solar cells. At temperatures of 10K we are able to observe both positively and negatively charged polarons in the pulsed EDMR spectrum and can identify them as partners in a spin-dependent pair process by experiments using two microwave frequencies. Using the time resolution and sensitivity of pulsed EDMR we are able to quantify the spin dynamics of the system and measure the lifetime of parallel spin pairs, the lifetime of antiparallel spin pairs, the spin decoherence time and the coupling strength between the spin partners. All of these microscopic parameters provide valuable information for an optimization of overall solar cell efficiencies.

DS 13.5 Tue 11:00 POT 081

Imaging the origin of S-shaped current-voltage characteristics of organic solar cells by scanning Kelvin probe microscopy — •Christian Müller[1,2,3], Rebecca Saive[1,2,3], Janusz Schinke[1,3], Robert Lovrincic[1,3], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab GmbH, Heidelberg, Germany — [2]Kirchhoff-Institut für Physik, University Heidelberg, Germany — [3]Institut für Hochfrequenztechnik, Technische Universität Braunschweig, Germany

We investigated organic bilayer solar cells consisting of poly(3-hexylthiophene)/1-(3-methoxycarbonyl)propyl-1-phenyl[6,6]C61 (P3HT/PCBM). Scanning Kelvin probe microscopy (SKPM) was performed on the solar cell cross sections which were exposed with a focused ion beam. We prepared the P3HT/PCBM bilayer solar cells by solution processing. These bilayer solar cells showed normal and anomalous, S-shaped current-voltage characteristics. Using SKPM on the device cross sections, we found that in normal bilayer solar cells the potential dropped at the ITO/PEDOT:PSS contact and over the active area, whereas in S-shaped bilayer solar cells the potential dropped exclusively at the aluminium contact. This behavior confirms the assumption that S-shaped curves are caused by hindered charge transport at electrode interfaces.

Coffee break (15 min.)

DS 13.6 Tue 11:30 POT 081

Improving the Charge Transport Parameters of Near-Infrared Absorbers — •Sebastian Radke[1,2], Frank Ortmann[1,2], Reinhard Scholz[2,3], and Gianaurelio Cuniberti[1,2,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, Germany — [3]Institut für Angewandte Photophysik, TU Dresden, Germany — [4]Center for Advancing Electronics Dresden, TU Dresden, Germany

For an improved performance of organic tandem solar cells, efficient organic infrared absorber materials are necessary. A promising class already used successfully in organic solar cells are 4,4'-difluoro-4-bora-3a,4a-diaza-s-indacenes (BODIPYs). Based on a comparative study of the intramolecular electronic properties as well as the intermolecular coupling in the crystal phase of three potential candidates, we find that the benzannulation of the molecular core improves both electron and hole transfer. As the frontier molecular orbitals are delocalized over the entire molecule also by attaching additional functional groups to the molecular core, the intermolecular coupling and especially the performance in amorphous phase can be optimized further. However, an immobilization of these substituents is necessary to regulate an increase in the reorganization energy for hole transfer. Based on these design rules, BODIPYs with optimized charge transfer properties can be synthesized increasing also the performance of the devices.

DS 13.7 Tue 11:45 POT 081

Qualitative und quantitative Auswertung von komplementären bildgebenden Methoden zur Degradationsuntersuchung und Qualitätskontrolle von Polymersolarzellen — •Roland Rösch, Marco Seeland, Daniel Fluhr, Burhan Muhsin, Peter Fischer, Rolf Öttking und Harald Hoppe — Institut für Physik, TU Ilmenau, Deutschland

Wir berichten über beschleunigte Alterungstests an modernen organischen und polymeren Solarzellen, ergänzt durch bildgebenden Methoden, wie z.B. bildgebende Lumineszenz, Lock-in Thermographie und lichtinduziertes Kurzschlussstrommapping. Neben einer qualitativen Interpretation der Daten, ist es durch die Kombination der verschiedenen Methoden möglich, auch eine quatitative Auswertung der Dynamiken der verschiedenen Degradationsmechanismen zu erhalten. Desweiteren vergleichen wir die experimentellen Ergebnisse mit theoretischen Modellen des Ladungsträgerflusses und -Rekombination. Daraus lassen sich intrinsische Paramter der Bauelemente, wie Elektrodenwiderstand und Diodenidealitätsfaktor bestimmen. Die wichtigste Erkenntnis aus diesen Untersuchungen ist, dass die Stabilität von modernen organischen Solarzellen vor allem durch die Elektrodendegradation und die Qualität der Versiegelung begrenzt ist. Diese Arbeit liefert einen Leitfaden für weitere Verbesserungen hin zu stabilen organischen Solarzellen.

DS 13.8 Tue 12:00 POT 081

Visualization of Lateral Phase Separation in Polymer: Fullerene Solar Cells by Quantitative Evaluation of Luminescence Imaging Measurements — •Marco Seeland, Christian Kästner, and Harald Hoppe — Institut für Physik, TU Ilmenau, Ilmenau, Germany

Luminescence imaging has evolved to a versatile characterization method for studying the laterally resolved behavior of polymer solar cells. Especially in degradation studies the use of luminescence imaging is beneficial as it is non-invasive and offers short measurement times. By either electrical or optical excitation separate characterization of the electrical contacts and the active layer is feasible. However, the data analysis so far is mainly qualitative, i.e. interpretation of the measured luminescence image by comparison with other techniques. In this work we present a quantitative analysis of electroluminescence images of laterally inhomogeneous polymer solar cells. By decoupling the local parameters within an iteration procedure this analysis allows calculation of the local current flow through and the local voltage applied to the active layer. Furthermore quantitative images of the local series resistance and the saturation current-density are achieved. The local saturation current-density contrast was found to correlate perfectly with the strong lateral phase separation occurring in PPE-PPV:PCBM based devices. Further analysis of the lateral difference in the saturation current-densities delivers information on the thermal activation of charge carriers at the donor/acceptor-interface and in the phase separated bulk.

DS 13.9 Tue 12:15 POT 081

The influence of fullerene loading on the photogeneration in intercalated polymer: fullerene bulk heterojunction solar cells — •Andreas Zusan[1], Koen Vandewal[2], Benedikt Allendorf[1], Nis Hauke Hansen[1], Jens Pflaum[1], Martin Heeney[3], Alberto Salleo[2], Vladimir Dyakonov[1,4], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Department of Materials Science and Engineering, Stanford University, Stanford, California 94305, USA — [3]Department of Chemistry, Imperial College, London, SW7 2AZ, UK — [4]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

The conjugated polymer, pBTTT, allows a systematic tuning of the blend morphology by varying the acceptor material and blend ratio, making it a well-suited structural model for studying the fundamental processes in organic BHJ solar cells. To analyze the correlation between photogeneration and intercalation, we have performed time delayed collection field (TDCF) measurements and Fourier-transform photocurrent spectroscopy (FTPS) on pBTTT:PCBM devices in various stoichiometries. An increased PCBM loading resulted in a less field dependent dissociation, which we attribute to enhanced electron delocalization along extended PCBM nanophases and energetically driven spatial separation of polarons due to the presence of pure acceptor domains. The highly efficient transfer of charge carriers from the intercalated phase into the pure phase has been studied further by extending TDCF measurements to include segregated pBTTT:bisPCBM blends.

DS 14: Focus Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale III (jointly with O)

Time: Tuesday 10:30–13:15 Location: TRE Ma

Topical Talk DS 14.1 Tue 10:30 TRE Ma

Ultrafast relaxation dynamics of Hubbard nanoclusters — •Michael Bonitz[1], Sebastian Hermanns[1], Christopher Hinz[1], and Denis Lacroix[2] — [1]Institut für Theoretische Physik und Astrophysk, CAU Kiel, Leibnizstr. 15, 24098 Kiel — [2]IPN Orsay, 15 Rue Georges Clemenceau, 91406 Orsay

With the growing availability of intense short-pulse radiation sources it becomes possible to drive interacting many-particle or few-particle systems out of equilibrium in a controlled way. The subsequent relaxation and equilibration dynamics is still poorly understood. From a theory point of view these processes are complicated due to the simultaneous dynamics of the occupation functions and of binary correlations. The problem becomes even more complicated when the system has finite size and is spatially inhomogeneous [1]. The Hubbard model is a prototype for treating correlation effects in condensed matter or molecular systems fully including finite size and inhomogeneity effects. We, therefore, concentrate on the relaxation dynamics of small 1D, 2D and 3D Hubbard clusters that contain from a few to several hundred electrons. We observe a complex multi-stage relaxation behavior that depends on the external excitation, on the coupling strength and on the geometry of the system. In this talk we present results from two complementary theoretical approaches: first, from nonequilibrium Green functions where we apply the Generalized Kadanoff Baym ansatz [1] and, second, from a stochastic mean field approach.

[1] K. Balzer, and M. Bonitz, “Nonequilibrium Green's Functions Approach to Inhomogeneous Systems”, Lect. Notes Phys. **867** (2013)

DS 14.2 Tue 11:00 TRE Ma

Exact adiabatic approximation in TDDFT — •Jeiran Jokar and Nicole Helbig — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The use of functionals from static density functional theory in an adiabatic way in a time-dependent framework is known to cause various problems due to the resulting exchange-correlation kernel being frequency independent. In order to isolate the effects which are due to the adiabatic approximation we calculate the exact static potential for two electron systems. Before using this potential in an adiabatic way in a time propagation we need to ensure that the potential is well defined also at those parts of space where the density is small as they might become more populated at a later time. We use the exact adiabatic approximation to describe Rabi oscillations, i.e. the oscillation between the ground state and an excited state when a monochromatic laser with a frequency close to the resonance is applied.

DS 14.3 Tue 11:15 TRE Ma

Real-time propagation of coupled Maxwell-Schrödinger and time-dependent Kohn-Sham-Maxwell systems — •René Jestädt[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Based on the Riemann-Silberstein vector of the electromagnetic field,

we formulate Maxwell's equations in a symplectic spinor representation similar to the Dirac equation. This spinor representation allows us to use standard unitary propagation techniques developed for the Schrödinger equation [1] also for Maxwell's equations and simplifies a coupled solution of Maxwell's and Schrödinger's equations. To illustrate our approach, we present the real-time evolution of atomic systems embedded in optical waveguides and dielectric nanostructures. The coupling of Maxwell's equations to the time-dependent Kohn-Sham equations is a basic ingredient for the development of a time-dependent density functional theory formulation of quantum electrodynamics [2]. As an extension of our work on coupled Maxwell-Schrödinger systems, we show first steps of an implementation of Maxwell's equations coupled to the time-dependent Kohn-Sham equations in the first principles real-space real-time code octopus [3].
[1] A. Castro et al., J. Chem. Phys. **121** (2004).
[2] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011); I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).
[3] X. Andrade et al., J. Phys. Cond. Mat. **24** (2012).

DS 14.4 Tue 11:30 TRE Ma

Nonlinear optics by means of the dynamical Berry phase: Application to second- and third-harmonic generation — •Claudio Attaccalite[1] and Myrta Gruning[2] — [1]Univ. Grenoble Alpes/CNRS, Institut Neel, F-38042 Grenoble, France — [2]School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK

We present an real-time approach to study nonlinear optical properties in Condensed Matter systems that is especially suitable for crystalline solids. The equation of motions and the coupling of the electrons with the external electric field are derived from the Berry phase formulation of the dynamical polarization. Many-body effects are introduced by adding single-particle operators to the independent-particle Hamiltonian. Specifically we include crystal local field effects, renormalization of the energy levels and excitonic effects. The approach is validated by calculating the second and third harmonic generation of bulk semiconductors. Finally we present second-harmonic generation spectrum of h-BN or MoS2 monolayers and show that correlation effects double the signal intensity at the excitonic resonances with respect to the contribution from independent electronic transitions.

References: [1] Nonlinear optics from ab-initio by means of the dynamical Berry-phase http://arxiv.org/abs/1309.4012 [2] Second Harmonic Generation in h-BN and MoS2 monolayers: the role of electron-hole interaction http://arxiv.org/abs/1310.7459

15 min. break

DS 14.5 Tue 12:00 TRE Ma

Accurate Correlation Energies from Adiabatic Time-Dependent Density Functional Theory with Renormalized Kernels — •Thomas Olsen[1] and Kristian S. Thygesen[2] — [1]Universidad del Pais Vasco — [2]Center for Atomic-scale Materials Design (CAMD), Technical University of Denmark

We demonstrate the accuracy of electronic correlation energies obtained from the adiabatic connection and Time-Dependent Density Functional Theory (TDDFT) using a non-empirical renormalized gradient-corrected exchange-correlation kernel. The method can be viewed as a natural step beyond the Random Phase Approximation (RPA) and captures the short-range correlation effects which are poorly described in RPA. In particular, we show that for molecules and solids the renormalized kernel gives a four and five fold improvement in binding energies respectively when compared to RPA. We also consider examples of barrier heights in chemical reactions, molecular adsorption and graphene interacting with metal surfaces, which are three examples where RPA has provided highly accurate results. In these cases, our novel kernel provides results that are of equal quality or even slightly better than RPA, with a similar computational cost. We finally note that the renormalization procedure can be applied to any known semi-local exchange-correlation functional and thus defines an entire new class of adiabatic non-local functionals for ground state calculations within TDDFT.

DS 14.6 Tue 12:15 TRE Ma

Low scaling algorithm for the random phase approximation — •Merzuk Kaltak, Jiri Klimeš, and Georg Kresse — University of Vienna, Computational Material Physics

The computationally most expensive step in conventional RPA implementations is the calculation of the independent particle polarizability χ. We present an RPA algorithm that calculates χ using the Green function G in real space and imaginary time. The systematic construction of optimized time and frequency grids for G is obtained by means of solving a fitting problem. Furthermore a non-uniform discrete Fourier transform between the two grids is introduced, which converges exponentially. We show that the usage of the Green function approach in combination with the optimized grids can be used for the calculation of the RPA correlation energy for large systems.

DS 14.7 Tue 12:30 TRE Ma

Long range correlation energy from coupled atomic response functions — •Alberto Ambrosetti and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Faradayweg 4-6 14195 Berlin, Germany

Electron correlation is an elusive and ubiquitous energy contribution that arises from transient collective electron fluctuations. Its reliable (accurate and efficient) modeling is central to the correct description of cohesive, structural, and response properties of molecules and solids. In this regard, the main challenge is to model the long-range correlation energy beyond (semi-)local density-functional approximations. Here we propose a very efficient method to compute the long-range correlation energy for non-metallic molecules and solids within a density functional theory framework, by using coupled atomic response functions (ARF). Extending the recent MBD method [1], we separate the coupling between ARFs into short and long range, allowing for a seamless many-body treatment of weakly and strongly polarizable systems. Thorough benchmarking on large data sets including small molecules (S22, S66x8), large supramolecular complexes (S12L), molecular crystals (X23) and bulk graphite shows consistently good agreement with high level theoretical and experimental reference binding energies (within the order of 6%). The uniform accuracy for molecules and solids represents a strong validation of our method, and further confirms the importance of modeling the truly collective nature of the long-range correlation energy. [1] A. Tkatchenko et al. PRL **108** 236402 (2012).

DS 14.8 Tue 12:45 TRE Ma

The exact Hohenberg-Kohn functional for a lattice model — •Tanja Dimitrov[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Standard local exchange-correlation and semi-local functionals in ground-state density functional theory are known for their shortcomings in describing correct charge transfer, dissociation energies of molecular ions, and barriers of chemical reactions [1,2]. To understand the failures of approximate functionals and to gain insight into the behavior of the exact functional, we investigate the exact solution of the many-body Schrödinger equation for a lattice model. Using exact diagonalization, we explicitely construct the exact Hohenberg-Kohn functional and the mapping from densities to wavefunctions. Besides the normal inter-system derivative discontinuity widely discussed in the density-functional theory community, we observe a new feature of the exact functional in the low-density limit. This "intra-system derivative discontinuity" resembles the inter-system derivative discontinuity, but is within the system (work in progress [3]). The description of many physical phenomena linked to charge-transfer processes (both in the static and dynamical regimes) require a proper account of this "intra-system derivative discontinuity".

[1] A. J. Cohen et al. Science **321**, 792 (2008).
[2] P. Mori-Sanchez et al., Phys. Rev. Lett. **100**, 146401 (2008).
[3] T. Dimitrov, H. Appel, A. Rubio to be published

DS 14.9 Tue 13:00 TRE Ma

Incorporating static correlation effects into density functional theory — Nektarios N. Lathiotakis[1], •Nicole Helbig[2], Nikitas I. Gidopoulos[3], and Angel Rubio[4,5] — [1]Theoretical and Physical Chemistry Institute, NHRF Athens, Greece — [2]Peter-Grünberg Institut, Forschungszentrum Jülich, Germany — [3]Department of Physics, Durham University, United Kingdom — [4]Nano-Bio Spectroscopy group, Universidad del Pais Vasco and DIPC, San Sebastian, Spain — [5]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We present a novel idea that builds on the knowledge acquired in Reduced density matrix functional theory (RDMFT) to construct a density-functional scheme which accurately incorporates static and left-right correlation effects. At the same time, the new scheme preserves the high quality of a density functional description at the equilibrium and keeps the computational costs at an acceptable level comparable to the costs when using hybrid functionals. Within this scheme the natural orbitals, i.e. the eigenfunctions of the one-body density matrix, are constrained to be solutions of a single-particle Schrödinger equation with a local effective potential. This provides a natural way to connect an energy eigenvalue spectrum to the natural orbitals. This energy spectrum is found to reproduce the ionization potentials of different atoms and molecules very well. In addition, the dissociation limit of diatomic molecules is well described without the need to break any spin symmetry, i.e. this attractive feature of RDMFT is preserved. The present scheme can be easily implemented in all first principles codes for electronic structure calculations.

DS 15: Organic semiconductors: Transistors and OLEDs (Jointly with HL, CPP)

Time: Tuesday 14:00–15:45 Location: POT 081

DS 15.1 Tue 14:00 POT 081

Solution-gated organic field effect transistors: small-molecule versus polymeric materials — •Hannah Schamoni[1], Rossella Porrazzo[1,2], Jose A. Garrido[1], and Maria Rosa Antognazza[2] — [1]Walter Schottky Institut, Technische Universität München, Deutschland — [2]Center for Nanoscience Technology (CNST) of IIT@Polimi, via Pascoli 70/3, 20133 Milano, Italy

Solution-gated organic field effect transistors (SGOFETs) are promising devices for biosensing applications featuring, amongst others, low production costs. For the organic semiconductor, two different kinds of materials are typically used, namely polymers like poly(2,5-bis(3-hexadecylthiophen-2-yl)thieno[3,2-b]thiophene) (pBTTT) and small molecules like α-sexithiophene (6T). In this work, we have investigated devices of both types regarding their performance, stability, and pH and ion sensitivity. A comparison of the two approaches is presented, taking also into account the differences in processing: While polymers can be spin-coated onto the substrate, small molecules are grown using organic molecular beam deposition. Finally, we will discuss the potential of SGOFETs as light sensors to stimulate nerve cells, which can pave the way towards the development of a new generation of retinal implants.

DS 15.2 Tue 14:15 POT 081

Light-induced switching mechanism of porphyrin-coated Si nanowire field effect transistors — •Eunhye Baek[1], Sebastian Pregl[1,2], Mehrdad Shaygan[3], Lotta Röhmhildt[1], Dmitry Ryndyk[1,2], Larysa Baraban[1], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Center for Advancing Electronics Dresden, TU Dresden, Germany — [3]Division of IT Convergence Engineering, Pohang University of Science and Technology, Pohang, Korea

We present light-induced switching mechanism of porphyrin-coated Si nanowire field effect transistors (Si NW FETs). Si NW FETs were fabricated by bottom-up methods and show ambipolar characteristics due to thermally annealed Schottky barrier on the contact between the electrode and NW channel. Si NW FETs are functionalized by porphyrin, a key dye molecule in photosynthetic process, to have photo-sensitive operation. Porphyrin-coated devices show clear current switching under light illumination that is not shown in bare devices. Switching time and switching current ratio depend on the concentration of porphyrin. Under light irradiation, electrical properties of molecular layer are changed; increased mobile charges by photo-excitation screen electrical field from the applied bias. In addition, molecules are polarized by charge separation that build vertical field towards the NWs. The electrical charge of porphyrin layer modifies the total applied field in NW, which induces current switching according to the concentration of porphyrin.

DS 15.3 Tue 14:30 POT 081

Lithographically processed vertical organic thin-film transistors (VOTFTs) — •Alrun Aline Günther[1], Hans Kleemann[2], Björn Lüssem[3], Daniel Kasemann[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden Germany — [2]Novaled AG, Tatzberg 49, 01307Dresden, Germany — [3]Department of Physics, Kent State University, Kent, OH 44242, USA

Vertical organic transistors are a novel type of organic semiconductor devices, the first of such devices having been presented by Ma et al. in 2004[1]. The idea of this novel device concept is to overcome the limitations often faced in conventional organic thin-film transistors (OTFTs), where performance parameters (e.g. cut-off frequency or transconductance) are limited by the channel length of the OTFT. The VOTFT concept developed at IAPP[2] allows for downscaling of this channel length to the order of nanometres, while using a novel photolithography approach[3] to achieve patterning of the source electrode. In the present work, the effects of semiconductor film morphology and addition of dopant molecules are investigated for pentacene VOTFTs. It is expected that knowledge of such effects will give a more detailed insight into the fundamental functional principles of the device, as these are not yet well understood.

References [1] L. Ma et al, Appl. Phys. Lett. 85, 21 (2004) [2] H. Kleemann et al, Small, Epub ahead of print (2013) [3] H. Kleemann et al, Org. Elec. 13, 3 (2012)

DS 15.4 Tue 14:45 POT 081

Controlling morphology of a Vertical Organic Transistor for enhanced current gain and very low operation voltages — •Felix Kaschura, Axel Fischer, Björn Lüssem, Daniel Kasemann, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden

Vertical Organic Triodes represent a novel transistor technology enabling high current densities without the need for expensive structuring techniques. These devices require a permeable base for highly efficient operation. Therefore, we place a morphology modifying gold layer underneath the organic semiconductor, which enhances charge carrier transmission and thus the current gain. We have further studied a geometry optimization of the device structure allowing to tune the built-in field of the device. This results in an increased transmission as the built-in field at the collector actively gathers charge carriers, as well as a very low minimum operation voltage - both desirable characteristics for practical applications.

DS 15.5 Tue 15:00 POT 081

Contact Resistance Adjustment in Top-Contact Organic Field Effect Transistors by Localized Doping — •Ji-Ling Hou, Björn Lüssem, Daniel Kasemann, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01069 Dresden, Germany

The contact resistance between metal and organic interface is a key challenge for Organic Field-Effect Transistors (OFETs) when short channel lengths are used to achieve low-cost and high-frequency. In this study, bottom-gate top-contact organic field effect transistors (OFETs) with different thickness of the p-dopant 2,2-(perfluoronaphthalene-2,6-diylidene) (F6-TCNNQ) under Au electrodes were fabricated by orthogonal photolithography to further investigate their impact on contact resistance. Extracted by the transmission line method (TLM), contact resistance was found to be significantly reduced from 50 kOhm*cm to 10 kOhm*cm by adding a 1nm thin dopant layer. Doping leads to an improved injection at low gate voltages, while the contact resistance is also reduced in the undoped reference device due to the applied field at higher gate voltages. Finally, we conducted temperature dependent I-V measurement to study the change of contact resistance at lower temperature. The result shows an abrupt transition in the linear region between 220K and 240K, which gives a direct evidence and link between contact resistance and doping effect.

DS 15.6 Tue 15:15 POT 081

IR spectroscopic investigation of charge transfer in organic semiconductors I: Doped layers — •Tobias Glaser[1,2], Sebastian Beck[1,2], David Gerbert[1,2], Johannes Zimmermann[1,2], and Annemarie Pucci[1,2,3] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab GmbH, Heidelberg — [3]Centre for Advanced Materials, Universität Heidelberg

Electrochemical doping of amorphous organic semiconductors is a frequently used technique in order to increase the amount of free charge carriers and thereby the conductivity of the doped layers. But for organic semiconductors, in general very low doping efficiencies in the range of only a few percent have been reported.

We performed infrared (IR) spectroscopy under ultrahigh vacuum conditions in order to investigate the process of charge transfer in various p-doped material systems. The charge transfer in doped layers can be determined with IR spectroscopy, as the new electronic structure of the charged molecules leads to a change in bond length and bond strength within the charged molecules that therefore exhibit a different vibrational spectrum compared to the neutral molecules. The appearance of broad electronic excitations in these systems shows the formation of new electronic states due to hybridization. We investigated the behavior of these electronic states after annealing as well as after degradation of the doped layers.

Financial support from the BMBF via the MESOMERIE Project (FKZ 13N10724) is gratefully acknowledged.

DS 15.7 Tue 15:30 POT 081

IR spectroscopic investigation of charge transfer in organic semiconductors II: Interfaces — •Sebastian Beck[1,2], David Gerbert[1,2], Tobias Glaser[1,2], and Annemarie Pucci[1,2,3] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab GmbH, Heidelberg — [3]Centre for Advanced Materials, Universität Heidelberg

In organic semiconductors charge transfer (CT) is crucial for all kinds of applications but its basic mechanisms are still under severe discussion. Especially a better knowledge of CT at organic/organic and inorganic/organic interfaces is essential for the design of new electronic devices with improved performance.

In this study we want to introduce a new approach to investigate CT at interfaces by means of in situ infrared (IR) spectroscopy. We investigated the system 4,4'-bis(N-carbazolyl)-1,1'-biphenyl (CBP)/MoO_3, as a prototypical example, and spectroscopically identified charged and non-charged species of CBP molecules, that were deposited onto MoO_3. Both species can be distinguished by their specific vibrational modes in the mid IR range. The inverted layer structure with MoO_3 deposited onto CBP shows a significantly different behavior that is attributed to the diffusion of MoO_3 into the organic film.

Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

DS 16: Focus Session: Sensoric Micro and Nano-systems II

Time: Tuesday 14:00–16:15 Location: CHE 89

Invited Talk DS 16.1 Tue 14:00 CHE 89

Carbon Wonderland from an Engineering Perspective — •Franz Kreupl, Stefan Kapser, and Sebastian Hübner — TUM, Department of Hybrid Electronic Systems, Munich, Germany

A fresh look on carbon-based materials like carbon nanotubes (CNTs) or graphene in microelectronic applications will be given. Graphene has just passed the peak of inflated expectations and is heading towards the trough of disillusionment from where CNTs are just recovering. In contrast to short scale SWCNTs, graphene nanoribbons - even with bandgap - are not promising candidates for a better transistor. However, interconnects made of multi-layer graphene show promise in a wide range of applications. Through-Silicon-Vias (TSV), capacitors, metal gate, diodes, membranes, memories and sensors will be discussed. These applications are heavily based on the direct deposition methods which we have developed over the past decade.

DS 16.2 Tue 14:30 CHE 89

Fabrication and characterization of nano-crystalline graphite/graphene membranes — •Andreas Geworski, Yuri Koval, and Paul Müller — Department of Physics and Interdisciplinary Center for Molecular Materials, Universität Erlangen

The newly emerging field of carbon-based micro electro-mechanical systems (C-MEMS) tries to utilize the diverse properties of carbon and to push the performance of MEMS devices further. We have developed a method to fabricate suspended micro and nano structures made of nanocrystalline graphite/graphene. The preparation includes low-energy ion irradiation and electron beam lithography at different electron energies. Two different polymers were used as precursors for the membrane fabrication: novolac and poly(methyl methacrylate) (PMMA). Both materials demonstrate similar results except for the thickness of the membranes, which is smaller for PMMA. The thickness of the nanocrystalline suspended membranes can be varied between 2 and 100 nm by process parameters. The membranes show outstanding thermal properties and stay intact even at more than 3000^oC in vacuum. A fine adjustment of the electrical conductivity of the membranes can be performed by an additional ion irradiation [1]. A sheet conductance as high as 10^{-3} S can be achieved. The conductance of the membranes can be varied by a gate electrode [2]. An integration of electrostatic actuation and field effect transistor effect opens a pathway for novel devices. [1] Y. Koval, I. Lazareva, P. Müller, Synthetic Metals 161 (2011) 528. [2] Y. Koval, I. Lazareva, P. Müller, Phys. Stat. Solidi (B) 248 (2011) 299.

DS 16.3 Tue 14:45 CHE 89

Abnormal Thermal Transport in Two-dimensional Silicon — •Ming Hu — Institute of Mineral Engineering, Division of Materials Science and Engineering, Faculty of Georesources and Materials Engineering, RWTH Aachen University, 52064 Aachen, Germany — Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, 52062 Aachen, Germany

Silicene, the silicon equivalent of graphene, has recently attracted significant attention because it has graphene-like electronic structures including the presence of the Dirac cone at the Fermi level and because of its compatibility with mature Si-based electronics. In this presentation, first I will describe my recent atomistic simulation on thermal transport of atomically thin two-dimensional silicon (silicene). We found that silicene has extremely low thermal conductivity, which is about 20 times smaller than bulk Si and two orders of magnitude less than that of its carbon counterpart graphene. Second, I will present the effect of strain on the thermal conductivity of this novel 2-D material. We discovered that, contrary to its counterpart of graphene and despite the similarity of their honeycomb lattice structure, silicene exhibits an anomalous thermal response to tensile strain. Finally, I will demonstrate the effect of length and impurity on the thermal transport of silicene, which makes silicene very promising for thermoelectrics. Our findings provide a guide of how to modulate the thermal transport properties of two-dimensional Si with nanoengineering and may be of use in tuning their electronic and optical properties for electronic, thermoelectric, photovoltaic, and opto-electronic applications.

DS 16.4 Tue 15:00 CHE 89

Magnetoresistive Emulsion Analyzer — •Gungun Lin[1], Larysa Baraban[2,3], Luyang Han[1], Daniil Karnaushenko[1], Denys Makarov[1], Gianaurelio Cuniberti[2,3], and Oliver.G. Schmidt[1] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [3]Center for Advancing Electronics Dresden (cfaed), TU Dresden, Germany

A substantial part of nanomedicine focuses on drug design and employing magnetic nanomaterials with multifunctional polymers, lipids or proteins. High-throughput drug discovery requires a tool which is able to analyze, manipulate, and sort objects containing known doses of magnetic nanoparticles associated with medications. A promising route relies on the implementation of magnetically-labeled biochemical species combining magnetoresistive sensors. In-flow detection based on magnetoresistive sensors has been demonstrated recently, representing first steps towards the integration of magnetic sensor elements into fluidic channels. However, up to date, progress is restrained to the mere sensing and counting of magnetic objects. Advanced and quantitative analysis, which is the main advantage of e.g. optical flow cytometry, has not been explored so far with magnetic sensors. Apart from detection and analysis, sorting of species is invaluable in diagnostic devices. We report a magnetoresistive emulsion analyzer which is capable of detection, multiparametric analysis and sorting of ferrofluid droplets. The device offers important complementarity to conventional optical approaches involving ferrofluids, and paves the way to the development of novel compact tools for diagnostics and nanomedicine.

DS 16.5 Tue 15:15 CHE 89

Building Blocks of a Micro and Nano Scale Tensile Testing Platform: Design, Technology, Numerical Simulation and Optimization — •Peter Meszmer, Karla Hiller, Raul David Rodriguez, Daniel May, Alexey Shaporin, Dietrich R. T. Zahn, Jan Mehner, and Bernhard Wunderle — Technische Universität Chemnitz, Germany

The presented tensile testing system targets to characterize functional sensor subcomponents such as CNTs, smart tubes, membrane structures, nanowires and their respective interconnections under thermo-mechanical loads to enable reliability predictions. The platform consists of three parts besides the specimen: actuator, force sensor and displacement sensor, integrated into a singe chip.

The thermal actuator is designed to ensure electrical insulation against the other components of the platform, passively heated using a thin aluminum meander, thus enabling the integration of all components, providing a travel range of up to $1\mu m$.

The displacement sensor is based on capacitive sensing, providing a resolution of $4fF$ and a sensitivity of $3\frac{fF}{nm}$.

The MEMS force sensor is based on the piezoresistive effect, capable of measuring nano-Newton sized forces mapped onto a micro-Volt scale and able to measure continuously while different loads are applied to the specimen.

All components are fabricated using SOI wafers processed by a BDRIE method, provide electrical readout and drive, are optimized using numerical methods providing experimentally verified results.

DS 16.6 Tue 15:30 CHE 89

Rolled-up antenna for on-chip aplication — •Dmitriy D. Karnaushenko, Daniil Karnaushenko, Denys Makarov, and Oliver G. Schmidt — Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, Dresden, Germany.

One of the severe limitations of the conventional inter- or intra-chip communication is the emergent parasitic reactance and resistance associated with interconnects at high frequencies, which prohibits further miniaturization of the functional elements. This issue can be overcome by wireless transceivers integrated directly on a chip [1]. The latter requires development of compact antennas with tunable emitting characteristics.

To achieve this goal, we realized helical antennas using rolled-up nanotechnology allowing straightforward on-chip integration. First, we performed full scale modeling to understand the impact of geometrical parameters on the antenna performance (gain, resonance frequency, directivity). Relying on the results of the simulations, we applied thin film deposition and lithography techniques to determine various 2D sample layouts, which are then successfully rolled-up into a 3D helical antenna. Measurements of the return loss characteristics up to 20 GHz demonstrate that the rolled-up antenna reveals better performance than the initial planar structure. Experimental data agrees well with the result of the simulations.

[1] T. Kikkawa, Microelectronic Eng. 88, 767 (2011).

DS 16.7 Tue 15:45 CHE 89

Multifunctional nanomembranes as sensitive optical sensors in compact MEMS devices — •Stefan M. Harazim[1], Vladimir Bolaños[1], Christian Helke[3], Tom Enderlein[3], Thomas Otto[2], Thomas Gessner[2,3], and Oliver G. Schmidt[1,4] — [1]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Fraunhofer ENAS, Technologie-Campus 3, 09126 Chemnitz, Germany — [3]TU Chemnitz, Zentrum für Mikrotechnologien, Reichenhainer Str. 70, 09126 Chemnitz, Germany — [4]TU Chemnitz, Material Systems for Nanoelectronics, Reichenhainer Str. 70, 09107 Chemnitz, Germany

Point of care (PoC) diagnostic is a method to test biological samples directly where the patient is. This method offers, compared to the slow and large stationary laboratory, the most spatial flexibility and is very efficient if not preservable, quickly perishable samples have to be analyzed. Micro-electro-mechanical systems (MEMS), especially Lab-on-a-Chip (LoC) systems, could be utilized to include all required process steps, starting from the sample preparation up to the analysis of the recorded data. Furthermore, if it is possible to develop a sensor and actuator technology, providing a broad spectrum of biomedical applications, that enables the fabrication of low cost and fast operational one-time analysis tools, a huge leap towards PoC diagnostic is done. Herein, we present the fabrication and microfluidic integration in a LoC system of easy and fast to fabricate multifunctional nanomembranes. The refractrometric sensor capabilities, signal stability, complete devices with sensitivities of up to 880 nm/refractive index unit (RIU), reliability and other key parameters of the device will be presented.

DS 16.8 Tue 16:00 CHE 89

Predicting the performance of all-metal AFM tips — •E. Sheremet[1], R.D. Rodriguez[1], V. Kolchuzhin[2], V. Desale[1], K. Bhattacharya[1], J. Mehner[2], S. Schulze[3], M. Hietschold[3], and D.R.T. Zahn[1] — [1]Semiconductor Physics, — [2]Microsystems and Precision Engineering, — [3]Solid Surfaces Analysis Group. Technische Universität Chemnitz, D-09107 Chemnitz, Germany

Atomic force microscopy (AFM) is one of the most common tools for nanoscale characterization. The quality of the information and the spatial resolution that can be achieved in the measurements are largely determined by the AFM tip used. Many applications, such as electrical AFM and tip-enhanced Raman spectroscopy (TERS), require metallic tips, which are normally prepared by covering Si or Si_3N_4 tips with a thin metal layer. Unfortunately, the coating readily goes away upon contact with the sample [1]. We developed all-metal gold and silver AFM tips [2], which provide much more robust performance. However, unconventional materials and shape of the cantilevers and tips makes it necessary to develop a model of their dynamical properties. We statistically analyzed custom-made gold and silver tips in order to develop a parametrical model which can predict their performance in AFM. The tips are simulated by the finite element method and the validity of the model is confirmed by comparing the simulated and measured tip resonance spectra. The model is then analyzed in order to extract empirical parametric quantities predicting the tip performance.

[1] S.S. Kharintsev, et al. Nanotechnol. 18, 315502 (2007).

[2] R.D. Rodriguez, et al. Rev. Sci. Instrum. 83, 123708 (2012).

DS 17: Ion and Electron Beam Induced Processes

Time: Tuesday 14:00–16:15 Location: CHE 91

DS 17.1 Tue 14:00 CHE 91

Reverse Epitaxy — •Xin Ou, Adrian Keller, Manfred Helm, Jürgen Fassbender, and Stefan Facsko — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR) e.V., P.O. Box 510119, 01314 Dresden, Germany.

Based on a self-organized ion beam erosion process, periodic ripple, hole, or dot arrays can be produced on various semiconductor surfaces. However, the main drawback of this method is that the irradiated semiconductor surfaces are amorphized. For device fabrication, a crystalline surface of high quality is indispensable. In this work we report the recent discovery of single crystal Ge nanopattern surface formation based on a *reverse epitaxy* process at elevated temperature.[1] The vacancies created during ion beam irradiation distribute according to the crystallographic anisotropy, which results in an orientation-dependent pattern formation on single crystal Ge surface. This process shows nicely the equivalence of epitaxy with deposited adatoms and *reverse epitaxy* with ion induced surface vacancies on semiconductors, and the formation of these patterns is interpreted as the result of a surface instability due to an Ehrlich-Schwoebel barrier for ion induced surface vacancies. The simulation of the pattern formation is performed by a continuum equation accounting for the effective surface currents. [1] Xin Ou et al., Phys. Rev. Lett. 111, 016101 (2013).

DS 17.2 Tue 14:15 CHE 91

Gallium Nitride Films by Ion-Beam Assisted MBE - Effects of Long-Term Ion Irradiation — •Annemarie Finzel, Jürgen Gerlach, Frank Frost, Jan Lorbeer, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e.V. (IOM Leipzig), Permoserstraße 15, D-04318 Leipzig, Germany

One technique to grow GaN thin films of high quality and purity is ion-beam assisted molecular-beam epitaxy (IBA-MBE). Ga is evaporated in an effusion cell and adsorbs at the heated substrate (superpolished 6H-SiC(0001) at 700 °C) surface, while it is bombarded by hyperthermal N ions ($E_{kin} \leq 25$ eV) generated by a hollow-anode plasma source. The aim of the present study is to examine whether a long-term irradiation with hyperthermal N ions has an effect on an already deposited GaN film. For this purpose, heated (700 °C , 600 °C) and non-heated (RT) GaN films were irradiated up to 6 h with N ions. To test that there is no thermal GaN decomposition one film was heated for several hours at the typical deposition temperature (700 °C) without ion irradiation. The investigations using RHEED, UHV-STM and AFM have shown that a long (2 h) irradiation with hyperthermal N ions after the film deposition has an effect on the surface of the GaN films. The roughness of the irradiated samples was increased and a large amount of holes and canyons was formed which could be due to sputtering or due to a rearrangement of atoms at the GaN film surface. It could be proven that a long heating of the GaN film at 700 °C and a long irradiation at RT has no visible influence on the surface structure and topography. The effects of the ion irradiation will be discussed.

DS 17.3 Tue 14:30 CHE 91

Systematic investigations of low energy ion beam sputtering of Ge — •Rene Feder, Horst Neumann, Carsten Bundesmann, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e.V, Leipzig, Germany

The ion beam sputter deposition (IBD) technique provides intrinsic features which influence the properties of the growing films. Ion properties and geometrical process conditions generate different kinetic energy and spatial distributions of both the sputtered and the scattered particles and consequently influence the properties of the growing films.

A vacuum deposition chamber has been set up which allows ion beam sputtering of different targets under variation of geometrical parameters (incidence and emission angles) and of ion beam parameters (species, energy) to make a systematic analysis of the correlation between the properties of the ion beam, the properties of the sputtered and scattered particles, and the properties of the deposited films. Several sets of samples were prepared and characterized with respect to selected film properties, such as thickness, optical properties, composition and surface topography. The experiments indicate a systematic influence of the deposition parameters on the film properties. For a better understanding of these correlations, the energy distribution of secondary particles was measured using an ESMS. Among others, experiments revealed high-energetic maxima for backscattered primary ions, which shift with increasing emission angle to higher energies. Experimental data are compared with MC simulations.

Financial support by DFG (BU2625/1-1) is gratefully acknowledged.

DS 17.4 Tue 14:45 CHE 91

Enhanced Sputtering Effects of Ion Irradiated Silicon Nanowires — •Stefan Noack[1], Andreas Johannes[1], Henry Holland-Moritz[1], Markus Glaser[2], Alois Lugstein[2], and Carsten Ronning[1] — [1]Institiut für Festkörperphysik, Friedrich-Schiller-Universität Jena — [2]Institut für Festkörperelektronik, Technische Universität Wien

While being easy to fabricate through both physical and chemical approaches, nanostructure customization often finds its limits due to thermal equilibrium. Ion implantation has become an important tool to circumvent this restriction, especially when doping semi-conductive materials. For the prediction of the behaviour of ion beam irradiated nanostructures, different approaches in theoretical calculation and computer simulation have been implemented, such as the Monte Carlo simulation program *iradina* [1]. The description of effects like sputtering, however, which differs greatly for nanostructures compared to bulk material, still has to be verified experimentally. With focus on this matter, etched silicon nanowires with a wide array of diameters were irradiated by argon ions of different energies, meeting conditions in order to preserve crystallinity and prevent bombardment induced bending. Subsequently, SEM investigations were made to quantify the sputter yield in comparison with the results from *iradina* simulations, all to be discussed in this presentation.

[1] C. Borschel, C. Ronning; Nucl. Instrum. Meth. Phys. Res. B 269, 2133 (2011)

DS 17.5 Tue 15:00 CHE 91

Investigation of dopant profiles, losses and heating using an energy filter for ion implantation — •Florian Krippendorf[1], Constantin Csato[1], Michael Rüb[1], Carsten Ronning[2], and Johannes von Borany[3] — [1]Ernst-Abbe-Fachhochschule Jena, Carl-Zeiss-Promenade 2, 07745 Jena — [2]Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [3]Helmholtz-Zentrum Dresden-Rossendorf e.V., Bautzner Landstraße 400, 01328 Dresden

Creating doped areas with depth distributions of several μm is difficult for some materials. A combination of a monoenergetic ion implantation (narrow depth distribution) and a subsequent diffusion step is not a suitable process, if diffusion coefficients are small. To overcome this problem a so called energy filter [1] has been developed. It consists of a micro patterned silicon membrane which modifies the ion beam in such a way, that the irradiated substrate is doped in a larger depth distribution. In the talk we show our results from the work on the energy filter. We demonstrate doping of a 7x7mm^2 Si substrate with 7MeV B ions in a depth distribution of 4 μm with only one implantation. SIMS and SRP measurements show the shape of the implanted profile and loss of ions due to scattering. To support these data the energy spectra of the ion beam after passing different microstructures and the resulting implantation profiles are simulated. The properties of the filter regarding heating, channelling, degradation etc. are discussed.

[1] F. Krippendorf et al., Proceedings MikroSystemTechnik Kongress 2013, 14.-16. Oktober 2013, Aachen: VDE Verlag, 2013, 8.12, 662-665

DS 17.6 Tue 15:15 CHE 91

Novel porous liquid metal ion source for surface modification with heavy polyatomic ions — •Daniel Bock[1], Wolfgang Pilz[1], Martin Tajmar[1], and Lothar Bischoff[2] — [1]Technische Universität Dresden, 01062 Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden

The most common Liquid Metal Ion Source emitters for focused ion beam (FIB) applications are from the tungsten needle type. Wetted with different elementary or alloy materials, a broad spectrum of mono- and polyatomic ions can be extracted and applied for surface modification purposes by using ion optics containing an ExB mass filter which is not restricted to FIB but to single ended ion accelerators as well. It was recently shown, that the impact of heavy polyatomic ions leads to quite different interactions on material surfaces as it is known up to now due to the enormous local energy deposition [1].

A new Micro-Powder Injection Molding technique allows the fabrication of porous tungsten emitters in nearly any shape, which is not accessible by mechanical machining [2]. Such porous tungsten emitters combine the advantages of needle and capillary type emitters. Due to their improved wettability and material flux, such an emitter can deliver ion currents of tens of μA concentrated in one beam focused by a special ion optics design. This new type of LMIS as well as its fabrication procedure and operational conditions will be discussed using a GaBi alloy liquid metal ion source.

[1] L. Bischoff, et al., Nucl. Instr. and Meth. B 272 (2012) 198.

[2] M. Tajmar, et al., Ultramicroscopy 111(2010)1.

DS 17.7 Tue 15:30 CHE 91

Charge exchange and energy loss of slow highly charged ions in 1nm thick carbon nanomembrane — •Richard A. Wilhelm[1], Elisabeth Gruber[2], Robert Ritter[2], René Heller[1], Stefan Facsko[1], and Friedrich Aumayr[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Technische Universität Wien, Wien, Österreich

It has been demonstrated in recent years that slow highly charged ions can be used as an efficient tool for nano-structure formation on insulating solid surfaces mainly by deposition of their potential energy. By reducing the solid thickness into the nano-meter range a limit is reached where on the one hand the ion may not be completely neutralized in the solid membrane and on the other hand dissipation of the deposited energy may be limited to two spacial dimensions. To investigate the energy deposition and neutralization processes in 2D-materials by slow highly charged ions we performed charge exchange and energy loss measurements of slow highly charged Xe ions transmitted through ultra thin polymeric carbon membranes. Surprisingly, two distinct exit charge state distributions accompanied by charge exchange dependent kinetic energy losses are observed. The energy loss for ions exhibiting large charge loss shows a quadratic dependency on the incident charge state, indicating that equilibrium stopping force values do not apply in this case. The combination of charge transfer and kinetic energy loss measurements allows us to link the two different exit charge state distributions to ion trajectories through distinct local electron densities distributions in the membrane.

DS 17.8 Tue 15:45 CHE 91

Comparison of proton and electron induced electronic excitations in thin metal films — •Lars Breuer[1], Andreas Wucher[1], and Detlef Diesing[2] — [1]Fakultät für Physik, Universität Duisburg-

Essen, Duisburg, Germany — [2]Fakultät für Chemie, Universität Duisburg-Essen, Essen, Germany

The electronic excitation in thin metal films by low energy protons and electrons ($60\,\mathrm{eV} < E < 1000\,\mathrm{eV}$) is detected as a current flowing from the ion or electron irradiated metal film through a thin oxide layer to an aluminium back electrode. Thus, the thin film metal–insulator–metal device couples the electronically excited metal (silver in the present work) to a metal (aluminium in the present work) in its electronic ground state. By the application of a bias voltage to the device in the course of ion irradiation a spectroscopy of the irradiation induced electronic excitation becomes possible. The device allows a characterisation of the excited electrons and of the excited holes as well in contrast to a conventional spectrometer with a retarding field. Proton induced excitations are found to store a significant amount of the energy in excited holes. Electron induced excitations on the other hand show only a negligible fraction of energy stored in holes, the main fraction of energy consists of secondary electrons in this type of excitations.

DS 17.9 Tue 16:00 CHE 91

Formation of PbTe nano particle by low energy ion beam mixing of Te/Pb bilayer — •Srashti Gupta[1,2], Dinesh Agarwal[3], Saif Khan[3], Sonathi Neeleshwar[2], Sunil Ohja[3], Ambuj Tripathi[3], S Amirthapandian[4], Binaya Panigrahi[4], and Devesh Avasthi[3] — [1]II. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]University School of Basic and Applied Sciences, G.G.S. Indraprastha University, Delhi- 110075, India — [3]Inter University Accelerator Centre, New Delhi-110067, India — [4]Materials Physics Division, Indira Gandhi Centre for Atomic Research, Kalpakkam-603102, India

The present work reports the formation of PbTe by low energy ion beam mixing of Te/Pb bilayer. Te/Pb bilayer samples are deposited using thermal evaporation technique with thicknesses (20 nm each) where Te is the top layer. These bilayer samples are irradiated at room temperature by 90 keV Ar and 140 keV Kr ion irradiation at different fluences ranging from $3*10^{15}$ ions/cm2 to $3*10^{16}$ ions/cm^2. The samples are characterized by resonant Rutherford backscattering spectrometry (RRBS) and reveal that PbTe starts forming at initial fluence of $3*10^{15}$ ions/cm2, and at fluence of $5*10^{15}$ ions/cm2 complete mixing takes place. RRBS also indicates the desorption of oxygen during irradiation. High-resolution transmission electron microscopy (HRTEM) and X-ray diffraction (XRD) are used to confirm the PbTe phase formation. HRTEM also confirms the formation of PbTe nanocrystals of 3-5 nm by Kr ion irradiation at fluence of $7*10^{15}$ ions/cm2.

DS 18: Organic Thin Films I

Time: Wednesday 9:30–12:45 Location: CHE 91

DS 18.1 Wed 9:30 CHE 91

Structural and photophysical properties of a two dimensional J-aggregate: MePTCDI on KCl — •Christian Marquardt, Alexander Paulheim, and Moritz Sokolowski — Institute for Physical and Theoretical Chemistry, University of Bonn, Wegelerstraße 12, 53115 Bonn, Germany

The structural and photophysical properties of the organic dye molecule MePTCDI (N,N-dimethylperylene-3,4,9,10-bis(dicarboximide)) adsorbed on KCl(100) surfaces have been investigated by low energy electron diffraction (LEED), fluorescence (FL) and FL excitation spectroscopy (FLE). Similar to the model molecule PTCDA the monolayer of MePTCDI forms a commensurate c(4×4) brickwall structure on KCl. In this structure, the transition-dipole moments of the molecules are arranged in a head to tail conformation forming two-dimensional J aggregates. This results in a superradiant electronic transition in optical emission- and absorption-spectra with a pronounced 0-0-transition and a red shift with respect to the spectra of isolated molecules. We will present the results on MePTCDI and compare them to those of PTCDA on KCl [1].

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

DS 18.2 Wed 9:45 CHE 91

The frontiers of organic metal epitaxy: TTF-TCNQ thin film preparation on KCl(100) substrates — •Alexander Mänz, Tobias Breuer, and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7, 35032 Marburg

The organic charge transfer complex Tetracyanoquinodimethane-Tetrathiafulvalene (TTF-TCNQ) exhibits interesting electronic properties and can be considered as a 1D organic metal. Although the epitaxial growth of TTF-TCNQ on alkali-halides is well known, the initial stages of film growth and thermal limitations of epitaxial ordering have yet not been studied systematically. While the crystallite size generally increases with substrate temperature upon growth, this process is limited by a sudden drop in the sticking coefficient. Alternatively, films at elevated temperatures were grown on seed layers that were deposited at low temperatures.

DS 18.3 Wed 10:00 CHE 91

Lead-phthalocyanine on graphite(0001): quantitative structural analysis via low-energy electron diffraction — •Matthias Meissner[1], Roman Forker[1], Torsten Fritz[1], Yu Watanabe[2], Noriaki Kawakita[2], Takashi Yamada[2], Hiroyuki S. Kato[2], and Toshiaki Munakata[2] — [1]Institute of Solid State Physics, Friedrich-Schiller University, Max-Wien-Platz 1, Jena 07743, Germany — [2]Department of Chemistry, Graduate School of Science, Osaka University, Osaka 560-0043, Japan

Thin layers of organic molecules have attracted a wide interest since the dawn of organic electronics because the performances of those devices critically depend on interface properties. The system of lead-phthalocyanine (PbPc) on graphite has been studied intensively with scanning tunneling microscopy (STM) [1], photoemission electron microscopy PEEM [2], and two photon photoemission spectroscopy (2PPE) [3]. It was found that the electronic properties of the interface are coverage dependent [2]. Thus, for a comprehensive understanding of the results the structure of the PbPc layer is of interest. Therefore, a quantitative analysis of LEED measurements was carried out under varying conditions like temperature and coverage graphite single crystals and will be compared to STM, PEEM, and 2PPE results.

[1] R. Yamamoto et al., Phys. Chem. Chem. Phys. 14, 9601 (2012).
[2] I. Yamamoto et al., Surf. Sci. 602, 2232 (2008).
[3] I. Yamamoto et al., Phys. Rev. B 77, 115404 (2008).

DS 18.4 Wed 10:15 CHE 91

Investigation of Rubrene Thin Films on Graphite — •Christian Udhardt[1], Yu Watanabe[2], Takashi Yamada[2], Roman Forker[1], Toshiaki Munakata[2], and Torsten Fritz[1] — [1]Friedrich Schiller University, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan

The aim of our present work is to localize electronic states on organic thin film surfaces and associate them with film structures. The object of study is a graphite surface covered with rubrene ($C_{42}H_{28}$), an organic dye from the class of polycyclic aromatic hydrocarbons (PAH). Previous studies of the graphite/rubrene interface with two-photon photoemission spectroscopy (2PPES) showed an enhanced, resonant excitation of a specific, unoccupied molecular orbital, which was labeled as Ln [J. Phys. Chem. C **116**, 5821 (2012)]. It is expected that the properties of the Ln excitation are influenced by an interaction with the image potential state of the graphite surface (IPS1). In this study, photoemission electron microscopy (PEEM) was used to localize the Ln excitation on the sample surface and gather further confirmations of the Ln-IPS mixing. Photon energy as well as film thickness dependence was investigated. In addition, the crystal structure at different thicknesses was characterized with low energy electron diffraction (LEED) and the light absorption behavior of the rubrene films was elucidated with differential reflectance spectroscopy (DRS).

DS 18.5 Wed 10:30 CHE 91

Interfaces between cobalt phthalocyanine and epitaxially grown ultrathin MnO films: Evidence for charge transfer. — •Mathias Glaser[1], Heiko Peisert[1], Hilmar Adler[1], Umut Aygül[1], Milutin Ivanovic[1], Peter Nagel[2], Michael Merz[2], Stefan Schuppler[2], and Thomas Chassé[1] — [1]Universität Tübingen, Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen, Germany — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany

The electronic properties of adsorbed transition metal phthalocyanines (TMPcs) on substrate surfaces are strongly affected by interactions at the interface [1,2]. Depending on the combination of the transition metal (TM) of the TMPc and the substrate, a charge transfer from the substrate to the TM may occur as observed, e.g. for CoPc/Ag(111) [2] and CoPc/Ni(111) [3]. Besides metals, transition metal oxide thin (TMO) films are promising substrates for applications of TMPcs - also in the view of a magnetic coupling between the molecules and the substrate. However, studies of these interfaces are rare. We performed photoemission and X-ray absorption experiments on the CoPc/MnO/Ag(100) system at different thicknesses of both oxide and organic films. The results are discussed in terms of local charge transfer processes across the interface.

[1] F. Petraki et al. *J. Phys. Chem. Letters* **1** (2010), 3380.
[2] F. Petraki et al. *J. Phys. Chem. C* **114** (2010), 17638.
[3] J. Uihlein et al. *J. Chem. Phys.* **138** (2013), 081101.

DS 18.6 Wed 10:45 CHE 91

Electronic and structural properties at the interface between a perylene di-imide-based molecule and gold — •Francesca Cicciullo[1], Sabine Antonia Savu[2], Antonio Cassinese[1], Thomas Chassé[2], and Maria Benedetta Casu[2] — [1]CNR-SPIN and Department of Physics Science, University of Naples, Piazzale Tecchio 80, Naples, Italy — [2]Institute of Physical and Theoretical Chemistry, Tübingen, Germany

Nowadays perylene di-imide derivatives are considered to be among the most promising n-type organic materials for high performance organic thin film transistors (OTFTs). However, the device behavior is strongly affected by interactions at the organic/substrate interface. A full understanding of these interactions is crucial to make these materials technologically appealing. In this work, we study N,N'-bis(n- ctyl)-x:y,dicyanoperylene-3,4:9,10-bis(dicarboximide) (PDI-8CN2) thin films deposited on Au(111) single crystals by using X-ray photoemission spectroscopy (XPS), near edge X-ray absorption fine structure (NEXAFS) spectroscopy, and atomic force microscopy (AFM). We focus on the investigation of morphology, molecular orientation, and electronic structure at the organic/metal interface. Our analysis reveals that the molecular bindings are perturbed when molecules come in direct contact with the gold surface, suggesting that PDI-8CN2 strongly interacts with gold atoms. At the state of the art, there is not any detailed comprehension of the PDI-8CN2/gold interface. We believe that our results are a relevant step forward to the full application of these materials in organic electronic devices.

Coffee break (15 min)

DS 18.7 Wed 11:15 CHE 91

The phthalocyanine heterojunction MnPc/F_{16}CoPc- An initial representative of a fascinating incipient material class? — •Susi Lindner[1], Benjamin Mahns[1], Uwe Treske[1], Martin Knupfer[1], Rico Friedrich[2], Torsten Hahn[2], Jens Kortus[2], Francisc Haidu[3], Michael Fronk[3], and Dietrich R.T. Zahn[3] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Str. 23, 09696 Freiberg, Germany — [3]Physics Department/ Semiconductor Physics, Chemnitz University of Technology, Reichenhainer Str. 70, 09126 Chemnitz, Germany

Using x-ray photoelectron and x-ray absorbtion spectroscopy we demonstrate charge transfer at an interface between two transition metal phthalocyanines, MnPc and F_{16}CoPc, resulting in charged MnPc$^{\delta+}$ and F_{16}CoPc$^{\delta-}$, species. Density functional theory calculations reveal that a hybrid state is formed between the two types of phthalocyanines, which causes this charge transfer. For the hybrid state the Mn $3d_{xz}$ interacts with the Co $3d_{z^2}$ orbital leading to a two-level system.

Moreover, we have prepared mixed films out of this pair, which were characterized also by means of electron energy-loss spectroscopy. Our data reveal the formation of MnPc/F_{16}CoPc charge transfer dimers in analogy to the heterojunction. The electronic excitation spectrum of these blends is characterized by a new low energy excitation at 0.6 eV.

This project is supported by the DFG (KN 393/14).

DS 18.8 Wed 11:30 CHE 91

An electron energy-loss study of picene based charge transfer salts — •Eric Müller, Benjamin Mahns, and Martin Knupfer — IFW-Dresden, P.O.Box 270116, DE-01171 Dresden, Germany

The electronic excitations of coevaporated thin films of TCNQ/picene and F4TCNQ/picene have been investigated using electron energy-loss spectroscopy. We demonstrate that the investigated molecular pairs support charge transfer which result in new electronic excitation features at low energy. We discuss the character and localization of these low energy excitations. This work was supported by the DFG (KN393/14).

DS 18.9 Wed 11:45 CHE 91

Real-time *in situ* growth study of organic semiconductor heterostructures relevant for organic photovoltaics — •Christopher Lorch, Rupak Banerjee, Johannes Dieterle, Christian Frank, Heiko Frank, Simon Weimer, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen

The organic semiconductors (OSCs) sexithiophene (6T), diindenoperylene (DIP) and buckminsterfullerene C_{60}, when used as active layers in organic photovoltaic cells, have recently shown promising device parameters [1,2]. We have performed real-time growth studies of different combinations and heterostructures [3] of these compounds (*i.e.* material A on material B, mixtures A:B) at various substrate temperatures and deposition rates. Using *in situ* X-ray reflectivity and grazing incidence X-ray diffraction we investigated the growth and the resulting film structure of these compounds in the out-of-plane and in-plane direction, respectively. We present the results of the growth measured in real-time and the structure of the compounds under different preparation conditions as well as for different material combinations. Surprising findings lead to viable routes for tailoring the film structure which might help to improve device parameters.

[1] J. Wagner *et al.*, Adv. Funct. Mater., **20**, 4295 (2010)
[2] U. Hörmann *et al.*, Phys. Status Solidi RRL, **5**, 241 (2011)
[3] A. Hinderhofer *et al.*, ChemPhysChem **13**, 628-643 (2012)

DS 18.10 Wed 12:00 CHE 91

Vibrational properties of fluorinated rubrene in thin films — •Falk Anger[1], Reinhard Scholz[2], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — [2]Institut für Angewandte Photophysik, TU Dresden, 01069 Dresden

One possibility of tuning the electronic properties of organic molecules is the substitution of hydrogen end groups by fluorine. Vibrational spectroscopy can be used to obtain information about the conformation of the molecules as well as intermolecular coupling in thin films. Rubrene ($C_{42}H_{28}$) has been shown to be a suitable semiconductor for applications, for which numerous experimental efforts have been made. In this study, we present FT-IR and Raman spectra of thin films of partly ($C_{42}H_{14}F_{14}$) and completely ($C_{42}F_{28}$) fluorinated rubrene. We show that there is a very good agreement of the experimental vibrational spectra with state-of-the-art DFT calculations.

[1] F. Anger *et al.*, Appl. Phys. Lett. **102**, 013308 (2013)
[2] T. Breuer *et al.*, J. Phys. Chem. C **116**, 14491-14503 (2012)

DS 18.11 Wed 12:15 CHE 91

Diffraction Limited Polarized Raman Microscopy for Probing Nanoscale Structural Order — •Xiao Wang[1], Katharina Broch[2], Reinhard Scholz[3], Frank Schreiber[2], Alfred J. Meixner[1], and Dai Zhang[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 18, 72076 Tübingen — [2]Institute of Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen — [3]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Straße 1, 01069, Dresden

Radially or azimuthally polarized doughnut laser beams (RPDB or APDB) are combined with topography studies of pentacene thin films, allowing to correlate Raman spectroscopy with intermolecular interactions depending on the particular pentacene modification. Polarization dependent Raman spectra of the C-H bending vibrations are resolved layer by layer within a thin film of approximately 20 nm thickness. The variation of the Raman peak positions indicates changes in the molecular orientation and in the local environment at different heights of the pentacene film. This method reveals the local structural order and the polymorph at different locations within the same pentacene thin film, depending mainly on its thickness: The first few monolayers grow in a thin film phase, but for larger film thicknesses, the morphology evolves towards the crystal bulk phase with a larger tilting angle of the pentacene molecules against the substrate normal.

DS 18.12 Wed 12:30 CHE 91

Real-time studies of the impact of intermolecular interactions and steric compatibility on structure-property relations in organic semiconductor blends — •Katharina Broch, Alexander Gerlach, Christopher Lorch, Johannes Dieterle, Jiří Novák, and Frank Schreiber — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

An understanding of the structure-property relation in binary blends of organic semiconductors (OSCs) is relevant for device optimization as well as for fundamental research [1]. Due to possible pronounced transient effects, post growth studies are often not sufficient for a detailed characterization of these complex systems [2,3]. Using grazing incidence X-ray diffraction simultaneously with optical spectroscopy techniques we follow the growth of binary blends of the three OSCs pentacene, perfluoropentacene and diindenoperylene *in situ* in real-time. Comparing the results obtained for the different combinations, we find significant differences in the structure formation during growth of the mixed films as well as pronounced transient effects in the absorption spectra. We discuss these observations in the context of the competing effects of favourable intermolecular interaction and steric incompatibilities [4].

[1] A. Hinderhofer and F. Schreiber, ChemPhysChem 13, (2012), [2] U. Heinemeyer et al., Phys. Rev. Lett. 104, (2010), [3] R. Forker and T. Fritz, Phys. Chem. Chem. Phys. 11, (2009), [4] K. Broch et al., J. Chem. Phys. 139, (2013).

DS 19: Multiferroics II (jointly with MA, DF,KR, TT)

Time: Wednesday 9:30–13:00 Location: HSZ 04

DS 19.1 Wed 9:30 HSZ 04

An Engineered Polar Oxide Heterostructure Built from Isosymmetric Magnetically Ordered Components — •Matthew S Dyer[1], Jonathan Alaria[1], Pavel Borisov[1,5], Troy D Manning[1], Serban Lepadatu[2], Markys G Cain[2], Elena D Mishina[3], Natalia E Sherstyuk[3], N A Ilyin[3], Joke Hadermann[4], David Lederman[5], John B Claridge[1], and Matthew J Rosseinsky[1] — [1]University of Liverpool, Liverpool, UK — [2]National Physical Laboratory, Teddington, UK — [3]Moscow State Technical University, Moscow, Russia — [4]University of Antwerp, Antwerp, Belgium — [5]West Virginia University, Morgantown, USA

Theory predicts that certain layered heterostructures consisting of perovskite blocks have non-centrosymmetric structures. The breaking of spatial inversion symmetry arises through a combination of octahedral tilting and A site ordering. Following this prediction, we grow a thin-film of the $[(YFeO_3)_5(LaFeO_3)_5]_{40}$ heterostructure using RHEED monitored pulsed layer deposition. Polar domains are present in the thin-film, as demonstrated by second harmonic generation and piezoelectric force microscopy measurements. We experimentally confirm that the heterostructure is also magnetically ordered at room temperature with a finite magnetization, retaining the magnetic structure of the individual $YFeO_3$ and $LaFeO_3$ components.

DS 19.2 Wed 9:45 HSZ 04

First-principles study of the $BaTiO_3/BaFeO_3$ perovskite interface — •Igor Maznichenko[1], Sergey Ostanin[2], Arthur Ernst[2], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Epitaxial growth can combine a robust ferroelectric, such as $BaTiO_3$, and strong ferromagnets into the so called composite multiferroic films. The switching properties of artificial multiferroics sandwiched between metallic contacts make them excellent candidates for the room temperature four-state memories.

Regarding the ferromagnetic side of composite multiferroics, we suggest to use the cubic perovskite $BaFeO_3$ whose epitaxial growth has been recently reported. Here, from the basis of *ab-initio* electronic structure calculations, within the Korringa-Kohn-Rostoker method, we study the magnetic properties of bulk $BaFeO_3$. The approach allows us to accurately monitor the evolution of the Curie temperature upon both the tetragonal distortions and presence of oxygen vacancies. Finally, we examine magnetoelectricity at the $BaTiO_3/BaFeO_3$ interface.

DS 19.3 Wed 10:00 HSZ 04

Behaviour of Raman modes in $BiFeO_3$ epitaxial thin films with respect to azimuthal orientation — •Andreas Talkenberger[1], Cameliu Himcinschi[1], Ionela Vrejoiu[2,3], Florian Johann[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09596 Freiberg, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — [3]Max Planck Institute for Solide State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany

$BiFeO_3$ (BFO) is an interesting candidate for multiferroic applications. In this work we focus on the Raman spectroscopic investigation of epitaxially grown thin films of BFO by pulsed laser deposition on different substrates, belonging to the group of scandates ($DyScO_3$, $SmScO_3$, $GdScO_3$). The Raman spectra were recorded using the 442 nm emission line of a He-Cd laser. Some phonon modes show changes in the position, full width at half maximum (FWHM) and intensity depending on the azimuthal angle. We found a 90 degree periodicity of the peak position and of the FWHM for particular modes. For both parallel and crossed polarisation the four maxima in positions correspond to the minima in FWHM. Such a behaviour can be explained considering a twin family of domains with a very well defined orientation to each other. Our results are supported by piezoresponse-force microscopy and X-ray diffraction measurements as well.

DS 19.4 Wed 10:15 HSZ 04

$BiFeO_3/LaFeO_3$: a magnetoelectric multiferroic — •Zeila Zanolli[1,3], Jacek Wojdel[2], Jorge Iniguez[2], and Philippe Ghosez[3] — [1]Forschungszentrum Jülich, PGI and IAS, Jülich, Germany — [2]ICMAB-CSIC, Bellaterra, Spain — [3]Université de Liège, Physics Department, Lieǵe, Belgium

Transition-metal oxides of perovskite structure present a wide variety of physical properties. In particular, there is a strong interest in multiferroic materials that are simultaneously ferroelectric and magnetic (*magnetoelectrics*). Due to the scarcity of natural magnetoelectric multiferroics and thanks to recent advances in epitaxial growth techniques, designing new magnetoelectric multiferroic heterostructures is a promising way to succeed in this quest.

First-principles techniques are used to investigate electric control of the magnetization in the $BiFeO_3/LaFeO_3$ perovskite oxide superlattice (SL) on a (001)-$SrTiO_3$ substrate. Our results [1] show that the $BiFeO_3/LaFeO_3$ SL exhibits a trilinear coupling of a polar mode with two different rotations of the oxygen cages (*hybrid improper ferroelectricity*). Non-collinear spin calculations reveal that the ferroelectric ground state also presents weak ferromagnetism with easy axis along the [1 -1 0] direction. The microscopic mechanism allowing one to manipulate the magnetization with an electric field in such systems is presented and its dependence on strain and chemical substitution is discussed. The $BiFeO_3/LaFeO_3$ SL is found to be a good candidate to attain electric switching of magnetization at room temperature.

[1] Phys. Rev. B **88**, 060102(R) (2013)

DS 19.5 Wed 10:30 HSZ 04

The influence of strain on the optical properties of pseudotetragonal $BiFeO_3$ thin films — •Cameliu Himcinschi[1], Akash Bhatnagar[2], Andreas Talkenberger[1], Dietrich R.T. Zahn[3], Jens Kortus[1], and Marin Alexe[2,4] — [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]Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [4]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

Tetragonally distorted $BiFeO_3$ recently attracted a lot of attention because of its interesting multiferroic properties and the larger spontaneous polarization as compared to its rhombohedral counterpart.

Highly strained (when grown on $LaAlO_3$ substrates) and nearly pseudomorphic (when grown on $TbScO_3$ substrates) $BiFeO_3$ films were deposited by pulsed laser deposition. The symmetry of the tetragonally distorted $BiFeO_3$ films is discussed based on polarisation dependent Raman measurements and the comparison with Raman spectra measured for films deposited on $TbScO_3$. The evaluation of ellipsometric spectra reveals that the films deposited on $LaAlO_3$ are optically less dense and the dielectric function is blue-shifted by more than 0.3 eV as compared to the films deposited on $TbScO_3$. By analyzing the absorption edge using a bandgap model, bandgaps of 3.10 eV and 2.75 eV were determined for the films deposited on $LaAlO_3$ and $TbScO_3$, respectively. This work is supported by the German Research Foundation DFG HI 1534/1-1.

DS 19.6 Wed 10:45 HSZ 04

Electrically induced magnetic transiton at the LSMO/BTO interface — •Markus Schmitz, Alexander Weber, Paul Zakalek, Markus Waschk, and Thomas Brückel — Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich Germany

The magnetoelectric coupling is one of the most fascinating and active research areas today. The control of the magnetism due to an applied electric field may lead to new device concepts. First principles calculations of $La_{(1-x)}Sr_xMnO_3/BaTiO_3(001)$ interfaces show magnetic reconstructions due to the change of the polarization of BTO by applying an external electric field. The different electron densities influence the equilibrium between super- and double-exchange favoring a ferromagnetic or an antiferromagnetic order at the interface for the two different orientations of the polarization. Here we report on LSMO/BTO, grown with an Oxide Molecular Beam Epitaxy system. The epitaxial layer-by-layer growth was confirmed by in-situ RHEED analysis and the crystalline quality of the surface was investigated by LEED and Atomic Force Microscopy. The structural characterization was carried out by X-ray reflectometry and diffraction. We could prove the possibility to electrically polarize $BaTiO_3$ substrates due to an applied voltage of 400V by optical methods. The macroscopic magnetic properties were determined by MOKE and SQUID magnetometry. The magnetic formation at the interface with respect to the polarization of the $BaTiO_3$ was investigated by Polarized Neutron reflectometry measurements performed at MARIA (FRM II).

15 min. break

DS 19.7 Wed 11:15 HSZ 04

Growth and structure characterization of double perovskite Sr2FeMoO6 thin films — •Hakan Deniz[1], Dietrich Hesse[1], Marin Alexe[1], Robert Lowndes[2], and Lucian Pintilie[2] — [1]Max-Planck Institute of Microstructure Physics, Weinberg 2, D-06120, Halle (Saale), Germany — [2]National Institute of Materials Physics, Atomistilor 105bis, Magurele 077125, Romania

The double perovskite Sr2FeMoO6 (SFMO) has drawn considerable attention recently owing to some of its unique features such as high Curie temperature (˜410K) and half-metallic ferrimagnetic nature with a high saturation moment of 4μB. The low-field room temperature magnetoresistance observed in SFMO makes it an attractive candidate for oxide spintronics applications. However, the broad distribution of results reported so far on SFMO films suggests that an optimal structure is attainable only within a narrow window of growth conditions; and magnetic/transport properties are highly akin to Fe and Mo atomic site disorder. Pulsed laser deposition was employed to grow SFMO thin films on vicinal SrTiO3 substrates from a custom-made stoichiometric target using argon as ambient gas. X-ray diffraction data revealed that the SFMO films were grown epitaxially with respect to the substrate, including, however, a small percentage of secondary phases. The morphology of the films shows flat plains with embedded grain- or needle-like structures, which are most likely the result of spurious phases. The nature of these defects and their interfaces with the SFMO matrix are under investigation by transmission electron microscopy. This work is supported by the EU-FP7 project IFOX.

DS 19.8 Wed 11:30 HSZ 04

Magnetic Anisotropy in Multiferroic Lu_2MnCoO_6 — •Martin Lonsky[1], Merlin Pohlit[1], María Antonia Señarís Rodríguez[2], and Jens Müller[1] — [1]Physikalisches Institut, Goethe-Universität, Frankfurt (M), Germany — [2]Dpto. Química Fundamental U. Coruña, Coruña, Spain

Lu_2MnCoO_6 recently has been introduced as a new type-II multiferroic with ferroelectricity due to charge ordering and magnetostriction related to magnetic Mn^{4+} and Co^{2+} ions which are arranged alternately in the form of Ising chains along the c-axis of the crystal [1]. The magnetic properties, however, remain puzzling, which in particular is due to the lack of measurements on single crystals, that have not yet successfully been synthesized. Here, we present for the first time measurements of the magnetic anisotropy by employing micro-Hall magnetometry on a few micrograins of dimensions $\sim 1\,\mu$m only. Our results reveal a strong dependence of magnetic hysteresis on temperature and the applied field direction. This anisotropy is also reflected in the observation of a variety of unusual effects as for instance wasp-waisted hysteresis loops, sharp jumps in magnetization at about $T = 300\,$mK and an exchange bias, ocurring in each case in only one field direction. Additionally, the observation of a pronounced maximum in the coercive field at $T_{\rm SF} \sim 12\,$K indicates a significant change in the spin dynamics of the system below $T_{\rm SF}$, similar to the behavior of the related compound $Ca_3Co_{2-x}Mn_xO_6$ ($x \approx 0.95$) [2].

[1] S. Yáñez-Vilar et al., Phys. Rev. B. 84, 134427 (2011).

[2] T. Lancaster et al., Phys. Rev. B 80, 020409 (2009).

DS 19.9 Wed 11:45 HSZ 04

The multiferroic $CuCrO_2$ compound: interlayer exchange and domain population — •Matthias Frontzek — Laboratory for Neutron Scattering, Paul Scherrer Institut, 5232 Villigen-PSI, Switzerland

Multiferroic materials have become of interest for their unusual low-temperature properties in general, and the tunability of the magnetic structure through an electric field and the electric polarization through a magnetic field in particular. The most promising candidates for such controllable multiferroics have been found among the materials with inherent geometric magnetic frustration.

Among these, the delafossite $CuCrO_2$, which crystallizes in the rhombohedral $R\bar{3}m$ space group, is a multiferroic compound with an apparent strong coupling of spin and charge. In contrast to other multiferroic compounds $CuCrO_2$ shows a spontaneous electric polarization upon antiferromagnetic ordering without an accompanying structural phase transition, thus the magnetic ordering alone breaks the inversion symmetry. The peculiar magnetic structure of $CuCrO_2$ allows the direct quantitative analysis of the domain population.

In our contribution, we present a detailed study on $CuCrO_2$ single crystals using neutron diffraction in applied electric and magnetic fields. With the fields we were able to tune the multiferroic states in $CuCrO_2$ and could directly relate them to the underlying domain physics. Our results allow the re-interpretation of macroscopic measurements and show that the $p-d$ hybridization is the dominant spin-charge coupling mechanism.

DS 19.10 Wed 12:00 HSZ 04

Structure and Magnetic Coupling in $YBaFeCuO_5$ — •Andrea Scaramucci[1], Mickael Morin[2], Ekaterina Pomjakushina[2], Marek Bartkowiak[2], Denis Sheptyakov[2], Lukas Keller[2], Juan Rodriguez-Carvajal[3], Michel Kenzelmann[2], Kazimierz Conder[2], Marisa Medarde[2], and Nicola A. Spaldin[1] — [1]Materials Theory, ETH-Zurich, Zurich, Switzerland — [2]Paul Scherrer Institute, Villigen, Switzerland — [3]Institute Laue Langevin, Grenoble, France

We theoretically study the structure and exchange couplings in multiferroic $YBaFeCuO_5$ (YBFCO). Using density functional theory we calculate energies of configurations with various Fe^{3+}/Cu^{2+} orderings in the bilayered perovskite structure of YBFCO. We find that configurations with different distribution of Fe^{3+} and Cu^{2+} ions fall into two groups with distinctly different energies. The energies of those in the lowest energy group are close to that of the ground state (relative to the growth temperature) suggesting Fe^{3+} and Cu^{2+} to be disordered in YBFCO. Finally, we calculate exchange coupling constants for all the low energy configurations and show that the magnetic ordering resulting from these couplings is compatible with the experimentally-observed high-temperature magnetic ordering. However, they do not explain the existence of the experimentally observed low-temperature incommensurate magnetic structure.

DS 19.11 Wed 12:15 HSZ 04

Hybrid-functional study of the structural, magnetic and electronic properties of rare-earth nickelates — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Rare-earth nickelates ($ReNiO_3$) are very promising functional perovskite crystalline materials, exhibiting metal-insulator (MI) transition, which can be continuously controlled by composition, bi-axial strain and(or) electric field. Unfortunately, conventional *ab initio* DFT+U results fail to reproduce their magnetic ground state as well as the effect of epitaxial strain on MI transition temperature. We present results of our comprehensive study of structural, magnetic and electronic properties of bulk $ReNiO_3$ (Re=Y, Gd, Eu, Sm, Nd and Pr) and strained $SmNiO_3$ films [1], performed with HSE06 functional. We show correlation between MI transition temperature and structural parameters of bulk and films, which nicely fits known experimental data. We also analyze the difference in the electronic structure obtained in DFT+U and with the hybrid functional and their influence on the resulting magnetic ordering in the ground state.

We acknowledge the support by Helmholtz Young Investigators Group Programme VH-NG-409, JSC and JARA-HPC.

[1] F.Y. Bruno, K.Z. Rushchanskii, S. Valencia, Y. Dumont, C. Carrétéro, E. Jacquet, R. Abrudan, S. Blügel, M. Ležaić, M. Bibes, and A. Barthélémy, Phys. Rev. B 88, 195108 (2013).

DS 19.12 Wed 12:30 HSZ 04

Magnetic properties of multiferroic $TbMnO_3$ — •Natalya Fedorova, Andrea Scaramucci, Claude Ederer, and Nicola Spaldin — ETH Zurich, Materials Theory, Wolfgang-Pauli-Strasse 27, CH-8093 Zurich, Switzerland

We use ab-initio calculations to investigate the magnetic properties of multiferroic $TbMnO_3$.

At low temperatures $TbMnO_3$ demonstrates an incommensurate spiral ordering of Mn spins which is accompanied by appearance of spontaneous electric polarization driven by applied magnetic field [1]. The establishment of such spin ordering is usually described within the framework of a Heisenberg model with competing nearest-neighbor and next-nearest-neighbor exchange interactions. However, our theoretical estimations of these interactions by ab-initio calculations demonstrate a clear deviation from Heisenberg model.

We consider first the coupling between magnetic and orbital orderings as a main source of non-Heisenberg behavior in $TbMnO_3$, but conclude that it does not explain the observed deviation. We find that higher order interactions (biquadratic and four-body spin couplings) should be taken into account for proper treatment of the magnetism in $TbMnO_3$.

[1] T. Kimura et al., Nature 426, 55-58 (2003)

DS 19.13 Wed 12:45 HSZ 04

Coupling of epitaxial strain and point-defect formation in perovskites — •Ulrich Aschauer, Philipp Baumli, and Nicola A. Spaldin — Materials Theory, ETH Zurich, Zürich, Switzerland

Using density functional theory calculations we recently established the existence of a strong coupling between epitaxial strain and the formation energy of oxygen vacancies in the model perovskite $CaMnO_3$ (Phys. Rev. B. 88, 054111, 2013). Here we investigate the generality of this concept for other oxides including metallic perovskites and also investigate the effect of strain on the formation of cation vacancies. We find that in general the response of the defect profile follows the behavior expected from chemical-expansion arguments, with tensile strain favoring oxygen vacancies and compressive strain favoring cation vacancies. We show, however, that material-specific details of the electronic structure can cause deviations from this trend under both tensile and compressive strain.

DS 20: Focus Session: Emerging oxide semiconductors I (jointly with HL, DF, O)

Oxides are increasingly explored for their semiconducting properties. This session sets a focus to the physics, material and surface science of oxides that have recently been considered as active material for n-type and p-type semiconductor devices. Besides the classical use in gas sensorsand as transparent contactsfor optoelectronics devices, novel applications of semiconducting oxides in power electronics, UV sensors, photovoltaics, and solar water splitting devicesare addressed.

Organizers: Oliver Bierwagen, Paul-Drude-Institut für Festkörperelektronik, Berlin, Norber Esser, Leibniz-Institut für Analytische Wissenschaften ISAS, Berlin, Rüdiger Goldhahn, Otto von-Guericke-Universität Magdeburg, and Marius Grundmann, Universität Leipzig.

Time: Wednesday 9:30–13:00 Location: POT 081

Topical Talk DS 20.1 Wed 9:30 POT 081

Computational design of oxide semiconductors — •Stephan Lany — National Renewable Energy Lab, Golden, CO, 80401

Traditional semiconductors are the group-V, III-V, and II-VI systems as well as their isovalent and isostructural alloys. Within the field of oxide semiconductors, there is a continuing interest in n-type wide gap compounds, such as ZnO, In2O3 and related materials, but there is also growing interest in oxide semiconductors for novel applications, e.g., for oxide photovoltaics or solar water splitting. This background leads us to explore the range of possible semiconducting properties within the realm of oxide semiconductor alloys. From a computational materials design perspective, this includes modeling of the alloy structure and energetics, prediction of band-structures, optical properties, and electrical properties (doping and defects). We will discuss two recent examples of this materials design effort, i.e., the realization of tetrahedral MnO alloys, and the optimization of the photovoltaic properties of Cu2O by aliovalent alloying through ultrahigh doping.

Work in collaboration with H. Peng, V. Stevanovic, and funded by the U.S. Dept. of Energy.

DS 20.2 Wed 10:00 POT 081

Phonon 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

We present *ab initio* investigations on phonon properties of the copper-oxide phases Cu_2O, CuO, and Cu_4O_3. Phonon bandstructure and density of states for all three phases are derived from a supercell small displacement method. This method relies on displacing atom(s) within a supercell and calculating resulting forces on all other atoms. As copper-oxides exhibit polar bonding the splitting of the LO and TO modes at the Γ point must be properly taken into account. We derive these splittings from Born effective charges and the dielectric tensor which enter the non-analytical contributions to the dynamical matrix in the limit $\mathbf{q} \to 0$.

DS 20.3 Wed 10:15 POT 081

Intrinsic point defects in Cu_2O - Lifting of Raman selection rules — •Thomas Sander, Christian T. Reindl, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität Gießen

The copper oxide system Cu_2O receives currently a renewed interest due to its potential photovoltaic applications. Its natural p-type conductivity is due to intrinsic defects. Understanding the formation and properties of such point defects is of major relevance for tuning the material for optoelectronic applications.

Crystalline cubic Cu_2O exhibits a very unusual feature which is up to now unexplained in the literature. Instead of showing just one optical mode expected for cubic symmetry, Raman spectra of Cu_2O are dominated by Raman forbidden phonons independent of the method used for growth. A group theoretical analysis will be presented showing that the forbidden phonons will become Raman allowed when the symmetry is lowered due to the formation of point defects. Furthermore, it will be shown that of all possible intrinsic defects the copper split vacancies cause the lifting of the Raman selection rules. The results are experimentally confirmed by making use of the full angle and polarization dependence called rotational Raman spectroscopy (RoRa). Low temperature Raman studies further reveal that the degeneracy of phonon modes is lifted which is in accordance with the results of the group theoretical analysis.

Thus the detailed Raman study of Cu_2O in combination with the group theoretical analysis yields much more insight than just a proof of selection rules or identification of lattice modes.

DS 20.4 Wed 10:30 POT 081

Effect of Chemical Precursors On the Optical and Electrical Propertiesof p-Type Transparent Conducting Cr_2O_3:(Mg,N) — Elisabetta Arca, •Karsten Fleischer, Sergey A. Krasnikov, and Igor V. Shvets — School of Physics, Trinity College Dublin, Ireland

Cr_2O_3:(Mg,N) has been reported as a p-type transparent conducting oxide. In this contribution the effect of each precursor used for deposition by spray-pyrolysis will be explored and their role in determining the optical and electrical properties of Cr_2O_3 will be outlined. A correlation between the structural, electrical, and optical properties upon introducing nitrogen precursors has been established. In particular it has been shown that the presence of ammonium salts in the deposition environment results in less absorbing films. By combining optical measurements and NEXAFS studies, a mechanism is proposed to explain the change in the optical properties. Moreover, it is shown that the presence of the nitrate moiety in the reaction environment is necessary to improve the electrical conductivity of the deposited films. The reaction of the nitrate moiety with the ammonium moiety has been proposed as the mechanism to explain the boost in conductivity.

DS 20.5 Wed 10:45 POT 081

Tailoring the electronic and magnetic structure of doped rutile-TiO_2 using p-elements (C,N); A Hybrid DFT study. — •Jacqueline Atanelov, Christoph Gruber, and Peter Mohn — Vienna University of Technology, Center for Computational Materials Science

We study the electronic and magnetic structure of carbon and nitrogen impurities and interstitials in rutile TiO_2. To this end we perform *ab-initio* calculations of a 48-atom supercell employing the VASP code. In order to obtain a realistic description of the electronic and magnetic structure, exchange and correlation are treated with the HSE06 hybrid functional. Substitutional carbon and nitrogen are found to have a magnetic moment of 2 and $1\mu_B$, respectively, with a tendency for anti-ferromagnetic long range order. For C/N on interstitial sites we find that carbon is non-magnetic while nitrogen always possesses a magnetic moment of $1\mu_B$. We find that these interstitial positions are on a saddle point of the total energy. The stable configuration is reached when both carbon and nitrogen form a C-O and N-O dimer with a bond length close to the double bond for CO and NO. This result is in agreement with earlier experimental investigations detecting such N-O entities from XPS measurements. The frequencies of the symmetric streching mode are calculated for these dimers, which could provide a means for expermental verification. For all configurations investigated both C and N states are found inside the TiO_2 gap. These new electronic states are discussed with respect to tuning doped TiO_2 for the application in photocatalysis.

DS 20.6 Wed 11:00 POT 081

Magneto-optical characterization of thin films of magnetic oxides prepared via aqueous solution processing — •Peter Richter[1], Michael Fronk[1], Paul N. Plassmeyer[2], Catherine J. Page[2], Dietrich R.T. Zahn[1], and Georgeta Salvan[1] — [1]Semiconductor Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [2]Department of Chemistry, University of Oregon, Eugene, Oregon 97403, USA

Ferromagnetic oxides are of great interest for a wide variety of applications. In spintronics, LaMnO3 and La1-xSrxMnO3 are now among the most commonly used materials for electrodes. Other oxides like the ferrites can show multiferroic properties and can be fabricated to be transparent and are therefore useful for optical and photovoltaic applications. However, the deposition of such magnetic oxide layers usually requires sophisticated instrumentation and may be expensive. We present a new approach to effectively prepare smooth thin films of metal oxides by spin coating them from aqueous precursor solutions. The full dielectric tensor (including the Voigt constant) of the obtained layers is determined from spectroscopic ellipsometry and magneto-optical Kerr effect (MOKE) spectroscopy measurements for a spectral range of 1.7 to 5.0 eV. The magnetic properties are investigated by MOKE magnetometry. Of particular interest, the ferrites $CoFe_2O_4$ and $NiFe_2O_4$ show characteristic spectral features and a ferromagnetic hysteresis at room temperature. We observe a variation of the optical and magnetic properties depending on the temperatures at which the samples were annealed after spin coating.

Coffee break (15 min.)

Topical Talk DS 20.7 Wed 11:30 POT 081

Beta-Ga2O3: Single crystal growth and semiconductor applications — •Encarnacion G. Villora[1], Daisuke Inomata[3], Stelian Arjoca[1,2], Kazuo Aoki[3], and Kiyoshi Shimamura[1,2] — [1]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan — [2]Graduate School of Advanced Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku, Tokyo 176-0022, Japan — [3]Koha Co., Ltd., Nerima, Tokyo 176-0022, Japan

β-Ga_2O_3 is a unique transparent conductive oxide, which is attracting an increasing attention in the recent years. It possesses two major features. The first is its very wide bandgap Eg=4.8 eV, which leads to a high transparency (>260 nm) and to a Baliga's figure of merit over three times that of GaN and SiC counterparts. The second feature is the capability to grow crystals from the melt, which makes possible the mass production of large substrates at low cost.

High quality 2 inch single crystals are grown by the EFG technique, and 4 inch are already in progress. N-type carrier concentration is controlled by Si- or Sn-doping. Conductive wafers are used as transparent conductive substrates for high-brightness vertically structured LEDs based on InGaN multi-quantum wells. Schottky barrier diodes and transistors have been demonstrated.

Additionally, a new phosphor concept for high-brightness white LEDs and LDs is presented. In contrast to currently used powder phosphors embedded in resins, single-crystal phosphors exhibit outstanding internal quantum efficiencies and do not degrade either under light irradiation or the increase of temperature.

DS 20.8 Wed 12:00 POT 081

MOCVD grown homo and heteroepitaxial β-Ga_2O_3 layer studied by transmission electron microscopy — •Robert Schewski, Martin Albrecht, Günter Wagner, Michele Baldini, Zbigniew Galazka, and Reinhard Uecker — Leibniz-Institut für Kristallzüchtung, Max-Born-Strasse 2, 12489 Berlin, Germany

We report on the structural properties of β-Ga_2O_3 layers, grown by MOCVD for various growth conditions. In detail, the influence of different precursors, namely pure oxygen, water, and CO_2 on the crystalline film quality has been investigated. Our studies were carried out for hetero- as well as homoepitaxially grown samples on (0001) sapphire and melt grown (100) β-Ga_2O_3 substrates, respectively. The conclusions are mainly based on transmission electron microscopy and x-ray data.

As main results, we found that pure oxygen in the growth ambient leads to the formation of nano-crystals in form of wires or agglomerates for both hetero- and homoepitaxial growth. However, by using water as oxygen precursor, smooth (rms: 6.5 nm) single crystalline layers can be achieved for homoepitaxial growth. Still, the structural quality of these thin films suffers from a substantial amount of stacking faults, which can be evidenced by TEM and x-ray data. However, annealing in oxidizing atmosphere at (900°C) leads to a reduction these stacking faults and thus improves the crystalline quality of the film. Another interesting observation is the formation of a pseudomorphic, 3 monolayers thick Ga_2O_3 layer in the alpha phase, directly at the interface between the sapphire substrate and the film.

Topical Talk DS 20.9 Wed 12:15 POT 081

Combinatorial approach to group-III sesquioxides — •Holger von Wenckstern — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Halbleiterphysik

Semiconducting group-III sesquioxides find potential application as chemical/biological sensors, deep-UV photo-detectors, and within transparent and high-power electronics. Technology for bulk growth of binary Me_2O_3 (Me=Al, Ga, In) exists and first promising devices on homoepitaxial layers have been demonstrated. For the exploration of ternary or quarternary systems thin film technology is required. In this contribution we introduce a facile approach to create lateral continuous composition spread(s) (CCS) within thin films on 2 inch wafers by pulsed-laser deposition (PLD) [1]. We ablate from a single, segmented, rotating target keeping the growth rate is for this approach as high as for conventional PLD. We will illustrate the potential of our CCS-technique and discuss structural, optical and electronic properties of $(In,Ga,Al)_2O_3$ thin films and their utilization in device demonstrations like rectifiers or photo-detectors.

[1] H. von Wenckstern *et al.*, CrystEngComm **15**, 10020 (2013)

DS 20.10 Wed 12:45 POT 081

Schottky contacts on β-Ga_2O_3 and In_2O_3 thin films — •Daniel Splith[1], Stefan Müller[1], Holger von Wenckstern[1], Oliver Bierwagen[2,3], James S. Speck[3], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany — [2]Paul Drude Institut, Berlin, Germany — [3]Materials Department, University of California, Santa Barbara, USA

Oxide semiconductors like β-Ga_2O_3 or In_2O_3 are promising materials for a new generation of transparent electronic devices. Oxide field-effect transistors but also the electrical characterization of these oxides by capacitance-voltage measurements or deep-level transient spectroscopy rely on Schottky contacts (SCs). For our study we fabricated SCs on β-Ga_2O_3 and In_2O_3 thin films and investigated their electrical properties. The β-Ga_2O_3 thin films were grown by pulsed laser deposition on highly conducting (00.1) oriented ZnO:Ga acting as a back contact layer. The In_2O_3 thin films were grown by molecular beam epitaxy on yttria-stabilized zirconia substrates. We prepared SCs by dc sputtering of different metals. On β-Ga_2O_3 the I-V characteristics of Cu SCs exhibit high rectification ratios up to 7 orders of magnitude. Temperature dependent measurements between 110 and 320 K yield a mean barrier height of 1.32 eV, which is in accordance to the effective barrier height at a temperature of 550 K, where the ideality factor decreases to 1.03. Due to surface electron accumulation, the realization of SCs on In_2O_3 is challenging. In a proof of principle experiment we fabricated SCs on In_2O_3 by reactive sputtering of Au, Pt and Pd with rectification ratios up to 3 orders of magnitude.

DS 21: Organic Electronics and Photovoltaics IV (joint session with CPP, HL, O)

Polymers, Solar Cells, OFETs, OLEDs, Spectroscopy

Time: Wednesday 9:30–12:45 Location: ZEU 260

DS 21.1 Wed 9:30 ZEU 260

Structural Degradation of Polymer Solar Cells — •Christoph J. Schaffer[1], Claudia M. Palumbiny[1], Martin A. Niedermeier[1], Christian Jendrzejewski[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

A major challenge in organic photovoltaics (OPV) is to elongate their lifetimes. Several mechanisms of organic solar cell degradation have been proposed in literature within the last years. However, insufficient research has been done on determining the role of transitions in the nanomorphology of the active layer of bulk-heterojunction (BHJ) polymer solar cells as an aspect of degradation. These transitions would strongly affect the properties of solar cells since the active layer morphology plays a crucial role in the energy conversion process.

We present a direct evidence of morphological degradation on a nanometer scale in polymeric solar cells by simultaneous in-situ GISAXS and current-voltage tracking on a running P3HT:PCBM solar cell. The loss of short-circuit current with time is fully modeled by the observed morphological transitions [1].

[1] C. J. Schaffer et al., *Adv. Mater.* **2013**, DOI: 10.1002/adma.201302854

DS 21.2 Wed 9:45 ZEU 260

Controlling nanomorphology in bulk heterojunction solar cells via addition of third component — •Eva M. Herzig[1], Ammara R. Akhtar[2], Anna Naumann[2], Shuai Guo[2], Gregory Tainter[2], Jianqi Zhan[2], Jan Perlich[3], Stephan V. Roth[3], Christine M. Papadakis[2], and Peter Müller-Buschbaum[2] — [1]TU München, MSE, Lichtenbergstr. 4, 85748 Garching — [2]TU München, Physik-Department,, James-Franck-Str. 1, 85748 Garching — [3]DESY, Notkestr. 85, 22603 Hamburg

Nanomorphology and effciency of organic solar cells are closely linked. It is therefore desirable to have control over the self-assembly process responsible for the morpholgy formation of the active material. Employing grazing incidence small and wide angle x-ray scattering(GISAXS & GIWAXS) as well as spectroscopy and microscopy methods allows us to characterize organic thin films on the nanoscale with high statistical relevance. Using these methods we thoroughly investigate the morphological changes upon the addition of a third polymeric component showing that the self-assembly process is altered. We find that the amount of the third component controls the phase separation in the bulk heterojunction active layer. Adjusting the preparation route to support crystallization of the active material leads to an increased solar cell performance for a tuned ternary solar cell system.

DS 21.3 Wed 10:00 ZEU 260

Layer by layer solution processing of nanostructured all-polymer solar cells — •Thomas Pfadler, Mihael Coric, Jonas Weickert, Karl-Philipp Strunk, and Lukas Schmidt-Mende — University of Konstanz

Organic solar cells have the potential to become an important low-cost alternative to conventional solar cells. However, before this can happen, the energy harvesting potential of organic solar cells must become more comparable with that of the pervading technology. This research is focusing on nanoimprint lithography (NIL), a low-cost lithographic method for high-throughput patterning applicable to organic semiconductors. This technique can be used to tailor an organic solar cells active material on a nanometer scale. A promising application of NIL aims to control the nanostructure of a donor-acceptor interface in an organic all-polymer device. The electron accepting polymer is structured. A stiff polymer network featuring a nanostructured topography is developed by the usage of a photoactivable crosslinker molecule (sFPA). The crosslinked polymer matrix is not dissolved during spincoating the donor polymer allowing fully solution processed device fabrication with controlled nanostructured donor-acceptor interfaces. Target of this approach is to investigate nanostructured bi-layer devices with controlled interfaces to finally enhance the overall efficiency by maximizing the interfacial area, increasing the exciton separation yield and ensuring direct pathways to the electrodes.

DS 21.4 Wed 10:15 ZEU 260

The role of processing additives in Organic Solar Cells after the preparation process — •Stefan Väth[1], Andreas Baumann[1], Andreas Sperlich[1], Carsten Deibel[1], Milutin Ivanovic[2], Heiko Peisert[2], Thomas Chassé[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Eberhard Karls University Tübingen, 72076 Tübingen — [3]ZAE Bayern, 97074 Würzburg

Processing additives are widely used in the preparation of new high performance bulk heterojunction organic solar cells to improve the power conversion efficiency (PCE) significantly. They act as selective solvent for fullerenes and are therefore improving the morphology of the active area. Nevertheless the question wether or not these co-solvents remain in the organic solar cells after the preparation process occurs. This question could be solved by investigating blends consisting of the material system PTB7:$PC_{60}BM$ processed with the additives diiodooctane (DIO), octanedithiol (ODT) and without additives as reference. We used the spin sensitive measurement technique light induced Electron Paramagnetic Resonance (LESR) to distinguish between positive polarons on the polymer and negative charges on the fullerene by their different g-factors. Together with Photoelectron Spectroscopy (PES) measurements we could show that the additive DIO remains partly inside the active layer of organic solar cells even after a high vacuum preparation step. We propose that they do not only lead to an improved morphology, but also to a doping effect.

DS 21.5 Wed 10:30 ZEU 260

Radiative and non-radiative recombination in organic solar cells — •Kristofer Tvingstedt, Philip Pelchmann, Vladimir Dyakonov, and Carsten Deibel — Experimental Physics VI Julius Maximilian University of Würzburg 97074 Würzburg

Although several organic solar cells has reached close to unity internal quantum efficiency at short circuit conditions, the open circuit voltage is still very far from its potential upper limit due to substantial charge recombination of various types, which remains to be accurately determined. In this work we evaluate the limiting mechanisms in OPVs by employing complementary steady state measurements of recombination as a function of charge carrier density by thoroughly evaluating the diode ideality factor. The diode ideality is directly related to the order of recombination and we first assess it via light intensity dependent open circuit voltage characterization under the influence of a varying temperature. We focus our study on the ratio between radiative and non-radiative recombination via the interfacial charge transfer state as determined by absolute CT electroluminescence efficiency measurements, also as a function of temperature. The charge transfer state governs the radiative recombination in OPV bulk heterojunctions and is therefore crucial to evaluate in this context. Improving the radiative efficiency of OPVs will substantially increase the open circuit voltage and eventually put these promising photovoltaic converters in efficiency parity with their inorganic counterparts.

DS 21.6 Wed 10:45 ZEU 260

Electronic Structure of Fullerene Heterodimer in Bulk-Heterojunction Blends — •Andreas Sperlich[1], Oleg G. Poluektov[2], Jens Niklas[2], Kristy L. Mardis[3], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg and ZAE Bayern, 97074 Würzburg — [2]Chemical Sciences and Engineering Division, ANL, Argonne, Illinois 60439, USA — [3]Department of Chemistry and Physics, Chicago State University, Chicago, Illinois 60628, USA

To increase performance of organic solar cells, the optimization of the electron-accepting fullerenes has received less attention. Here, we report an electronic structure study of a novel covalently linked C_{60}-C_{70}-heterodimer in blend with the polymer PCDTBT. Upon optical excitation of polymer:heterodimer solid films, the electron is shared between both C_{60} and C_{70} cages. In contrast, in the solution the electron is localized on one half of the dimer. Electronic structure calculations reveal that for the heterodimer two nearly iso-energetic minima exist, essentially the cis and trans conformers. These conformers have different edge-to-edge distance between the two cages and therefor the electron is either shared between two dimer halves (cis) or localized on one half of the heterodimer (trans). By comparison with the experimental data, we conclude that the cis conformation is preferable in films, and the trans conformation in solution. These findings demonstrate how electronic coupling of the fullerene acceptor molecules is influenced by their packing in blends, which may have an impact on the charge carrier generation efficiency in solar cells.

15 min. break

DS 21.7 Wed 11:15 ZEU 260

Cyclic potential growth mechanism for electropolymerized polythiophenes as anode buffer layers in P3HT-PCBM solar cells — •Sidhant Bom, Marlis Ortel, and Veit Wagner — Research Center for Functional Materials and Nanomolecular Science, Jacobs University, Bremen, Germany

A new method for electro-polymerization of polythiophenes as anode buffer layer (ABL) is presented. The ABL is used in a bulk-heterojunction solar cell with P3HT-PCBM as active material. Electro-polymerized thiophenes (ePT) are grown electrochemically with a standard three electrodes system on conductive contacts. We find a distinct impact of the time variation of the growth potential on the obtained layer properties. A new time dependent cyclic potential electro-polymerization method is systematically compared to a standard constant potential method. AFM topography reveals that a uniform homogeneous film of ePT is obtained by the time dependent cyclic potential growth method. The devices were fabricated with a 10 nm ePT between the active layer and PEDOT:PSS with aluminum as cathode. With a cyclic potential method, about 20% enhancement in short circuit current was observed in contrast to 10% enhancement with constant potential method. Improvements by the ePT layer are attributed to better band alignment of the HOMO levels and a LUMO offset of 0.2eV which gives its electron blocking characteristics. In summary, the cyclic potential method results in a better quality of ePT layers with good homogeneity and area coverage leading to further improvements in device performance.

DS 21.8 Wed 11:30 ZEU 260

Intrinsic charge carrier mobility in PCDTBT:PC$_{71}$BM blend thin films investigated by simultaneous transient absorption and transient microwave conductivity measurements — •Andreas Fritze[1], Jeremias Weinrich[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

PCDTBT is a promising low-bandgap polymer for photovoltaic applications that has demonstrated unique recombination dynamics compared to the model P3HT system. Usually, the recombination dynamics in organics blends is expected to be proportional to the macroscopic charge carrier mobility, which is influenced by trapping and therefore potentially depends on the charge carrier concentration. For PCDTBT blends, we want to determine if the recombination dynamics are indeed governed exclusively by the low macroscopic mobility or if it is dominated by the, high local mobility. Therefor, we performed simultaneous measurements of transient absorption (TAS) and transient microwave conductivity on PCDTBT:PC$_{71}$BM thin films on a 10 ns to 1 ms time scale. TAS probes the charge carrier density, whereas the microwave experiment is sensitive to the intrinsic, high frequency conductivity. By investigating the charge carrier dynamics and conductivity at different laser pump intensities and temperatures, we can separate the effects of mobility relaxation from carrier concentration dependent mobility in order to understand the dominant loss mechanism in organic solar cells.

DS 21.9 Wed 11:45 ZEU 260

On the role of the effectiv mass, ground state complexes and interfacial dipoles on exciton dissocitation in organic donor-acceptor systems — •Anna Köhler — University of Bayreuth, Bayreuth, Germany

Efficient exciton dissociation at a donor-acceptor interface is a necessary condition for obtaining high efficiency polymeric solar cells. Despite its importance, this step is still not fully understood. A central question is how and why, after photoexcitation of the donor and transfer of an electron onto the acceptor, the the e-h pair can overcome their considerable mutual Coulomb potential. Possibilities that are currently discussed include the degree of delocalization of both an exciton and a charge in a conjugated polymer, ground state charge transfer complexes as well as interfacial dipoles that may exist at the donor-acceptor interface in the ground state, and the degree of energetic and structural order/disorder. In this talk I will show how we combine insight gained from ultrafast pump-probe spectroscopy, field dependent photocurrent measurements, photoemission measurements and modeling to assess which factors control the dissociation process.

DS 21.10 Wed 12:00 ZEU 260

Non-photochemical self-quenching mechanism in conjugated polymers revealed by control of chain length and morphology — •Florian Steiner, Jan Vogelsang, and John M. Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D- 93040 Regensburg

Unraveling the complex photophysics of multichromophoric systems like conjugated polymers (CPs) is an ongoing interdisciplinary task. Some of the pressing questions in CP photophysics are: (i) what unit absorbs and emits the light in a CP? (ii) What processes take place between the absorption and emission event? And (iii) what is the interplay between excitation energy transfer between chromophores and non-radiative fluorescence decay? Answering these questions will lead to a fundamental understanding of the photophysics of CPs, which in turn can highlight important loss mechanisms regarding the efficiency in CP-based devices, such as self-quenching.

We illustrate that control of size and morphology in combination with several single-molecule techniques leads to a universal picture of the self-quenching mechanism in CPs by addressing these questions. As a model system we chose the device-relevant prototypical CP poly(3-hexylthiophene). Morphological control, combined with well-defined sub-populations of different sizes, enabled us to correlate a diverse set of photophysical observables (brightness, emission polarization, emission spectra, photon antibunching) with each other and the size. Finally, the increasing fluorescence self-quenching with size and morphological order is rationalized with a comprehensive photophysical model.

DS 21.11 Wed 12:15 ZEU 260

Conformations and electronic structure of Oligo-PPEs Investigated by Pulsed Electron Paramagnetic Resonance Spectroscopy — Patrick Korf, Friederike Schütze, Christian

Hintze, Stefan Mecking, and •Malte Drescher — Department of Chemistry, University of Konstanz, Germany

Poly(para-phenyleneethynylene)s (PPE) are versatile polymers that are synthetically easily accessible.

Owing to their application in organic electronics and cell microscopy their microscopic and electronic properties are of high interest.

Herein we report the investigation of the electronic structure including the photo-excited triplet state of rod-like Oligo-PPEs. The lifetime, relaxation rates and populations of the triplet sublevels are quantitatively analyzed at cryogenic temperatures in a glassy toluene matrix via time-resolved EPR with synchronized UV laser flash excitation. The photo-physical properties are studied depending on the size of the delocalized π-electron system by varying the number of repeat units in the Oligo-PPEs.

In addition, their microscopic material properties are studied in particles with confined size constituted by block coplymers of PEGylated Oligo-PPEs. The molecular conformation is investigated by EPR distance measurements in solution, in bulk material as well as in particles. The data suggest that the rod-like Oligo-PPEs are present in a collapsed state in the particles.

DS 21.12 Wed 12:30 ZEU 260

Structural and electrical characterization of Hex-5T-Hex oligothiophene thin films during film formation — •Eduard Mikayelyan[1], Linda Grodd[1], Ullrich Pietsch[1], Artem. V. Bakirov[2], Maxim. A. Shcherbina[2], Sergei N. Chvalun[2], and Souren Grigorian[1] — [1]University of Siegen — [2]Enikolopov Institute of Synthetic Polymeric Materials of Russian Academy of Sciences

Organic semiconductors are attractive for electronics due to the low cost processing methods and their high electrical conductivity. Thiophene based polymers and oligomers are demonstrating relatively high mobility, excellent luminescence properties which used for application in solar cells, radio-frequency identification, etc. [1, 2]. We have investigated the thiophene based oligomer Hex-5T-Hex. Structural characterization has been performed by grazing incidence x-ray diffraction (GIXD)method, in particular we probed the crystallite orientations in prefabricated thin films. The 3D structure of Hex-5T-Hex oligomer evaluated from the in-plane (010), (020) and (021) reflections is consistent with 2D structure suggested from 5T based oligomer self-assembled monolayer (SAM) [3]. Additionally, we found the (100) and (100)' reflections in out-of-plane direction characterizing two different stacking along thiophene backbone axis. In order to correlate the structural properties of oligothiophene thin films with the electrical characteristics both properties were probed simultaneous during film formation. This work was supported by BMBF, project number 05K10PSC.

DS 22: Focus Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale IV (jointly with O)

Time: Wednesday 10:30–13:15 Location: TRE Ma

Topical Talk DS 22.1 Wed 10:30 TRE Ma

From Rydberg Crystals to Bound Magnons - Probing the Non-Equilibrium Dynamics of Ultracold Atoms in Optical Lattices — •Immanuel Bloch — Max-Planck Institut für Quantenoptik, Garching, Germany — Ludwig-Maximilians-Universität, Munich, Germany

Ultracold atoms in optical lattice form an ideal testbed to probe the non-equilibrium dynamics of quantum many-body systems. In particular recent high-resolution imaging and control techniques allow to probe dynamically evolving non-local correlations in an unprecedented way. As an example, I will focus in my talk on the dynamical excitation of spatially ordered Rydberg structures that are formed through laser exctiation from ground state Mott insulating atoms. In addition, I will show how single-spin and spin-pair impuritites can be used to directly reveal polaron dynamics in a strongy interacting superfluid or the bound state of two magnons in a Heisenberg ferromagnet - a problem discussed first theoretically more than 80 years ago by H.A. Bethe. New atom interferometric schemes to directly probe the Green's function of a many-body system through the impurity dynamics will be discussed.

DS 22.2 Wed 11:00 TRE Ma

Correlated Light-Matter Interactions in Cavity QED — •Johannes Flick[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

In the electronic structure community, the quantized nature of the electrons is usually (approximately) incorporated, whereas the electromagnetic field is mostly treated classically. In contrast, in quantum optics, matter is typically simplified to models with a few levels, while the quantized nature of light is fully explored. In this work, we aim at treating both, matter and light, on an equal quantized footing.

We present exact solutions for fully quantized prototype systems consisting of atoms or molecules placed in optical one- or two-dimensional high-Q cavities and coupled to the quantized electromagnetic modes in the dipole or quadrupole coupling regime. We focus on spontaneous emission, strong-coupling phenomena, dipole-dipole couplings including van-der-Waals interactions, and Förster resonance energy transfer (FRET), all beyond the rotating-wave approximation.

This work has implications for a future development of a time-dependent density functional theory formulation of QED [1,2] for correlated multi-photon configurations.

[1] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011).

[2] I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).

DS 22.3 Wed 11:15 TRE Ma

Optimized effective potential approach to time-dependent density functional theory for many-electron systems interacting with cavity photons — •Camilla Pellegrini[1], Johannes Flick[2], Heiko Appel[2], Ilya V. Tokatly[1,3], and Angel Rubio[1,2] — [1]Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, E-20018 San Sebastían, Spain — [2]Fritz-Haber Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany — [3]IKERBASQUE, Bilbao, Spain

In a recent paper [1] time dependent density functional theory has been generalized to many-electron systems strongly coupled to quantum electromagnetic modes of a microcavity. Here we construct an approximation for the corresponding exchange-correlation (xc) potential by extending the optimized effective potential (OEP) method to the electron-photon system. The derivation of the OEP equation employing the non-equilibrium Green's function formalism, and the first order approximation for the electronic self-energy is presented. Beyond the mean field level, the electron-photon coupling generates a time non-local photon-mediated interaction between the electrons, whose propagator enters the exchange-like diagram. We further show the approximated xc-potential for a model two-level diatomic molecule with one electron coupled to photon modes. The comparison between the obtained results and the exact numerical ones in the different coupling regimes (from weak up to ultra-strong) is discussed. [1] I.V. Tokatly, Phys. Rev. Lett. 110, 233001(2013)

DS 22.4 Wed 11:30 TRE Ma

Correlated photon-electron wavefunctions in cavity Quantum Electrodynamics — •Heiko Appel[1], Johannes Flick[1], Rene Jestaedt[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Experimental progress in recent years has enabled the fabrication of Fabry-Perot resonators with high optical quality factors (high-Q). Such cavities allow to study the interaction of matter with a quantized light field at the single-photon level (Nobel prize 2012). In this talk we present the real-time evolution of correlated photon-electron wavefunctions in optical one- and two-dimensional high-Q cavities. We discuss implications for a multi-component density functional theory for Quantum Electrodynamics [1,2] based on the time-dependent electron density and the photon energy density.

[1] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011).
[2] I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).

DS 22.5 Wed 11:45 TRE Ma

Photoelectron driven plasmaron excitations in (2x2)K/Graphite — •Bo Hellsing — Department of Physics, Gothenburg University, Sweden

A new type of plasmarons formed by the compound of photoelec- trons and acoustic surface plasmon (ASP) excitations is investigated in the system p(2 * 2)-K/Graphite. The physics behind these types of plasmarons, e-plasmarons, is different from the ones re- cently found in graphene and quantum well systems, where the loss features results from the photohole-plasmon interaction in the material, h-plasmarons. Based on the first principles scheme, Time dependent density functional (TDDFT), we calculated the linear response due to the presence of the escaping photo-electron and determine the ASP dispersion. The coupling between the photoelectron and the ASP gives rise to excitation of the e- plasmarons manifested by a broad dispersive feature shifted about 0.5 eV below parabolic K induced quantum well band (QWB) in agreement with the ARPES experiment by Agdal et al. The e-plasmarons should be considered as a source of the loss satellite structure in ARPES for 2D systems. In addition they are important to take into account in theoretical studies of different compounds as they reflect an additional channel for excitations of plasmons. This could then increase the photon-plasmon conversion yield which obviously is of interest in the field of plasmonics.

DS 22.6 Wed 12:00 TRE Ma

Charge-transfer excitations in organic systems from many-body perturbation theory — •Xavier Blase[1], Carina Faber[1,2], Paul Boulanger[1], Claudio Attaccalite[1], and Ivan Duchemin[2] — [1]Institut Néel, CNRS and UJF, Grenoble, France — [2]L_SIM/INAC, CEA, Grenoble, France

Charge-transfer excitations in organic systems lies at the heart of a large variety of physical phenomena, from photosynthesis to photovoltaics, photocatalysis or DNA denaturation. From a theoretical point of view, such nonlocal excitations are well known to lead to difficulties within the TDDFT framework, leading to the development of range-separated hybrids. We present here the merits of the Bethe-Salpeter formalism and demonstrate its ability to reproduce *cold* and *hot* Frenkel or charge-transfer excitations with remarkable accuracy [1-3]. Our calculations are based on a recent Gaussian basis implementation of the GW and Bethe-Salpeter formalism, the Fiesta initiative [1-4], allowing all-electron or pseudopotential excited states calculations for systems comprising several hundred atoms. Recent developments towards discrete and continuous embedding techniques within the many-body perturbation framework will be presented.

References: [1] C. Faber, I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. B, 86, 155315 (2012). [2] I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. 109, 167801 (2012). [3] I. Duchemin and X. Blase, Phys. Rev. B 87, 245412 (2013). [4] X. Blase, C. Attaccalite, V. Olevano, Phys. Rev. B 83, 115103 (2011).

DS 22.7 Wed 12:15 TRE Ma

Charge transfer from first principles: self-consistent *GW* applied to donor-acceptor systems — •Fabio Caruso[1,2], Viktor Atalla[1], Angel Rubio[1,3], Matthias Scheffler[1], and Patrick Rinke[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]University of Oxford, UK — [3]Universidad del País Vasco, San Sebastián, Spain

Charge transfer in donor-acceptor systems (DAS) is determined by the relative alignment between the frontier orbitals of the donor and the acceptor. Semi-local approximations to density functional theory (DFT) may give a qualitatively wrong level alignment in DAS, if the ionisation potential of one molecule erroneously ends up above the electron affinity of the other. An unphysical fractional electron transfer will then result in weakly interacting DAS [1]. *GW* calculations based on first-order perturbation theory (G_0W_0) correct the level alignment. However, the ground state is unaffected by the G_0W_0 approach, and the charge-transfer properties remain on the level of the initial DFT calculation [1]. We demonstrate that self-consistent *GW* (sc*GW*) – based on the iterative solution of the Dyson's equation – provides an ideal framework for the description of charge transfer in DAS. The sc*GW* level alignment is in agreement with experimental reference data. In addition ground- and excited-state properties are described at the same level of theory. As a result, the electron density in DAS is consistent with the level alignment between donor and acceptor, leading to a qualitatively correct description of charge-transfer properties.

[1] V. Atalla, M. Yoon, F. Caruso, P. Rinke, and M. Scheffler, Phys. Rev. B **88**, 165122 (2013).

DS 22.8 Wed 12:30 TRE Ma

What Koopmans' compliant orbital-density dependent functionals can do for you: a comprehensive benchmark of the G2-set — •Giovanni Borghi[1], Ngoc Linh Nguyen[1], Andrea Ferretti[2], Ismaila Dabo[3], and Nicola Marzari[1] — [1]École Polytechnique Fédérale de Lausanne, Lausanne (VD), CH — [2]Centro S3, CNR–NANO, Modena, IT — [3]Department of Materials Science and Engineering, Penn State University, University Park (PA), USA

In this talk we present the results of benchmark calculations of the structure and electronic-structure of all molecules in the g2 set, using different flavours for Koopmans' compliant (KC) functionals. Results are compared not only to LDA and PBE, but also to orbital-density dependent calculations with the Perdew-Zunger self-interaction correction.

Our results assess the accuracy of Koopmans' compliant functionals in improving semilocal functionals to predict electronic eigenvalues and in particular ionization energies, with an accuracy that for molecules seems to be comparable or superior to that of many-body (GW) approaches. We also highlight how the Koopmans' condition tends to preserve the potential energy surface of the underlying functional, with higher reliability than e.g. PBE in structural predictions, while also providing good estimates of atomization energies.

The talk will also provide a general introduction to the theory of Koopmans' compliant functionals and their implementation in existing electronic structure codes.
Ref. Dabo *et al.*, PRB 82, 115121 (2010), and Psik highlight (2012).

DS 22.9 Wed 12:45 TRE Ma

The electronic structure of quinacridone: Optimally tuned range-separated hybrid functional versus GW results — Daniel Lüftner[1], Sivan Refaely-Abramson[2], Michael Pachler[1], Michael G. Ramsey[1], Leeor Kronik[2], and •Peter Puschnig[1] — [1]Institut für Physik, Karl-Franzens-Universität Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, Israel

Quinacridone is an organic molecule (C20H12N2O2) utilized in the formation of organic pigments. It has also been discussed for usage in organic electronics particularly due to its stability under ambient conditions and its tendency to form self-assembled supramolecular networks. Here, we report on its electronic structure, both, for the isolated molecule as well as for the alpha- and beta- bulk molecular crystal polymorphs. We employ an optimally tuned range-separated hybrid functional (OT-RSH) within density functional theory as well as GW corrections within a many-body perturbation theory framework. A comparison of the theoretical results obtained with the different levels of theory and a subsequent comparison with experimental data from angle-resolved photoemission spectroscopy emphasize the need for going beyond simple semi-local DFT-functionals in order to obtain the correct orbital ordering. Furthermore the comparison indicates that the results obtained with OT-RSH greatly improve those of standard DFT functionals and achieve an agreement with experiment at the level of GW calculations, thus making the OT-RSH an alternative to the computationally more expensive GW approach.

DS 22.10 Wed 13:00 TRE Ma

GW many-body perturbation theory for electron-phonon coupling calculations — •Carina Faber[1,2], Paul Boulanger[1], Ivan Duchemin[1,2], and Xavier Blase[1] — [1]Institut Néel, CNRS, Grenoble, France — [2]INAC, CEA, Grenoble, France

We study within many-body perturbation theory the electron-phonon coupling in organic systems, taking as paradigmatic examples the fullerene molecule and the pentacene crystal [1,2]. We show that the strength of the electron-phonon coupling potential is dramatically underestimated at the LDA level, while GW calculations offer an excellent agreement with experiments [1]. Further, combining GW calculations of the electronic band structure and of the electron-phonon coupling in crystalline pentacene, we show that the hole bands dispersion can be reconciled with photoemission experiments, by solving non-perturbatively (DMFT) the effect of electron-phonon coupling on the electronic self-energy [2]. We finally explore various approximations that may allow to combine the GW formalism with convenient linear response formalisms beyond the frozen-phonon techniques. Our calculations are performed with the Fiesta package, a Gaussian based GW and Bethe-Salpeter code allowing all-electron or pseudopotential calculations with various resolution of the identity techniques and without any plasmon pole approximation [3,4].

[1] C. Faber et al., Phys. Rev. B 84, 155104 (2011) [2] S. Ciuchi et al., Phys. Rev. Lett. 108, 256401 (2012) [3] C. Faber, I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. B, 86, 155315 (2012). [4] I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. 109, 167801 (2012).

DS 23: Invited Talk - Stefan Förster (Joint Session with DF, O, KR, MM)

Time: Wednesday 10:30–11:15 Location: GER 37

Invited Talk DS 23.1 Wed 10:30 GER 37

Two-dimensional Oxide Quasicrystals: A new class of materials? — •Stefan Förster[1], Klaus Meinel[1], Rene Hammer[1], Martin Trautmann[1], and Wolf Widdra[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Two-dimensional materials - like graphene, hexagonal boron nitride, or topological insulators - have recently pioneered a new field of materials science. Their peculiar properties are often related to their specific two-dimensional periodic structure.

Here we report the first observation of a two-dimensional oxide quasicrystal (QC), a new member in the family of 2D materials [1]. The QC is derived from $BaTiO_3$ thin films on a hexagonal Pt(111) substrate. Low-energy electron diffraction (LEED) reveals a twelve-fold rotational symmetry. Scanning tunneling microscopy (STM) at room temperature as well as at low temperatures (80 K) allow to resolve the atomic structure. The aperiodic structure is formed by primitive atomic arrangements in squares, triangles, and rhombi with a universal edge length of 0.69 nm. In addition to this dodecagonal atomic arrangement, building blocks of squares, triangles,and rhombi are also found on $(2+\sqrt{3})$ and $(2+\sqrt{3})^2$ larger scales indicating the characteristic self-similarity of an ordered QC. The observed interface-driven formation of a 2D QC from a perovskite oxide in contact with a hexagonal substrate is expected to be a general phenomenon.

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, *Nature 502*, 215 (2013).

DS 24: Focus Session: Resistive Switching by Redox and Phase Change Phenomena I (Memristive devices and new circuit concepts)

The focussed session will give a comprehensive introduction into the physical mechanisms of redox based and phase change based resistive switching phenomena observed in oxides and higher chalcogenides. These phenomena have developed into a mega-trend in nanoelectronics in recent years because of their potential application in energy-efficient high-density memory devices. Methods for the accurate crystallographic determination of the involved defect structures and experimental proves for field-induced crystallographic and valence changes will be reviewed, and issues concerning the integration of such elements within a nanoelectronics environment and the assessment of the device properties will be discussed. In addition, cells based on these phenomena may possibly offer application opportunities which reach into logic and neuromorphic computational concepts. (Organizers: Rainer Waser, RWTH Aachen / FZ Jülich, Matthias Wuttig, RWTH Aachen / FZ Jülich)

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

Invited Talk DS 24.1 Wed 9:30 CHE 89

Scaling limits and future prospects of resistive switching devices: From materials to systems — •Victor Zhirnov — Semiconductor Research Corp., Durham, NC, USA

Device scaling and energy consumption during computation has become a matter of strategic importance for modern Information and Communication Technologies (ICT). The central question addressed in this talk is: What is the smallest volume of matter needed for ICT devices, such as memory or logic? The scaling limits of electron-based devices, such as transistors are˜5-7 nm due to quantum-mechanical tunneling. Smaller devices can be made, if information-bearing particles are used whose mass is greater than the mass of an electron. Therefore the new principles for ICT devices, scalable to ˜1 nm, could be 'moving atoms' instead of 'moving electrons', for example using nanoinonic structures. The nanoionic resistive switching devices may offer a promising path to replace the foundation of today's computing technologies. Examples include memory (ReRAM) and logic (atomic/ionic switches). A related concept, the memristor, is currently being actively explored for different information processing tasks. As will be discussed in this presentation, biological computation is extensively based on heavy particles to represent and process information. Based on the biological computing analogy, future 'neuromorphic' computational architectures could be implemented by using nanoionic devices.

DS 24.2 Wed 10:00 CHE 89

BiFeO3 bilayer structures for implementing beyond von-Neumann computing — •Tiangui You[1], Yao Shuai[2], Wenbo Luo[2], Nan Du[1], Danilo Bürger[1], Ilona Skorupa[3], René Hübner[3], Stephan Henker[4], Christian Mayr[4], René Schüffny[4], Thomas Mikolajick[5], Oliver G. Schmidt[1,6], and Heidemarie Schmidt[1] — [1]TU Chemnitz, Chemnitz — [2]UESTC, Chengdu, China — [3]HZDR, Dresden — [4]TU Dresden, Dresden — [5]NaMLab gGmbH, Dresden — [6]IFW Dresden, Dresden

The conventional von-Neumann architecture, which physically separates processing and memory operations, is limited in so much as the processor cannot execute a program faster than instructions and data can be fetched from and returned to memory[1]. Resistive switching devices[2] are considered as one of the most promising candidates for carrying out the processing and storage simultaneously and at the same device cell. In this work, we present a BiFeO3:Ti/BiFeO3 bilayer structure which shows stable and nonvolatile resistive switching behaviour under both positive and negative bias. With the same writing bias, the bilayer structure shows different resistance state for the different polarity of reading bias. The resistance states are distinguishable and stable enough for the practical applications. For the logic applications, the polarity of reading bias can be used as an additional logic variable, which makes it feasible to program and store all 16 Boolean logic functions simultaneously and into a same single bilayer structure cell in three logic cycles. [1] C. D. Wright, et al., Adv. Funct. Mater., 2013, 23, 2248 [2] A. Bogusz, T. You, et al., accepted in Proc. IEEE (2013)

DS 24.3 Wed 10:15 CHE 89

Application of the metal-to-insulator transition in VO_2 for neuromorphic circuits — •Marina Ignatov, Martin Ziegler, Mirko Hansen, Adrian Petraru, and Hermann Kohlstedt — Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel, Germany

The negative differential resistance of two-terminal vanadium dioxide

(VO_2) devices are investigated for possible applications in neuromorphic circuit architectures. VO_2 was deposited by Pulse Laser Deposition on TiO_2 and Al_2O_3 single crystal substrates. The VO_2 film thickness ranged between 50 nm to 100 nm. Lateral electrodes with a seperation-width ranging from 1 μm to 4 μm were patterned by optical lithography. The observed negative differential resistance is a result of the reversible insulator to metal phase transition in vanadium dioxide due to local Joule heating. In particular, structural and electrical characteristics of different VO_2 devices are discussed in detail. Further, by adding a capacitor in parallel to those devices electrical oscillations at room-temperature were obtained, which enable the emulation of the all-or-nothing spiking behavior of neurons.

DS 24.4 Wed 10:30 CHE 89

High On/Off ratio in ReRAM cells from TiN/TiO_x/Al_2O_3/Pt by atomic layer deposition — •Hehe Zhang, Nabeel Aslam, Rainer Waser, and Susanne Hoffmann-Eifert — Forschungszentrum Juelich, PGI-7 und JARA-FIT, 52425 Juelich, Germany

The bilayer of TiO_x/Al_2O_3 was integrated into micro-cross point TiN/bilayer/Pt devices and investigated for resistive switching memory application. Liquid injection Atomic Layer Deposition (ALD) was used for the deposition of Al_2O_3 and TiO_x in this work. Amorphous Al_2O_3 films with thickness in the nano meter range were prepared using DMAI[$(CH_3)_2AlOCH(CH_3)_2$] and water as oxide source. Al_2O_3 thin films grown on Pt/Si substrates under optimized parameters have sharp interface, low roughness, low impurity level and high insulating properties. Integrated into the TiN/TiO_x/Al_2O_3/Pt micro-cross point structures, the insulting behaviour of Al_2O_3 improved the resistive switching behaviour of the cells. The variation of TiO_x thickness has a significant effect on the R_{off}/R_{on} ratio during switching, whereas the change of Al_2O_3 thickness mainly affects the forming and reset voltage. Bilayer-cells with about 3 to 4 nm Al_2O_3 and 5 to 10 nm TiO_x exhibited a stable bipolar type resistive switching behaviour with resistance ratios of about 10^4 to 10^5.

This work was supported in part by the Deutsche Forschungsgemeinschaft (SFB917), and by the Global Research Laboratory program (2012040157) through the National Research Foundation (NRF) of Korea.

DS 24.5 Wed 10:45 CHE 89

Higher harmonics generation using Au/BiFeO3/Pt metal-insulator-metal (MIM) structure — •N. Du[1], N. Manjunath[1], T. You[1], Y. Shuai[2], W. Luo[2], D. Bürger[1,3], I. Skorupa[3], R. Schüffny[4], C. Mayr[5], M. Di Ventra[6], O. Schmidt[1,7], and H. Schmidt[1,3] — [1]Faculty of Electrical Engineering and Information Technology, TU Chemnitz — [2]State Key Laboratory of Electronic Thin Films and Integrated Devices, UESTC — [3]Institute of Ion Beam Physics and Materials Research, HZDR — [4]Department of Electrical Engineering and Information Technology, TU Dresden — [5]Computational Systems Biology Group, ETH Zürich — [6]Department of Physics, University of California — [7]Institute for Integrative Nanosciences, IFW Dresden

Memristive systems can be used for the generation of higher harmonics [1]. We investigated the second and higher harmonics generation by means of a passive circuit with a sinusoidal input voltage source in series with a load resistor and a single memristor (Au/BiFeO3/Pt) that exhibits nonvolatile bipolar resistive switching. We found that a single memristor in high resistance state and in low resistance state can be used to generate two clearly distinguishable sets of second and higher harmonics. The power conversion efficiencies (PCEs) for higher harmonics generation can be derived from the normalized charge-flux curves of the single memristor [2]. The PCEs can be possibly used in neuromorphic computing. [1] G.Z. Cohen et al., Appl. Phys. Lett. 100, 133109 (2012) [2] N. Du et al., Rev. Sci. Instrum. 84, 023903 (2013)

DS 25: Focus Session: Resistive Switching by Redox and Phase Change Phenomena II (Valence and phase change in oxides)

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

Invited Talk DS 25.1 Wed 11:15 CHE 89

Nanoscale redox-processes in resistive switching oxide devices — •Regina Dittmann — Peter Gruenberg Institut (PGI-7), Forschungszentrum Juelich GmbH, 5425 Juelich

Although there exists a general consensus that bipolar resistive switching in transition metal oxides is in most cases connected with a redox-process, the details of the underlying physical mechanism are only poorly understood up to now. One of the obstacles for its further elucidation is that the net changes of structure, stoichiometry and valence state during electroforming and switching are very small and occur primarily at the electrode interface ore within nanoscale filaments. Besides electron microscopy and- spectroscopy, different Synchrotron radiation based spectroscopy and scattering techniques have been employed so far in order to detect local redox-processes and/or filament formation caused by the electrical treatment of resistive switching oxide devices. This talk will give an overview over electrically-induced structural and stoichiometric changes detected in different types of oxide thin film devices and will discuss their implications on device scaling and stability.

DS 25.2 Wed 11:45 CHE 89

First principles investigation of Sr-rich phases in $SrTiO_3$ — •Ivetta Slipukhina, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Perovskite-type oxides exhibit a whole variety of functionlities, among which resistive switching is one of the most interesting due to the potential use in non-volatile random access memory. In many of these materials the unintentionally formed secondary phases are known to be responsible for the observed resistive switching phenomena. Recently, Sr-rich secondary phases were observed during electroforming in $SrTiO_3$ thin films grown by pulsed laser deposition [A. Köhl, PhD thesis]. The structure and composition of these phases are unknown so far. By means of ab initio calculations, we have considered possible mechanisms for the formation of Sr-rich phases in $SrTiO_3$ and compared the calculated electronic structures with the existing experimental XPS and XAS data.

This work was supported by the SFB917-Nanoswitches.

DS 25.3 Wed 12:00 CHE 89

Correlation of Local Conductivity and Imaging X-ray Photoelectron Spectroscopy in Resistively Switching SrTiO Thin Films — •Christoph Baeumer[1], Annemarie Koehl[1], Marco Moors[1], Marten Patt[1], Vitaliy Feyer[1], Carsten Wiemann[1], Claus Michael Schneider[1], Rainer Waser[1,2], and Regina Dittmann[1] — [1]Peter Grünberg Institut, Forschungszentrum Juelich GmbH, Germany — [2]Institut für Werkstoffe der Elektrotechnik (IWE-2), RWTH Aachen, Germany

Resistively switching oxides are investigated extensively as a possible route towards future non-volatile memory or as basis for the design of novel neuromorphic circuits. Despite the existing strong experimental evidence that resistive switching in transition metal oxides is caused by nanoscale redox reactions, many fundamental details are not yet understood. In particular, the electronic and chemical structure of the resistively switching regions after electroforming and after each switching event remains elusive.

Here we will present a direct correlation of localized chemical composition alterations in $SrTiO_3$ thin films with local conductivity measurements. Imaging X-ray photoelectron spectroscopy after *in-situ* top electrode delamination revealed sub-micrometer regions characterized by an altered cation stoichiometry and increased surface potential, which form after electrical treatments. UHV-LC-AFM measurements showed that these regions possess strongly increased electrical conductivity. This observation hints at a non-negligible contribution of cation diffusion in the formation of conducting channels.

DS 25.4 Wed 12:15 CHE 89

Vacancy-vacancy interaction in $SrTiO_3$ bulk and surfaces — •Ali Al-Zubi, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut (PGI) & Institute for Advanced Simulation (IAS), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We employ the density functional theory (DFT) to model point defects, in particular oxygen vacancies, in the perovskite $SrTiO_3$. We use a bulk super-cell model to calculate the formation energy of single and double O-vacancies for different arrangements in the unit cell. Our results indicate a clear trend of the defects to form one-dimensional extended structures in the ground state.

We extend the study to surfaces and calculate the interaction energy of homogeneously distributed O-vacancies on SrO- and TiO_2-terminated (001) surfaces. To compare to the bulk, we investigate clustering effects, in particular on the TiO_2-terminated surface. For an analysis of the results, we study the role of structural relaxations and estimate the importance of electronic effects by comparison to DFT+U calculations that simulate correlation effects via a Hubbard-U parameter. Furthermore, interaction energies on the SrO-terminated surface are compared to results for O-vacancies in the SrO plane in the Ruddlesden-Popper phases, exhibiting the importance of screening effects in the bulk matrix.

We acknowledge the DFG, SFB 917 project A4, for financial support.

DS 25.5 Wed 12:30 CHE 89

Resistive switching in $SrTiO_3$:Nb single crystals related to phase transformations — •Christian Rodenbücher, Gustav Bihlmayer, Rainer Waser, and Kristof Szot — Peter-Grünberg-Institut 1 + 7, Forschungszentrum Jülich, 52425 Jülich, Germany

The understanding of the nanoscale origin of resistive switching is of particular importance for the development of non-volatile memories. While investigations of the model material $SrTiO_3$ using LC-AFM revealed a filamentary type of switching, the switching type changes upon doping with the donor Nb to a cluster-like switching mechanism related to Nb segregation effects in Verneuil-grown single crystals. We show that the switching itself takes place in the surface layer that can change its properties under the influence of external gradients easily. In particular, we demonstrate that during electrodegradation, which can be used as an emulation of switching, fundamental chemical and crystallographic phase transformations from $SrTiO_3$ towards different substoichiometric TiO_x phases take place in the surface layer under electrical gradients. Based on ab-initio calculations and analyses by various surface-sensitive methods such as XPS, LEED, EBSD and LC-AFM with atomic resolution, we present a potential nanoscale model of the cluster-like resistive switching assuming a phase transformation mechanism inside a nano-filament acting as a switch between the conducting clusters.

DS 26: Gaede Prize Talk

Time: Wednesday 12:30–13:00 Location: HSZ 02

DS 26.1 Wed 12:30 HSZ 02

Spectroscopy and microscopy of graphene on metals — •Yuriy Dedkov — SPECS Surface Nano Analysis GmbH, Berlin, Germany

Graphene on metals, which structure can vary from simple lattice matched to commensurate moiré structures, is an ideal system for different kinds of surface science experiments allowing to study many fascinating phenomena. Here we present several examples on the application of electron spectroscopy (NEXAFS, XMCD, XPS, ARPES) and scanning probe methods (STM and AFM) for the investigation of the electronic structure of these systems. These combined approaches allow to understand the bonding mechanism at the graphene-metal interface, the main features of the graphene-derived electronic structure as well as the imaging contrasts in the scanning probe experiments. All experimental data are compared with the state-of-the-art DFT calculations that lead to the deep understanding of the observed phenomena.

DS 27: Organic Thin Films II

Time: Wednesday 15:00–18:30 Location: CHE 91

DS 27.1 Wed 15:00 CHE 91

All-UHV growth of organic/ZnO hybrid structures — •Mino Sparenberg, Sylke Blumstengel, and Fritz Henneberger — HU zu Berlin, Institut für Physik, AG Photonik

Conjugated organic molecules have a great potential for opto-electronic devices when used in hybrid components together with inorganic semiconductors where the advantages of both materials are combined. Crucial for the fabrication of hybrid structures is the understanding of the interaction at the interface between the organics and the inorganics. To achieve this the growth is conducted and observed in an all-UHV MBE system where growth conditions of the conjugated molecules can be controlled and analysed in-situ with electron diffraction techniques as well as scanning probe microscopes. The inorganic semiconductor investigated here is epitaxially grown ZnO which has been proven for its suitability in hybrid structures with several conjugated molecules. As model systems of the present study, serve aromatic hydrocarbons like the linear sexiphenyl (6P) and its fluorinated derivatives to investigate how the electrostatic interaction at the interface of the ZnO substrate influences the growth of the molecules, as it is predicted in theory, as well as the planar molecule hexabenzocoronene (HBC), which is due to its hexagonal symmetry a promising candidate to create an epitaxial-like growth on top of the ZnO crystal. Our measurements have shown that the fluorination of 6P leads to an interaction with the substrate surface, changing the growth mode in comparison unfluorinated 6P species. Furthermore STM and LEED investigations of HBC samples indicate a predominant growth direction correlated with the substrate.

DS 27.2 Wed 15:15 CHE 91

The role of a molecular dipole in thin-film growth kinetics: *In situ* X-ray studies of 6P and 6P-3,5-F_2 — •Anton Zykov[1], Sebastian Bommel[1,2], Peter Schäfer[1], Francesco Carlà[3], Roberto Felici[3], and Stefan Kowarik[1] — [1]Inst. f. Physik,Humboldt Universität Berlin — [2]DESY, Deutsches Elektronen-Synchrotron, Hamburg — [3]ESRF, Grenoble

An understanding and ideally a control of thin-film growth is needed to rationally fabricate organic-inorganic heterostructures for optimized devices like efficient OLEDs. However, growth control is up to now almost exclusively limited to substrate temperature and growth rate. The incorporation of tunable static dipoles into well-known organic molecules may thus establish a new degree of freedom to design the thin-film morphology. Here we want to present first results of a growth study of 6P and its dipolar derivative 6P-3,5-F_2 on SiO_2. The films were deposited in a vacuum chamber by OMDB under variation of the growth rate and the substrate temperature. Simultaneous *in situ* X-ray measurements of the growth oscillations and GISAXS were carried out at the ID03 beamline at the ESRF to access growth-mode, island-sizes and -densities, which in the end determine the film morphology. We find that films from the dipolar molecule 6P-3,5-F_2 form smaller islands while at the same time yielding smoother films than 6P. Interestingly the inter-layer crystallographic orientation is also lost in 6P-3,5-F_2. These results suggest a different growth mode due to the additional source of disorder through random orientation of dipoles.

DS 27.3 Wed 15:30 CHE 91

Investigation of Interfaces between Pentacene and C60 - Diffusion-Controlled Growth of Two-, One-, and Zero-Dimensional C60-Nanostructures — •Tobias Breuer and Gregor Witte — Philipps-Universität Marburg, Deutschland

A variety of low dimensional C60 structures has been grown on supporting pentacene multilayers. By choice of substrate temperature during growth the effective diffusion length of evaporated fullerenes and their nucleation at terraces or step edges can be precisely controlled. AFM and SEM measurements show that this enables the fabrication of either 2D adlayers or solely 1D chains decorating substrate steps, while at elevated growth temperature continuous wetting of step edges is prohibited and instead the formation of separated C60 clusters pinned at the pentacene step edges occurs. Remarkably, all structures remain thermally stable at room temperature once they are formed. In addition, the various fullerene structures have been overgrown by an additional pentacene capping layer. Utilizing the different probe depth of XRD and NEXAFS we found that no contiguous pentacene film is formed on the 2D C60 structure, whereas an encapsulation of the 1D and 0D structures with uniformly upright oriented pentacene is achieved, hence allowing the fabrication of low dimensional buried organic hetero-structures.

[1] T. Breuer, G. Witte, ACS Applied Materials & Interfaces 5, 9740 - 9745 (2013)

DS 27.4 Wed 15:45 CHE 91

Dynamics at Pentacene/C_{60} interfaces studied by time resolved photoluminescence — •Nils Rosemann, Andrea Karthäuser, Gregor Witte, and Sangam Chatterjee — Philipps-Universität Marburg, Marburg, Germany

The combination of Pentacene (PEN) and C_{60} is a promising model system for next-generation solar cells based on organic semiconductors. Here, the C_{60} acts as an electron acceptor while PEN, on the other hand, attracts the holes. One of the remaining challenges in this system is the underlying charge-transfer mechanism. In general the efficiency of this charge separation will depend on the structural and electronic states at the interface. To study these dynamics, we performed time-resolved photoluminescence measurements on a thin PEN layer of standing molecules covered by C_{60}. The data indicate the formation of correlated states across the interface.

DS 27.5 Wed 16:00 CHE 91

Order in functional self-assembled monolayers for transistor applications — •Thomas Schmaltz[1], Hans-Georg Steinrück[2], Artoem Khassanov[1], and Marcus Halik[1] — [1]Organic Materials & Devices (OMD), University Erlangen- Nürnberg, Germany — [2]Crystallography and Structural Physics, University Erlangen-Nürnberg, Germany

Self-assembled monolayers (SAMs) of functionalized molecules containing semiconducting moieties can be utilized to fabricate monolayer transistor devices (SAMFETs) by a simple, solution based process. However, the order in such systems is not always inherently as desired. For example, C60 functionalized alkylphosphonic acids (C60C18-PA) tend to arrange in a poor 2D order, but it can be increased by introducing alkyl-based monolayers in mixed SAMs as a supporting matrix [1]. In other systems, in which the size of the head group matches better to alkyl chain and anchor group, e.g. in (benzo[b]benzo[4,5]thieno[2,3-d]thiophene)-functionalized alkylphosphonic acids (BTBT-C12-PA), self-assembly of the pure molecules already yields highly ordered layers [2]. To obtain a deeper insight into the order of those monolayers, X-ray reflectivity and X-ray grazing incidence diffraction measurements on those SAMs were performed. Information from those analytical investigations is crucial to understand the relation between the chemical structure, the molecular order and electrical properties of those systems.

[1] C.M. Jaeger, T. Schmaltz et al., JACS, 135, 4893-4900 (2013).

[2] T. Schmaltz, A. Y. Amin et al., Adv Mater, 25, 4511-4514 (2013).

DS 27.6 Wed 16:15 CHE 91

Study of the structure of solution processed bulk heterojunction organic solar cells — •Thaer Kassar[1], Torben Schindler[1], Tilo Schmutzler[1], Christoph Brabec[2], and Tobias Unruh[1] — [1]LKS FAU, Erlangen, Germany — [2]i-MEET FAU,Erlangen, Germany

Solution processed bulk heterojunction polymer solar cells are becoming viable technology due to their potential as a low-cost, printable, and flexible renewable energy source. Little is known about their structure formation and how it can be controlled. It was thought that conjugated polymers and fullerene derivatives separate into pure domains. However, recent reports suggest that intercalation of fullerenes between the side chains of the polymers is possible. Our working group has built a dedicated cell with an integrated doctor blading coater to perform in situ measurements of the evolution of the blend structure during the drying process. To access the 3D structure of the studied thin films from the molecular to the mesoscale, we probe the inner structure through the methods of grazing incidence X-ray diffraction (GIXD) and grazing incidence small angles X-ray scattering (GISAXS). Grazing incidence geometry is used to enhance the scattered intensity and limit it to the films. We exploit SAXS to study the solutions before coating them. We also study ternary cells which overcome the absorption limitation of organic semiconductors and how solvent mixtures, processing additives, thermal/solvent annealing and multilayer stack build-up of the device affect the final dried blend structure. In this talk, first results on the structure formation of active layers of solution processed solar cells will be presented.

DS 27.7 Wed 16:30 CHE 91

Correlation between exciton diffusion and morphology in thin films of Diindenoperylene — •Alexander Steeger[1], Anna Katharina Topczak[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

The exciton diffusion length (EDL) of organic thin films is known to strongly depend on the respective organic compound and can be attributed to a combination of intrinsic material properties and morphological impacts. In order to investigate the latter, we controlled the morphology of thin films of diindenoperylene (DIP) during evaporation by means of the substrate temperature T_S. The EDL was extracted from film thickness dependent photoluminescence measurements in consideration of quenching quality, interference effects and interface roughness. In good agreement with atomic force microscopy and X-ray diffraction measurements showing an enhanced dewetting and significantly larger crystallite sizes at higher T_S, polycrystalline DIP layers grown at $T_\mathrm{S} = 300\,\mathrm{K}$ and $400\,\mathrm{K}$ exhibit high EDLs of 59 nm and 115 nm, respectively. In contrast, X-ray amorphous DIP deposited at $T_\mathrm{S} = 100\,\mathrm{K}$ shows minor transport properties of excitons. This result emphasizes that exciton diffusion is substantially promoted by the long range order in molecular thin films. Financial support by the DFG focus program SPP 1355 is gratefully acknowledged.

Coffee break (15 min)

DS 27.8 Wed 17:00 CHE 91

In-situ GIWAXS on slot die coated highly conductive PEDOT:PSS as electrode for ITO-free organic electronics: Crystallinity and molecular orientation — •Claudia M. Palumbiny[1], Feng Liu[2], Cheng Wang[3], Alexander Hexemer[3], Eric Schaible[3], Thomas P. Russel[2], and Peter Müller-Buschabum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]UMass Amherst, Department of Polymer Science and Engineering, Amherst, MA 01003, USA — [3]Advanced Light Source, LBNL, Berkeley, CA 94720, USA

The potential to manufacture organic photovoltaic devices on flexible substrates enables roll-to-roll mass production. Thereby, techniques such as slot die coating are used. In this study, we use a mini slot die coater, specially designed and made at ALS Berkeley in collaboration with UMass Amherst and Jema Technology, Berkeley, for the implementation at a synchrotron facility. This enables in-situ Grazing Incident Wide Angle X-ray Scattering measurements during the slot die coating process. It allows us to follow the changes in molecular orientation and crystallinity. Further, there are still challenges for roll-to-roll processed flexible devices such as the brittleness of ITO. In this study we therefore investigate PEDOT:PSS modified with the co-solvent ethylene glycol (EG) during the slot die process with in-situ GIWAXS. The results are correlated to the conductivity of the thin films. Doping with EG increases the conductivity of PEDOT:PSS films up to the value of ITO conductivity[1] and can thereby replace ITO as a stand-alone electrode. [1] Palumbiny, C.M. et al., 2014 (submitted)

DS 27.9 Wed 17:15 CHE 91

Island size evolution and molecular diffusion during growth of organic thin films followed by time-resolved specular and off-specular scattering — Christian Frank[1], Jiří Novák[1], Rupak Banerjee[1], •Alexander Gerlach[1], Frank Schreiber[1], Alexei Vorobiev[2], and Stefan Kowarik[3] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France — [3]Institut für Physik, Humboldt Universität Berlin, Germany

We report on a combined off-specular and specular X-ray scattering growth study of ultra-thin films of the prototypical organic semiconductor diindenoperylene (DIP, $C_{32}H_{16}$) [1,2]. We investigate the evolution of the in-plane correlation length and the growth kinetics of the films including their dependence on the substrate temperature and the growth rate. We observe a temperature dependent collective re-

arrangement of DIP molecules from the thin-film to the bulk phase, which can be rationalized by incorporating a thickness-dependent out-of-plane lattice parameter. We further observe that the nucleation behavior of DIP changes from the 1st to the 2nd monolayer, which we relate to a difference in the diffusion of the molecules.
[1] S. Kowarik et al., Phys. Rev. Lett. **96** (2006) 125504
[2] A. Aufderheide et al., Phys. Rev. Lett. **109** (2012) 156102

DS 27.10 Wed 17:30 CHE 91

Telechelic polymers and magnetic nanoparticles nanocomposites: thin dry films and hydrogels — •Antonella Campanella — JCNS Institute of Forschungszentrum Jülich GmbH, Lichtenbergstraße 1 85747 Garching, Germany

The incorporation of inorganic nanoparticles into polymer matrix has extended the particle application because of the several advantages of the polymer thin films like homogeneity and tunable physicochemical properties by increasing mechanical, magnetic and conductive properties. Such kind of nanocomposites are suitable for several modern applications, e.g. as electromagnetic wave absorbers, photovoltaic cells, OLED, data storage. In this context, the object of our study are nanocomposite systems composed of a polymer matrix which consists of hydrophobically modified ethoxylated urethane polymers (a relatively new class of industrially important macromolecules, which are gaining increasing industrial use due to their ability to impart improved rheological behavior to particulate dispersions) with core-shell magnetite nanoparticles embedded. The shell of the magnetite nanoparticles is composed by oleic acid and oleylamine, in order to provide more stability in organic solvent. We are now focusing on the structural characterization of such nanocomposites in two different morphologies: as thin dry films and as hydrogels, in order to understand the influence of the water on the structural organization of the system. The presence of magnetic nanoparticles in the dry polymer matrix shows also an interesting magnetic aspect of the system, which could be interesting for specific applications mentioned above.

DS 27.11 Wed 17:45 CHE 91

Synthesis of Two-Dimensional Polymer/Copolymers Sheets — •Zhikun Zheng[1], Lothar Opilik[2], Florian Schiffmann[1], Wei Liu[3], Renato Zenobi[2], Joost Vandevondele[1], and A. Dieter Schlüter[1] — [1]Department of Materials, ETH Zürich, Wolfgang-Pauli-Strasse 10, 8093 Zürich, Switzerland — [2]Department of Chemistry and Applied Biosciencs, ETH Zürich, Wolfgang-Pauli-Strasse 10, 8093 Zürich, Switzerland — [3]Physical Chemsitry and Electrochemistry, Technical University Dresden, 01062, Dresden, Germany

The current interest in graphene, a naturally occurring two-dimensional polymer (2DP), highlights the necessity to produce other chemically different analogues. Until very recently there was no organic synthetic method available that would allow accessing a laterally infinite, one-monomer-unit thick, freestanding, unimolecular network with a defined internal periodicity. This talk will overview current efforts towards 2DPs with detailed discussion of our concepts, which rest upon carefully designed monomers, interfacial ordering, and both metal-complexation and light-induced polymerizations. In addition, we will report the synthesis of 2D random copolymers and a 2D block copolymer, which provide unprecedented structural diversity of 2DPs.

DS 27.12 Wed 18:00 CHE 91

Film Growth, Adsorption and Desorption Kinetics of Indigo on SiO2 — •Boris Scherwitzl, Roland Resel, and Adolf Winkler — Institute of Solid State Physics, Petersgasse 16, A-8010 Graz, Austria

Understanding the initial stages of organic film growth is the first step of manufacturing organic microelectronic devices. Due to hydrogen bonding and π-stacking, unlike most organic materials, the natural dyes indigo and tyrian purple form highly crystalline films with interesting semiconducting characteristics. In this contribution we report our recent efforts and studies on the initial growth behavior of thin indigo films (C16H10N2O2) on a silicon dioxide substrate under UHV conditions with respect to sample treatments. Films from sub-monolayer up to multilayer range were created using physical vapor deposition and subsequently analyzed with Auger Electron Spectroscopy, Thermal Desorption Spectroscopy, Atomic Force Microscopy and X-Ray Diffraction. It could be shown that indigo films tend to dewet at sub-monolayer coverages and form bulk-like structures bound by hydrogen bonds once a certain film thickness is reached. Repeating the measurements on a sputter-cleaned surface and considering heat of evaporation calculations, yields interesting results regarding growth kinetics and surface diffusion.

DS 27.13 Wed 18:15 CHE 91

Organic surface nano-patterns prepared by using nanoporous templates — •Yan Zheng, Wenxin Wang, Ahmed Al-Haddad, Huaping Zhao, Chengliang Wang, and Yong Lei — Ilmenau University of Technology, Institute of Physics & IMN MacroNano* (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau (Germany)

Tris(8-hydroxyquinoline) aluminum (Alq3) is an organic semiconductor which attracted considerable attention for the applications in optical and electrical devices. Nanostructured metallic surface associated with organic semiconductor molecule can result unique electronic and optical properties. In this work, large area of Alq3 nanoparticle pattern with high uniformity and periodicity was successfully prepared using ultra-thin alumina membranes (UTAMs) through organic molecular sublimation under ultrahigh vacuum conditions. The various photoluminescence properties of Alq3 nanoparticle pattern can be realized from the particle diameters by adjusting the pore size of the alumina template. Enhanced photoluminescence was observed when Alq3 deposited onto metallic nanoparticle arrays. The PL enhancement of Alq3 material covered on metallic nanoparticle arrays could be attributed to the increased absorption and quantum yield of surface plasmon resonance. All the results indicate that the controllable highly ordered Alq3 nanoparticle pattern, which is based on the low cost and convenient method of UTAMs template-directed by organic molecular sublimation with PL enhancement performance, has potential applications in nano-optoelectronic devices.

DS 28: Invited Talk - Heidemarie Schmidt (Joint Session with DF, MA, HL, KR, MM)

Time: Wednesday 15:00–15:45 Location: GER 37

Invited Talk DS 28.1 Wed 15:00 GER 37

Smart multiferroic thin films for cognitive computing — •Heidemarie Schmidt — Technische Universität Chemnitz, Department of Materials for Nanoelectronics, Reichenhainer Str. 39, 09126 Chemnitz

Cognitive systems promise to penetrate complexity and assist people and organizations in better decision making [1]. We have successfully prepared metal-multiferroic-metal (MMM) structures with the multiferroic material BiFeO3 and BiFeTiO3. All those MMM structures exhibit nonvolatile resistive (meristive) switching. Investigations of memristive switching is driven by promising applications of power-efficient memristive nanostructures including data storage, logic systems, cognitive computing and artificial neural networks. Prominence of work on memristive systems might be visualized by the near-future breakthrough in computing technology, where classical Von Neumann architecture is replaced by cognitive systems. In this talk I present three new functionalities of smart MMM structures including nonvolatile multilevel resistive switching [2], nonvolatile reconfigurable logics and nonvolatile second and higher harmonics generation [3] which are very promising for the development of cognitive computing. [1] J. E. Kelly III, S. Hamm, Smart Machines: IBM*s Watson and the Era of Cognitive Computing, Columbia University Press, 2013 [2] Y. Shuai et al., J. Appl. Phys. 109 (2011); Appl. Phys. Lett. 98 (2011); Appl. Phys. Exp. 4 (2011); 111 (2012); IEEE Electron Device Letters 34 (2013); Scientific Reports 3 (2013) [3] N. Du et al., Rev. Sci. Instr. 84 (2013)

DS 29: Organic Electronics and Photovoltaics V (joint session with CPP, HL, O)

Spectroscopy, OFETs, OLEDs, Photo switches

Time: Wednesday 15:00–18:15 Location: ZEU 260

DS 29.1 Wed 15:00 ZEU 260

Comprehensive efficiency analysis of organic light-emitting diodes featuring horizontal emitter orientation and triplet-to-singlet up-conversion — •Tobias Schmidt[1], Bert Scholz[1], Christian Mayr[1], Andreas Rausch[2], Thomas Wehlus[2], Dirk Michaelis[3], Norbert Danz[3], Thilo Reusch[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]OSRAM Opto Semiconductors GmbH, Leibnizstrasse 4, 93055 Regensburg, Germany — [3]Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

The external quantum efficiency (EQE) of an organic light-emitting diode can strongly be affected by orientation of the emissive dipole moments, and for fluorescent dyes, by triplet-to-singlet up-conversion leading to an enhanced radiative exciton fraction (η_r), exceeding the spin-statistical limit of 25 %. By a combination of EQE investigations with time resolved photo- and electroluminescence measurements we are able to quantify the lower limit of the additionally created singlet excitons, e.g. by thermally activated delayed fluorescence, as well as the factors being responsible for light-outcoupling. For the investigated fluorescent system the EQE is boosted by two effects. First, due to horizontal alignment of the transition dipole moments, the outcoupling factor is enhanced by a factor of 1.3. Second, the enhanced η_r value of 36 %, results in an additional efficiency increase by a factor of 1.44. As a consequence of the combination of both effects the EQE almost doubles and values up to 5 % are achieved for direct emission in spite of a comparatively low emitter efficiency of 40 % only.

DS 29.2 Wed 15:15 ZEU 260

Multi-analytical investigation of SAM formation in printing relevant timescales III: OFET devices — •Milan Alt[1,2,6], Janusz Schinke[2,3], Sabina Hillebrandt[2,5], Marc Hänsel[2,4], Kaja Deing[2,6], Uli Lemmer[1,2], and Norman Mechau[1,2] — [1]Karlsruher Institute of Technology — [2]InnovationLab, Heidelberg — [3]TU Braunschweig — [4]TU Darmstadt — [5]Uni Heidelberg — [6]Merck KGaA

Self-assembled monolayers (SAMs) can be used to effectively reduce contact resistances originating from energetic misalignments at metal-semiconductor interfaces. Solution processing of SAMs has been intensively studied and is in principle compatible with high throughput printing techniques. However, most studies on SAMs feature immersion in very dilute solutions for many hours, in some cases up to several days. The objective of this work is to understand SAM accumulation with a focus on short time scales in order to estimate weather the deposition of well performing SAMs can be speeded up sufficiently to be compatible with typical film drying times in printing. We combined analytical characterization of SAM treated metal surfaces via photoelectron- and IR-spectroscopy, as well as Kelvin Probe with measurements of the actual injection barriers in OFET devices. We chose the widely used 1H,1H,2H,2H-Perfluorodecanethiol SAM and investigated its quality and charge injection performance in dependency of the process parameters immersion time and molecular concentration. Additionally, we studied the impact of ambient condition on SAM deposition and the resulting SAM performance, in order to account for a realistic fabrication environment.

DS 29.3 Wed 15:30 ZEU 260

Multi-analytical investigation of SAM formation on printing-relevant time scales I: Kelvin probe and photoelectron spectroscopy — •Janusz Schinke[1,5], Marc Hänsel[2,5], Milan Alt[3,4,5], Sabina Hillebrandt[2,5], Eric Mankel[6,5], Wolfram Jaegermann[6,5], Wolfgang Kowalsky[1,5], and Robert Lovrincic[1,5] — [1]TUBS, Inst. f. Hochfrequenztechnik — [2]Uni HD, Kirchhoff-Inst. für Physik — [3]Karlsruher Inst. f. Technologie — [4]Merck KGaA — [5]InnovationLab GmbH, Heidelberg — [6]TUD, Materials Science Inst.

In organic electronic devices, charge injection at the contacts is crucial for electrical performance. The devices require electrodes with a sufficiently low contact resistance at the metal-semiconductor interface to inject into or collect charge carriers from the transporting layer. A smart way to align the energetics at the interface is the use of self-assembled monolayers (SAMs). We have studied the properties of 1H,1H,2H,2H-Perfluorodecanethiol using photoelectron spectroscopy (XPS/UPS), infrared spectroscopy (IR), ambient Kelvin probe (KP), and contact angle (CA) measurements and the injection barriers were also measured in actual devices - organic field effect transistors. Using these methods we were able to obtain a very deep understanding of the whole SAM adsorption process, as well as the impact of immersion time, concentration and the influence of ambient conditions on the resulting monolayer and its performance. With this knowledge we estimate optimized parameters to speed up the treatment process, in contrast to most studies where long immersion times are used, to be compatible with typical times used in standard printing methods.

DS 29.4 Wed 15:45 ZEU 260

Multi-analytical investigation of SAM formation on printing-relevant time scales II: infrared-reflection-absorption-spectroscopy — •Sabina Hillebrandt[1,5], Janusz Schinke[2,5], Milan Alt[3,4,5], Robert Lovrincic[2,5], Tobias Glaser[1,5], and Annemarie Pucci[1,5] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik — [3]Karlsruher Institut für Technologie — [4]Merck KGaA, Darmstadt — [5]Innovationlab GmbH, Heidelberg

In organic semiconductor devices the improvement of charge carrier injection between metal contact and organic semiconductor is a major concern. Self-assembled monolayers (SAMs) built up interface dipoles on metal surfaces that can increase or lower the work function of the material. Therefore SAMs can be used as injection layers. The properties of solution-processed SAMs such as orientation and interface dipole are influenced by various factors like concentration of the molecule in solution, immersion time and purity of the solution or substrate.

Infrared-reflection-absorption-spectroscopy (IRRAS) is very sensitive to changes in the orientation of SAMs on metal surfaces, thus we performed IRRAS measurements on SAMs consisting of 1H,1H,2H,2H-perfluorinated decanethiol on evaporated gold substrates. Orientation, ordering and quality of the SAM were investigated under systematic variation of immersion time and concentration of the molecule in solution. Taking into account realistic printing conditions we also investigated very short immersion times and high concentrations as well as the impact of oxygen in solvent and substrate on the layer formation.

DS 29.5 Wed 16:00 ZEU 260

Towards fully printed organic light-emitting diodes: investigation of solution processed electron injection layers — •Sebastian Stolz[1,4], Gerardo Hernandez-Sosa[1,4], Michael Scherer[2,4], Eric Mankel[3,4], Robert Lovrinčić[2,4], Janusz Schinke[2,4], Uli Lemmer[1,4], and Norman Mechau[1,4] — [1]Karlsruhe Institute of Technology, Light Technology Institute — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik — [3]Technische Universität Darmstadt, Materials Science Institute, Surface Science Division — [4]InnovationLab GmbH, Heidelberg

The fabrication of organic light-emitting diodes (OLEDs) by high throughput printing techniques requires the development of solution processable electron injection layers. Today, either alkali salts or low work-function alkaline earth metals are used as cathode layers in OLEDs. As these materials are highly reactive, they cannot be easily solution processed. In this work, we present blue fluorescent light-emitting diodes which use silver in combination with Polyethylenimine (PEI) and Polyethylenimine-ethoxylated (PEIE) as cathode layer. We demonstrate that both materials can be effectively used as electron injection layers in OLEDs and correlate the performance of the devices to the characteristics of the PEI(E) layers. Photoelectron spectroscopy is used to estimate the polymer thickness and the corresponding change in cathode work-function while the homogeneity of the layers is evaluated by AFM measurements. We show that OLEDs using PEI/PEIE and silver as cathode layer yield an improved performance and shelf lifetime compared to reference devices that use calcium, instead.

15 min. break

DS 29.6 Wed 16:30 ZEU 260

Micro-structured organic field effect transistor on commercial poly(urethane) resin as substrate and gate dielectric — Jan

Hartel, Derck Schlettwein, and •Christopher Keil — Institute of Applied Physics, Laboratory of Materials Research, Justus-Liebig-University Giessen, Germany.

Dielectric layers of a commercial cross-linked poly (urethane) (PU) were prepared on a conductively coated film and served as gate dielectric and as substrate for the growth of an organic semiconductor film in an alternative approach to all-organic field effect transistors (OFET). A method was developed to process micro-structured electrodes on top of the PU dielectric layer which proved superior to the traditional lift-off-procedure. The influence of the aspect ratio of the electrodes within the organic transistor on a given dielectric layer will be discussed with respect to the calculation of the relative permittivity and the gate capacitance. A method is proposed to compensate short electrode effects which would otherwise lead to an underestimation of the gate capacitance and hence to a miscalculation of the OFET properties.

DS 29.7 Wed 16:45 ZEU 260

Time-resolved potentiometry of organic thin film transistors — •Jan Murawski, Tobias Mönch, Moritz Philipp Hein, Peter Milde, and Lukas M. Eng — Technische Universität Dresden, Institut für Angewandte Photophysik

High speed application still poses a challenge for organic thin film transistors (OTFTs) due to their low charge carrier mobilities, high driving voltages, and low on/off-current ratios. Few investigations have been reported on the switching dynamics of OTFTs on the nanoscale, even fewer in the relevant temporal operation regime as required for high speed applications. Yet, such investigations are crucial for understanding the bottle-necks in OTFTs dynamic performance.

Here, we introduce time-resolved Kelvin probe force microscopy (tr-KPFM) to track the time evolution of surface potential wave fronts inside the channel of a pentacene-based bottom-gate coplanar OTFT. The relevant dynamical evolution proceeds in the microsecond regime and is easily resolved by our quantitative tr-KPFM method. Comparing our experiment with simulations reveals the presence of Schottky barriers in the real device to be responsible not only for a reduced effective electric field across the transistor channel (and thus a reduced field mobility) but also for inducing a delayed re-injection of charge carriers at the electrode-semiconductor interface. Although the charge-carrier mobility would allow for faster switching, charging the Schottky barrier constitutes the bottle-neck to be overcome for higher working frequencies in OTFTs.

DS 29.8 Wed 17:00 ZEU 260

High-Mobility, Low-Voltage Organic TFTs based on Air-Stable DNTT Derivatives: Time-Dependent Improvement in Contact Resistance and Dynamic Performance — •Ulrike Kraft[1,3], Ute Zschieschang[1], Kazuo Takimiya[2], Edwin Weber[3], and Hagen Klauk[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]RIKEN Advanced Science Institute, Wako, Japan — [3]Technical University Bergakademie Freiberg, Germany

The organic semiconductor dinaphtothienothiophene and its derivatives C10-DNTT and diphenyl-DNTT provide larger carrier mobilities and better air stability than, e.g., pentacene. We present a detailed comparison of the thin-film morphology, static and dynamic performance and stability of low-voltage (3 V) thin film transistors based on vacuum-deposited films. Freshly fabricated TFTs (channel length: 100 um) have hole mobilities ranging from 3 cm2/Vs (DNTT) to 5 cm2/Vs (diphenyl-DNTT), with on/off ratios of 10ˆ7.

During the first few hours after fabrication, the effective mobility of short-channel TFTs (L=1 um) increases by about 20-30%, due to an improvement in the contact resistance (measured with TLM). The dependence of this effect on the exposure to different gas atmospheres, humidity and to light was investigated. To study the impact on the dynamic performance of the TFTs, we fabricated unipolar ring oscillators on flexible PEN substrates. The stage delay of DNTT TFTs (L=1 um) measured at 3 V drops from 920 to 410 ns during the first 4 days of exposure to ambient air, which is the shortest delay reported for flexible organic TFTs at supply voltages <10 V.

DS 29.9 Wed 17:15 ZEU 260

Continuously tunable organic semiconductor distributed Feedback (DFB) lasers as an example for optical components built from shape-memory polymers — •Senta Schauer[1], Xin Liu[2], Tobias Meier[1], Marc Schneider[1], Matthias Worgull[1], Uli Lemmer[1,2], and Hendrik Hölscher[1] — [1]Karlsruhe Institute of Technology, Institute of Microstructure Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Karlsruhe Institute of Technology, Light Technology Institute, Engesserstraße 13, 76131 Karlsruhe, Germany

Phase gratings are important tools for many applications in optics and photonics, e.g., they serve as resonators in DFB-lasers. We manufactured Bragg gratings from a shape-memory polymer (SMP) to tune their period over a wide range without any mechanical components. SMPs can remember a predefined shape and recover to it even after strong deformations, if they are triggered by a stimulus. We used the polyurethane Tecoflex(R), which is a thermally triggered SMP, to fabricate nanostructured gratings via hot embossing. After stretching, these gratings feature an increased period which shrinks back to its original length after the activation of the recovery process. In order to demonstrate the practical applicability of these gratings as useful components for photonics, we successfully fabricated continuously tunable DFB-lasers based on SMP grating substrates with Alq3:DCM serving as active material. By changing the grating period via the shape-memory effect, the emitted wavelength of the laser changes likewise. So far we demonstrated shifts of the emission spectrum by 30nm.

DS 29.10 Wed 17:30 ZEU 260

Optical studies of excitonic precursor spin species under magnetic resonance in organic light emitting diodes. — •Hermann Kraus, Sebastian Bange, and John M. Lupton — Universität Regensburg, 93040 Regensburg, Deutschland

Large magnetoresistance effects e.g. due to spin-dependent recombination rates are well-known for OLEDs [C. Boehme et al., Nat. Nano 8, 612 (2013)], although models are still under debate given that they remain hard to verify from a measurement of integrated current and luminance values[J. M. Lupton et al., Nature Mat. 7, 598 (2008)]. Spin resonance of paramagnetic species enables direct manipulation of carrier and excitonic precursor spins, providing a wealth of new insight into dynamic spin properties. Previous work on electrical or optical detection of spin manipulation [W. J. Baker et al., Nature Comm. 3, 898 (2012); W. J. Baker et al., Phys. Rev. B 84, 165205 (2011)] misses out on the opportunity to directly observe the presence of triplet exciton species that are at the heart of spin-dependent recombination models. A few polymeric and small-molecular compounds are now known to exhibit reasonable triplet emission without modification of the polaron pair and exciton dynamics by strong spin-orbit interaction [D. Chaudhuri et al., Angew. Chem. Int. Ed. DOI 10.1002/anie.201307601(2013); J. M. Lupton et al., Phys. Rev. Lett. 89 167401(2002)]. Those materials are ideal candidates to directly track spin singlet and triplet excitonic species in organic light-emitting diodes under conditions of magnetic resonance, by comparing the fluorescence (singlet) to phosphorescence (triplet) intensity.

DS 29.11 Wed 17:45 ZEU 260

***Ab-initio* quantum dynamics simulation of photo-induced molecular switching: Azobenzene on coinage metals** — •Reinhard J. Maurer and Karsten Reuter — Department Chemie, Technische Universität München, Germany

The constant pursuit towards further miniaturization of electronic devices slowly reaches the point where individual molecules may serve as the main functional units. Unfortunately, more often than not, an inherent molecular function is quenched by overly strong coupling to the environment; a permanent danger, specifically in the case of metal surface adsorption. Nevertheless, metal surface adsorption may also introduce new functionality, such as in the case of photo-induced molecular switching of tetra-*tert*-butyl-functionalized Azobenzene (TBA) on Au(111). In this work we attempt a full *ab-initio* description of the explicit nuclear and electronic dynamics to analyze a novel substrate-mediated process that was suggested for this system [1]. The immense system size and a continuum of electronic states demand an effective modelling approach explicitly accounting only for the most important degrees of freedom. Employing an efficient density-functional theory based ΔSCF approach [2] we construct and analyze the involved excited-state potential energy surfaces (PESs), and establish a mixed-quantum classical dynamics simulation. A particular focus is the effect of the image-charge induced changes on the excited-state PESs and the excited-state lifetime- and temperature-dependence of the quantum yield. [1] Wolf, Tegeder, Surf. Sci. **603**, 1506–1517 (2009); [2] Maurer, Reuter, J. Chem. Phys. **139**, 014708 (2013)

DS 29.12 Wed 18:00 ZEU 260

Reversible switching and light-induced structural changes in spin-coated thin films of Azobenzene-polymers —

•Christopher Weber[1], Tobias Liebig[1], David Bléger[2], Stefan Hecht[2], Jürgen Rabe[1], and Stefan Kowarik[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik — [2]Humboldt-Universität zu Berlin, Institut für Chemie

Functionalized surfaces with molecules whose conformation can be reversibly switched between two isomeric forms by light are relevant for future devices -e.g. for switching adaptive materials, storing two states in memory applications, and switching current in molecular electronics. Here we use grazing incidence x-ray diffraction (GIXD), atomic force microscopy (AFM) and differential reflectance spectroscopy (DRS) to study light-induced structural changes in spin-coated thin films of Azobenzene-polymers with Alkyl side-chains. In solution, the individual Azobenzene-polymer shrinks upon UV-irradiation. Submonolayers of Azobenzene-polymers on Silicon oxide are still switchable with high efficiency, but do not show the same shrinking behavior, as suggested by AFM measurements before and after UV-illumination. Increasing the thickness to multilayers drastically changes the switching behavior, because of strong sterical hindrance. Interestingly, GIXD shows that the in-plane Bragg peaks corresponding to the coherent ordering of the Alkyl side-chains disappear when the sample is illuminated with UV-light and partially reappear after a few minutes in the dark, showing that switching is still possible in the crystalline state albeit with slower kinetics.

DS 30: Focus Session: Emerging oxide semiconductors II (jointly with HL, DF, O)

Continuation of the morning session 'Emerging oxide semiconductors I'

Organizers: Oliver Bierwagen, Paul-Drude-Institut für Festkörperelektronik, Berlin, Norber Esser, Leibniz-Institut für Analytische Wissenschaften ISAS, Berlin, Rüdiger Goldhahn, Otto von-Guericke-Universität Magdeburg, and Marius Grundmann, Universität Leipzig.

Time: Wednesday 15:00–18:45 Location: POT 081

Topical Talk DS 30.1 Wed 15:00 POT 081

Electronic properties of the transparent semiconducting oxides Ga2O3 and In2O3 — •Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

The exploration of oxides from the perspective of semiconductor science and technology offers great opportunities for uncovering new physics as well as developing novel devices with unprecedented performance and functionality. In this talk the transparent semiconducting oxides (TSO) Ga2O3 and In2O3 will be presented. Regarding the electronic structure respectively band structure, crucial progress has been reached in the last years. Here Ga2O3 and, in particular, the (100) surface behaves like expected for a large-gap semiconductor. Against this, for In2O3 the occurrence of a charge accumulation layer is heavily debated. This possibly will restrict their potential for applications.

DS 30.2 Wed 15:30 POT 081

Dielectric function of In_2O_3 from the mid-infrared into the vacuum ultraviolet — •Rüdiger Goldhahn[1], Jakob Nixdorf[1], Christian Lidig[1], Klaus Irmscher[2], Zbigniew Gałazka[2], Oliver Bierwagen[3,4], James S. Speck[4], Christoph Cobet[5], and Martin Feneberg[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg — [2]Leibniz-Institut für Kristallzüchtung, Berlin — [3]Paul Drude Institut für Festkörperelektronik — [4]University of California, Santa Barbara — [5]Johannes Kepler Universität, Linz

The optical properties of cubic bixbyite In_2O_3 are under intense discussion. There is not even a consensus about the direct or indirect nature of the fundamental band gap and the corresponding energies. Here, we present spectroscopic ellipsometry from the phonon region in the mid-infrared up to 10 eV using several different instruments including synchrotron radiation. The studies comprise bulk (111) crystals and epitaxial (001) thin films on (001) yttria-stabilized zirconia covering a wide range of electron concentrations (N_s). The dielectric function of In_2O_3 at high energies exhibits pronounced features related to critical points. By analyzing certain peculiarities of ellipsometric data, the fundamental band gap energy to be 2.77 ± 0.02 eV for low N_s. A continuous Burstein-Moss shift is found for increasing N_s. The analysis of the plasma frequency yields an electron effective mass of about $0.23m_0$.

DS 30.3 Wed 15:45 POT 081

Barrier height of Ag on In_2O_3 (111) single crystals — •maryam nazarzadehmoafi[1], stephan machulik[1], florian Neske[1], christoph janowitz[1], zbigniew galazka[2], and recardo manzke[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, Berlin, Germany

The barrier height of a metal-semiconductor contact was studied by means of angle-resolved photoemission spectroscopy, which was implemented through stepwise Ag deposition on the (111) surface of In_2O_3 single crystals. Work function of Ag and electron affinity of In_2O_3 were measured in situ, being 4.21 ± 0.05 eV and 4.24 ± 0.05 eV, respectively. A slight barrier height of 0.15 ± 0.07 eV was determined by following the band bending of valence band and core level spectra with Ag coverage. Good agreement was observed when comparing the results to a calculation of the height by applying the Schottky-Mott rule, yielding the negligible value of 0.03 ± 0.05 eV. Therefore, the character of the contact is ohmic like. Additionally, the results revealed the existence of diffuse band-gap states for In_2O_3(111) and a Fermi level shift by 0.09 ± 0.02 eV due to the photovoltage effect with Ag deposition.

DS 30.4 Wed 16:00 POT 081

Metal contacts on the beta-Ga2O3 single crystal (001) surface — •Stephan Machulik[1], Maryam Nazarzadehmoafi[1], Mansour Mohamed[2], Andreas Siebert[1], Christoph Janowitz[1], Zbigniew Galazka[3], and Recardo Manzke[1] — [1]Humboldt Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin — [2]Assiut University, Physics Department, Faculty of Science, Assiut 71516, Egypt — [3]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, Berlin, Germany

Results of band structure measurements on beta-Ga2O3 single crystals were in good agreement with theoretical calculations [1], indicating a good theoretical understanding of this material. For application purposes in semiconductor technologies both Schottky and Ohmic metal-semiconductor contacts are required. ARPES and I/U measurements performed on n-doped Au-beta-Ga2O3(001) contacts confirmed Schottky-like behavior with a barrier height of 1.01 eV [2]. Motivated by the lower work function of silver we performed an ARPES study of Ag-beta-Ga2O3(001). The results point to a distinctly lower Schottky barrier, but the contact was not yet Ohmic. Additionally the work function depending on the layer thickness of Ag was studied.

[1] M. Mohamed, C. Janowitz, I. Unger, R. Manzke, Z. Galazka, R. Uecker, R. Fornari, J.R. Weber, J.B. Varley, C.G. van de Walle, Appl. Phys. Lett. 97, 211903 (2010)

[2] M. Mohamed, K. Irmscher, C. Janowitz, Z. Galazka, R. Manzke, R. Fornari, Appl. Phys. Lett. 101, 132106 (2012)

DS 30.5 Wed 16:15 POT 081

Sputtered SnO_2 degenerately doped with Ta or Sb - A comparative study for applications in transparent electronics — •Mirko Weidner and Andreas Klein — Technische Universität Darmstadt

In the emerging field of transparent electronics, indium oxide doped with tin (ITO) is still the predominately used electrode material, due to its high conductivity at low deposition temperatures. Due to the relative scarcity and high cost of Indium, alternatives are highly sought after. Tin oxide (SnO_2) is one of the few other materials that combine the properties of optical transparency and electrical conductivity. The material may serve as a transparent electrode in optoelectronic devices such as displays, touch screens, LEDs and thin film solar cells. In recent years, SnO_2 doped with Tantalum (TTO) has been shown to be a valid alternative to the established SnO_2 systems doped with Fluorine

(FTO) or Antimony (ATO). However, little work has been published on the material, and thus far the question as to why Tantalum doping can yield better electrical conductivity than Antimony doping has not been raised or answered.
In this study, TTO and ATO thin films where sputter-deposited and characterized under similar conditions to maximize comparability between the two materials. Characterization of electrical conductivity and optical transmissivity was complimented by probing the materials' electronic structure by in-situ Photoelectron Spectroscopy (XPS/UPS) of the sample surfaces and by structural characterization by AFM and XRD.

DS 30.6 Wed 16:30 POT 081

Structural and electrical properties of Nb doped TiO_2 anatase films (2 - 17 at.%) sputtered with plasma emission control — •Sebastian Schipporeit[1], Sanat Kumar Mukherjee[1], Hans-Werner Becker[2], Andrew Paolo Cádiz Bedini[1], Christian Notthoff[1], Abdelkader Nebatti[1], Detlef Rogalla[1], Azadeh Soleimani-Estafani[1], and Dieter Mergel[1] — [1]Thin Film Technology Group, Faculty of Physics, University Duisburg-Essen — [2]University Bochum

Nb doped TiO_2 films were deposited using radio frequency magnetron sputtering with a metallic Ti target and introducing O_2 and Ar gas into the chamber. Nb wires were put onto the sputter track of the Ti target and the oxidation state of the target was controlled using a Ti line of the plasma emission. The films were analysed with XRD, RBS, SEM, EDX and XPS. After annealing at 400 °C, all films are polycrystalline and inhibit anatase structure. The Nb/(Nb+Ti) content varies from 2 to 17 at.%. The lattice parameter a and the unit cell volume increase in a similar manner compared to TiO_2:Nb single crystals.

The films with the lowest resistivity of $7{\cdot}10^{-4}$ Ωcm (Nb content: 10 at.%) were coated with an oxidation state of the target in the transition region between metallic and oxidic modes. The Nb is incorporated as Nb^{5+} into the anatase lattice. In films with higher resistivity, the donor effect of Nb might be compensated by Ti vacancies (acceptors). The oxygen content is higher than in stoichiometric TiO_2. Ogyxen interstitials might increase the mass density in the films.

Coffee break (15 min.)

Topical Talk DS 30.7 Wed 17:00 POT 081

Surface properties of In_2O_3 and other semiconducting metal oxides — •Ulrike Diebold — Institute of Applied Physics, TU Vienna, Austria

The atomic-scale surface properties of semiconducting oxides influence, and often even dominate, their performance in a variety of applications. Often, local effects such as defects can severely affect the local electronic structure and surface chemistry. Our group uses STM in combination with DFT and area-averaging spectroscopies to investigate such phenomena at the atomic scale. Recent results on single crystalline In_2O_3 and other metal oxides will be discussed.

DS 30.8 Wed 17:30 POT 081

STM and STS at the InO(111) cleavage surface — Robert Zielinski, Andrea Lenz, Josephine Schuppang, Mario Dähne, and •Holger Eisele — Technische Universität Berlin, Institut für Festkörperphysik, 10623 Berlin, Germany

The freshly cleaved In2O3(111) surface is investigated by UHV cross-sectional scanning tunneling microscopy and spectroscopy in order to achieve knowledge about its intrinsic electronic surface states. Atomically resolved STM images show a topographic contrast, which can be related with recent density functional theory calculations, and indicate a local charge enhancement within the surface unit cell. Scanning tunneling spectra reveil intrinsic states within the fundamental bulk band gap. Furthermore, the Fermi level is energetically located within the bulk band gap. This finding leads to the assumption that electron accumulation at this surface is not an intrinsic property, but related to extrinsic effects, such as e.g., non-stoichiometric material re-organization.

DS 30.9 Wed 17:45 POT 081

Electrical properties of In2O3 single crystals: distinction between surface and bulk conductivity — •Klaus Irmscher, Mike Pietsch, Wolfram Troeder, and Zbigniew Galazka — Leibniz-Institut für Kristallzüchtung, Berlin

Transparent semiconducting oxides such as In2O3, SnO2 or ZnO have the tendency to form surface electron accumulation layers. The highly conductive surface layers may have strong implications in the emerging field of transparent oxide electronics. For instance, the implementation of active elements like Schottky diodes depends on whether the accumulation of electrons at the surface can be suppressed in a controlled manner. Investigations on the origin of the surface electron accumulation in In2O3 were hitherto performed on thin crystalline films. Here, we present temperature dependent Hall effect measurements of melt-grown In2O3 bulk single crystals. The samples had electron concentrations between 10^16 and 10^19 cm-3 at room temperature depending on post-growth annealing conditions. The temperature dependent electron concentrations measured from 15 to 750 K show clear contributions due to surface electron accumulation. To differentiate between bulk and surface proportions the data evaluation is based on a two-layer model. This enables a clear attribution of donor concentration changes due to sample annealing under oxidizing or reducing conditions to surface-near and bulk regions, respectively. We discuss the possible influence of oxygen vacancies, hydrogen donors and surface adsorbates.

DS 30.10 Wed 18:00 POT 081

Electronic surface properties of stoichiometric and defect-rich indium oxide films prepared by MOCVD — •Marcel Himmerlich[1], Chunyu Wang[2], Volker Cimalla[2], Oliver Ambacher[2], and Stefan Krischok[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, PF 100565, 98684 Ilmenau, Germany — [2]Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastraße 72, 79108 Freiburg, Germany

The influence of metalorganic chemical vapor deposition conditions on the indium oxide surface properties is investigated using photoelectron spectroscopy (PES). It is shown that the growth conditions have a strong influence on the physical properties and that films prepared at 200°C or below are highly oxygen-deficient and rich in defects, influencing the surface chemical and electronic properties and resulting in the existence of excess electrons, which are partially localized at the remaining indium atoms. This configuration results in the existence of reactive defect sites, which cause high ozone sensitivity. The PES results are compared to the electronic properties of crystalline In_2O_3 films in cubic bixbyite and rhombohedral structure. The influences of the surface stoichiometry and high defect density, ozone oxidation and UV photoreduction on variations in surface band bending, electron accumulation, work function and formed surface dipoles as well electron transport and sensor characteristics are analyzed.

DS 30.11 Wed 18:15 POT 081

Stability of low-index bcc-In_2O_3 surfaces under O-Rich-, In-Rich-, and Sn-doping molecular beam epitaxy conditions: An Experimental Study — •Oliver Bierwagen[1,2], Patrick Vogt[1], and James S. Speck[2] — [1]Paul-Drude-Institut, Berlin,Germany. — [2]University of California, Santa Barbara, USA.

Molecular beam epitaxy of bixbiyte In_2O_3 on (001) oriented ZrO_2:Y (YSZ) substrates typically results in {111} faceted surfaces whereas on (111) smooth films are obtained [1]. This behavior has been explained by theory calculations that found the surface free energies of low index bixbiyte surfaces to increase from (111) to (011) to (001) surfaces [2]. On the other hand, it was found that In-rich growth conditions [1] or high Sn-doping [6] lead to the formation of smooth, unfaceted (001) In_2O_3 films on YSZ(001). These results are in-line calculations of stoichiometry-dependent surface free energy [5]. Our experimental study of In_2O_3 on YSZ(001), (011), (111) grown by MBE under O-rich, In-rich and high Sn-doping conditions suggest the following relative surface free energies: (111) lowest under all conditions, (001) significantly lowered by In-rich conditions and Sn-doping. A flat (011) surface was not observed suggesting a higher surface free energy than predicted by theory. Our experimental results compare well to theory of [5]. [1] Bierwagen, Appl. Phys. Lett. 95, 262105 (2009). [2] Walsh and Catlow, J. Mater. Chem. 20, 10438 (2010). [4] Bierwagen and Speck, J. Appl. Phys. 107, 113519 (2010). [5] Agoston and Albe, Phys. Rev. B 84, 045311 (2011). [6] Taga, Jpn. J. Appl. Phys. 37, 6585 (1998).

DS 30.12 Wed 18:30 POT 081

Surface structure of metal oxides via classical and quantum mechanical rainbow scattering — •Marco Busch[1], Eric Meyer[1], Jan Seifert[1], Helmut Winter[1], Klaus Irmscher[2], and Zbigniew Galazka[2] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstrasse 15, D-12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Strasse 2, D-12489 Berlin, Germany

Fast light atoms and molecules with energies from 200 eV up to several tens of keV are grazingly scattered from clean and flat metal oxide surfaces. 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. As examples, we present investigations of the quantum scattering from the cleaved (100) surface of β-Ga$_2$O$_3$ 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 atoms in the topmost surface layer. Furthermore, diffraction effects were present in the regime of surface channeling, where quantum scattering is considered for the motion parallel to the surface. For the thermal induced reconstruction of the (11$\bar{2}$0) and (0001) surface of Al$_2$O$_3$ we found also a preservation of the longitudinal coherence and observed Laue circles of higher orders.

DS 31: Focus Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale V (jointly with O)

Time: Wednesday 16:00–19:15 Location: TRE Ma

Topical Talk DS 31.1 Wed 16:00 TRE Ma

Theory of nonlinear phononics for coherent light-control of solids — •Antoine Georges[1,2,3], Alaska Subedi[2], and Andrea Cavalleri[4] — [1]College de France, Paris, France — [2]Ecole Polytechnique - CPHT, Palaiseau, France — [3]University of Geneva, DPMC, Switzerland — [4]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

The use of light to control the structural and electronic properties of solids is an area of great current interest. We present a microscopic theory [arXiv:1311.0544] for ultrafast control of solids with high-intensity Tera-Hertz frequency optical pulses. When resonant with selected infrared-active vibrations, these pulses transiently modify the crystal structure and lead to new collective electronic properties. The theory predicts the dynamical path taken by the crystal lattice using first-principles calculations of the energy surface and classical equations of motion, as well as symmetry considerations. Two classes of dynamics are identified. In the perturbative regime, displacements along the normal mode coordinate of symmetry-preserving Raman-active mode can be achieved by cubic anharmonicities. This validates the mechanism proposed by Först et al. [Nature Physics 7, 854 (2011)] and explains the light-induced insulator-to-metal transition of manganites reported experimentally by Rini et al. [Rini et al. Nature 449, 72 (2007)]. We also predict a new non-perturbative regime in which ultra-fast instabilities that break crystal symmetry can be induced.

DS 31.2 Wed 16:30 TRE Ma

DFT+Frontier Orbital U — •Emine Kucukbenli and Nicola Marzari — Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH)

Piecewise linearity of the total energy with respect to occupations is not only a fundamental property that should be obeyed by any exact energy functional, but also a starting point to improve approximate functionals that are used in practical applications.

DFT+U enforces piecewise linearity on the Hubbard manifold [1], and it has been shown to greatly improve the accuracy of density-functional theory for transition-metal complexes, thanks to its correction of self-interaction errors [2]. However, it still performs poorly in complexes where significant covalency is present, and intersite corrections (so-called DFT+U+V) have been introduced to improve these challenging cases [3].

Here, we revisit piecewise linearity within the DFT+U and DFT+U+V correction schemes, and explore a novel approach where self-interaction corrections are applied directly to the frontier orbitals. We test this approach on model transition metal complexes, where highly accurate reference results can be established, and on small molecules with varying degrees of covalency.

References: [1] M. Coccoccioni and S. de Gironcoli, Phys. Rev. B 71, 35105 (2005). [2] H. J. Kulik, M. Cococcioni, D. A. Scherlis and N. Marzari, Phys. Rev. Lett. 97, 103001 (2006). [3] V. Leiria Campo Jr and M. Cococcioni, J. Phys. Cond. Matt. 22, 055602 (2010); H. J. Kulik and N. Marzari, J. Chem. Phys. 134, 094103 (2011).

DS 31.3 Wed 16:45 TRE Ma

Quasiparticle self-consistent *GW* method with spin-orbit coupling applied to Bi and HgTe — •Christoph Friedrich, Irene Aguilera, Markus Betzinger, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present an implementation of the quasiparticle self-consistent (QS) *GW* method where the spin-orbit coupling (SOC) is fully taken into account in each iteration rather than being added *a posteriori*. The implementation is based on the FLAPW method. The SOC gives rise to spin off-diagonal blocks in the Green function G^{SOC} and the self-energy $\Sigma^{\mathrm{SOC}} = iG^{\mathrm{SOC}}W^{\mathrm{SOC}}$. We applied the QS$G^{\mathrm{SOC}}W^{\mathrm{SOC}}$ method to the semimetal Bi, which presents in experiment small electron and hole pockets and a tiny band gap (11-15 meV) at the L point, all of them largely overestimated by LDA (e.g., the gap is 86 meV). The QS$G^{\mathrm{SOC}}W^{\mathrm{SOC}}$ approach predicts a value of the band gap of 8 meV and electron and hole pockets in very good agreement with experiment. The *a posteriori* treatment of the SOC (QS*GW*+SOC), on the other hand, yields an unphysical result for Bi, predicting it to be a topological insulator with a very large gap at L (260 meV) instead of a trivial semimetal. Similarly, for HgTe, QS*GW*+SOC reorders the bands in a wrong way and opens a gap at the Γ point in disagreement with experiment. In contrast, the QS$G^{\mathrm{SOC}}W^{\mathrm{SOC}}$ approach yields a qualitatively and quantitatively correct description of the electronic band structure. We acknowledge support from the Helmholtz Association through the Virtual Institute for Topological Insulators (VITI).

DS 31.4 Wed 17:00 TRE Ma

Studies of semiconducting pyrite and marcasite compounds using many-body perturbation theory in the *GW* approximation — •Timo Schena, Gustav Bihlmayer, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Germany

FeS$_2$ pyrite and marcasite have recently gained renewed interest as materials for photovoltaic applications, due to their large optical absorption and abundance. Therefore, a reliable description of the fundamental band gap of these compounds within first-principles calculations is desirable. However, common density functional theory (DFT) often suffers from an underestimation of band gaps. This calls for beyond-DFT methods, *e.g.*, the *GW* approximation, which is known to yield gaps in much better agreement with experiment. Although this is widely accepted for "simple" semiconductors, the situation is not well understood for more complicated cases, where the band edges differ in atomic and orbital character. In fact, we observe an uncommon band gap reduction in FeS$_2$ when applying single-shot *GW* on top of DFT, which might be problematic for photovoltaic applications [1]. In this work, we investigate the effects of the *GW* approximation on a couple of pyrite and marcasite compounds, employing the FLAPW code `FLEUR` and the *GW* code `SPEX` (www.flapw.de). In addition to single-shot *GW*, we also compare to the results of the recently implemented quasi-particle self-consistent *GW* approximation. We gratefully acknowledge funding from BMBF of the NADNuM project 03SF0402A.

[1] T. Schena *et al.* Physical Review B (accepted 2013)

15 min. break

DS 31.5 Wed 17:30 TRE Ma

Probing d-band Quantum Well States in Palladium Nanofilms — •Srijan Kumar Saha[1], Sujit Manna[1], Marek Przybylski[1,2], Valeri Stepanyuk[1], and Jurgen Kirschener[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, 30-059 Kraków, Poland — [3]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

We present the results of our new study which probes the d-bands quantum well (QW) states in Pd nanofilms grown on Cu(001) using first-principles density functional theory (DFT) calculations combined with scanning tunneling spectroscopy (STS) experiments. This study reveals that QW states occur in the overlayer films of Pd over a strikingly large film thickness (up to 17 monolayers) and in a large binding energy range (from 0.1 to 3.0 eV below Fermi level), thanks to its distinct and broad 4d-bands. The orbital characters of these states are unambiguously identified by our DFT calculations. Calculations also demonstrate oscillatory multilayer relaxations and d-derived quantum size oscillations in Pd films. The pseudomorphic growth, well-defined interface, and spatially resolved STS allows us to probe individual occupied QW states and extract the accurate dispersion of the (Δ_5-like) d electronic band, as these states are laterally highly localized and give rise to distinct and sharp feature in the tunneling spectra.

DS 31.6 Wed 17:45 TRE Ma

Implementation and analysis of a plane wave and real space pseudopotential method including an efficient spin-orbit coupling treatment tailored to calculate the electronic structure of large-scale semiconductor nanostructures — •Frank Zirkelbach, Pierre-Yves Prodhomme, Jerome Jackson, and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

The implementation of the *large-scale atomic effective pseudopotential program* to solve the Schrödinger equation of an electronic system is discussed. *Atomic effective pseudopotentials* that are derived from screened local effective crystal potentials of self-consistent density functional theory (DFT) calculations are utilized, which ensure an accurate treatment at reduced computational costs. The capability of describing relevant electronic eigenstates of a quantum dot structure consisting of hundred thousand atoms at an atomistic *ab initio* level comparable to DFT is demonstrated. The possibility to represent the wavefunction and to evaluate parts of the Hamiltonian either in a plane wave or real space basis allows for a coherent analysis of various different approaches. In the fully real space treatment, linear scaling with respect to the system size is achieved. The convergence behavior of the different methods and utilized approximations is shown. Furthermore, an efficient spin-orbit treatment different to previously existing implementations within the pseudopotential formalism is outlined. The accuracy of the method is demonstrated via direct comparison to standard DFT codes.

DS 31.7 Wed 18:00 TRE Ma

Strong Parallelization of Real-Space DFT Calculations — •Andrea Nobile[1,2], Paul Baumeister[1,2], Daniel Wortmann[1], and Stefan Blügel[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Jülich Supercomputing Center, Forschungszentrum Jülich, 52425 Jülich, Germany

The rapid change in modern supercomputing architectures poses a challenge to well established DFT codes. In particular, the increase in raw floating point power obtained through parallelism at different levels is not easily exploitable by using the traditional direct diagonalization methods. We will present our new real-space Projector Augmented Wave (PAW) implementation. The real-space representation of the wave functions, densities and potentials, enables the usage of very flexible boundary conditions and naturally adapts to massively parallel architectures. Parallelism can be exploited in the form of domain decomposition of the three dimensional grid, k-point sampling and bands. The kinetic energy operator, realized as a finite difference stencil, is localized. As a consequence the real-space representation of the Hamiltonian is sparse. This limits the amount of necessary communications and allows an application of the operator to a trial vector in order(N) operations. We will present results about the efficiency of the most numerical intensive parts of the code and we will compare the accuracy of the calculations for reference systems with other established DFT methods.

DS 31.8 Wed 18:15 TRE Ma

Rare Earth Metals in Density-Functional Theory — •Marco Casadei[1], Xinguo Ren[2], Patrick Rinke[1], Angel Rubio[1,3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Technology, Hefei, China — [3]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

The presence of f electrons in the rare earths and their interaction with the s and p electrons give rise to several physical phenomena. One prominent example is the isostructural α-γ phase transition in cerium (Ce). We have shown that density-functional theory (DFT) captures the volume collapse associated with the transition, but only if advanced functionals such as exact exchange plus correlation in the random-phase approximation (EX+cRPA) are used [1]. The volume collapse is understood in terms of a *localization/delocalization* of the f electrons. We then addressed the question: *is the isostructural volume collapse in cerium unique*? By applying DFT, we studied lanthanum (La), praseodymium (Pr) and neodymium (Nd), which undergo several structural changes with pressure. We find that the transitions are already captured at a lower level of DFT (i.e. with (semi)-local functionals) and therefore conclude that f-electrons are not the driving force in this case. Within hybrid functionals, we find only one phase in lanthanum, which has no f-electrons, and more than one stable solution in the fcc crystal for Pr and Nd, as found for Ce. Unlike in Ce, however, there is always one solution that is the most stable, thus no isostructural volume collapse emerges in agreement with experiments. [1] M. Casadei *et al.*, Phys. Rev. Lett. **109**, 14642 (2012).

DS 31.9 Wed 18:30 TRE Ma

Electronic Structure and van der Waals Interactions in the Stability and Mobility of Point Defects in Semiconductors — •Wang Gao and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Point defects are abundant in materials, and significantly affect the electronic, optical, and magnetic properties of solids. However, our understanding of the stability and mobility of point defects remains incomplete, despite decades of intensive work on the subject. In the framework of density-functional theory, Perdew-Burke-Ernzerhof functional underestimates formation energies by 0.7 eV due to the electron self-interaction error, while Heyd-Scuseria-Ernzerhof (HSE) functional yields formation energies in better agreement with high-level many-body methods, but often overestimates migration barriers by up to 0.4 eV.

Using HSE coupled with screened long-range vdW interactions [1], we demonstrate that HSE+vdW can simultaneously and accurately describe the formation energies and migration barriers of point defects. The inclusion of vdW interactions significantly changes the transition state geometries, and brings migration barrier into close agreement with experimental values for six different defects. For multiatom vacancies and point defects in heavier semiconductors, vdW interactions play an increasingly larger role [2].

[1] G. X. Zhang, *et al.*, PRL **107**, 245501 (2011); A. Tkatchenko, *et al.*, PRL **108**, 236402 (2012).

[2] W. Gao and A. Tkatchenko, PRL **111**, 045501 (2013).

DS 31.10 Wed 18:45 TRE Ma

Scaling Laws for van der Waals Interactions in Nanostructured Materials — •Vivekanand Gobre and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Berlin

Accurate description of van der Waals (vdW) interactions is crucial for precise prediction of structure and stability of complex materials. VdW forces originate from interactions between fluctuating multipoles in matter and play a significant role in the self-assembly of nanostructured materials. Many models used to describe vdW interactions in nanomaterials are based on a simple pairwise-additive approximation, neglecting the strong electrodynamic response effects caused by long-range fluctuations in matter. We develop and utilize an efficient microscopic method [1,2] to demonstrate that vdW interactions in nanomaterials act at distances greater than typically assumed, and can be characterized by different scaling laws depending on the dimensionality and size of the system. Specifically, we study the behaviour of vdW interactions in single-layer and multilayer graphene, fullerenes of varying size, single-wall carbon nanotubes and graphene nanoribbons. As a function of nanostructure size, the van der Waals coefficients follow unusual trends for all of the considered systems, and deviate significantly from the conventionally employed pairwise-additive picture. We propose that the peculiar van der Waals interactions in nanostructured materials could be exploited to control their self-assembly. [1] Tkatchenko, DiStasio, Car, and Scheffler, PRL (2012); [2] Gobre, Tkatchenko, Nat. Commun. (2013).

DS 31.11 Wed 19:00 TRE Ma

2D nanopatterns of shape-persistent molecular polygons on

HOPG — •Stefan-S. Jester, Nina Schönfelder, Eva Sigmund, and Sigurd Höger — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Shape-persistent organic molecules with flexible side chains self-assemble at the solution/solid interface to form 2D nanoarchitectures. Scanning tunneling microscopy yields a submolecularly resolved insight into the adsorbate structures. A key issue is how the shape and symmetry of the backbones and their alkyl chain substitution pattern determine the shape and symmetry of the adsorbate patterns. Recently we focused on molecular polygons (triangles, squares, pentagons, and hexagons) with dithiophene corners and phenylene-alkynylene sides.[1] In my talk I will give insight into the relation between Archimedean surface patterns and supramolecular 2D adlayers. [1] S.-S. Jester, E. Sigmund, S. Höger *J. Am. Chem. Soc.* **2011**, *133*, 11062.

DS 32: Focus session: Resistive Switching by Redox and Phase Change Phenomena III (Defect and material engineering in oxides)

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

DS 32.1 Wed 15:00 CHE 89

Towards selective ion beam modification of vanadium dioxide — •Jura Rensberg, Ronny Nawrodt, Sebastian Vatterodt, Jana Sommerfeld, Alexander von Müller, and Carsten Ronning — Institut of Solid State Physics, Friedrich Schiller University Jena, Germany

Vanadium dioxide VO_2 undergoes a metal-insulator transition (MIT) at a critical temperature of about 68°C. The MIT induces significant changes in electrical, optical and structural properties making VO_2 thin films promising for integrated devices as switches, sensors, and memories. The critical temperature can be decreased by doping with electron donors like tungsten. However, doping of VO_2 thin films during growth is limited to vertical incorporation of dopant profiles. In contrast, ion beam doping allows also for lateral doping using suitable masking technique. Furthermore, the dopant concentration and implantation depth can be well controlled. The major disadvantage of doping by ion implantation is the creation of irradiation damage, making in-situ or post implantation annealing necessary. Here we report on noble gas ion irradiation of VO_2 thin films. Damage formation was studied using Rutherford backscattering spectrometry. Electrical and optical measurements were performed in order to investigate the change of MIT properties. It was found that damage formation leads to a degradation of MIT properties. Irradiation at higher temperatures utilizing dynamic annealing is not applicable due to oxygen outdiffusion in high-vacuum. Furthermore, post implantation annealing studies will be discussed in this contribution.

DS 32.2 Wed 15:15 CHE 89

Towards forming free switching in HfO_{2-x}/TiN thin films grown by molecular beam epitaxy — •S Ulhas Sharath[1], Thomas Bertaud[2], Jose Kurian[1], Erwin Hildebrandt[1], Christian Walczyk[2], Pauline Calka[2], Peter Zaumseil[2], Malgorzata Sowinska[2], Damian Walczyk[2], Andrei Gloskovskii[3], Thomas Schroeder[2], and Lambert Alff[1] — [1]Materialwissenschaft, Technische Univerität, Darmstadt — [2]IHP, Frankfurt/Oder, Germany — [3]Deutsches Elektronen-Synchroton DESY, Hamburg, Germany

Oxygen deficient thin films of hafnium dioxide (HfO_2) were grown using reactive molecular beam epitaxy on epitaxial and polycrystalline titanium nitride films with varying thicknesses and deposition temperatures. The oxygen content was engineered by controlled oxidation using RF-activated oxygen during growth [1]. The crystallinity of the films was studied using X-ray diffraction. Under oxygen deficient conditions, a mixture of monoclinic and tetragonal or cubic phases of HfO_2 was stabilized whereas close to stoichiometric films were purely monoclinic. The films were further probed using hard X-ray photoelectron spectroscopy (HAXPES) confirming the presence of sub-stoichiometric hafnium oxide and defect states near the Fermi level. Resistive switching in Pt/HfO_{2-x}/TiN stack devices was then studied for different electrode size, thickness and crystallinity of the HfO_2 thin films. Oxygen deficient hafnium oxide thin films show bipolar switching with an electroforming step occurring at voltages less than 2V and slightly higher than the set voltage. [1] E. Hildebrandt et al., Appl. Phys. Lett. 99, 112902 (2011).

DS 32.3 Wed 15:30 CHE 89

Defects behavior in HfO_2-based resistive switching devices — •Małgorzata Sowińska[1], Thomas Bertaud[1], Damian Walczyk[1], Andrei Gloskovskii[2], Pauline Calka[1], Lambert Alff[3], Christian Walczyk[1], and Thomas Schroeder[1,4] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]P09 beamline at Petra III (DESY), Notkestrasse 85, 22607 Hamburg, Germany — [3]Institute of Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Str. 2, 64287 Darmstadt, Germany — [4]Brandenburgische Technische Universität, Konrad-Zuse-Strasse 1, 03046 Cottbus, Germany

In-operando hard X-ray photoelectron spectroscopy (HAXPES)[1,2] is applied to non-destructively study the influence of current compliance and switching cycles on the Ti/HfO_2 interface chemistry and physics of resistive switching Ti/HfO_2/TiN cells. The HAXPES studies confirm theoretical results that current compliance is a crucial parameter to create a critical amount of oxygen vacancies in order to achieve stable resistive switching. Furthermore, HAXPES clearly detects an interface segregation of carbon impurities from the HfO_2 film towards the Ti/HfO_2 interface under electrical stress by current compliance and over the cycling. As carbon impurities may thus alter the oxygen vacancy defect balance in the HfO_2 film during resistive switching, materials engineering approaches need to include all major impurities in the dielectric to achieve reproducible and reliable resistive random access memory performance.

[1] M. Sowinska et al., Appl. Phys. Lett. 100, 233509 (2012).

[2] T. Bertaud et al., Appl. Phys. Lett. 101,143501 (2012).

DS 32.4 Wed 15:45 CHE 89

Oxygen engineered HfO_{2-x} as a CMOS compatible candidate for resistive switching — •Erwin Hildebrandt[1], S. U. Sharath[1], Jose Kurian[1], Mathis M. Mueller[1], Thomas Schroeder[2], Hans-Joachim Kleebe[1], and Lambert Alff[1] — [1]Institute of Material Science, Technische Universität Darmstadt, Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany — [2]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

Reactive molecular beam epitaxy has been applied to grow stoichiometric and oxygen deficient thin films of hafnium oxide. Films as thin as 10 nm were grown epitaxially on *c*-cut sapphire, proven by grazing incidence in-plane X-ray studies and high resolution transmission electron microscopy. As a function of oxygen vacancy concentration, the optical band gap varies by more than 1 eV and a sharp metal-insulator transition occurs. Hall-effect measurements indicate *p*-type conductivity with a mobility of 2 $cm^2/(Vs)$ for highly deficient thin films [1, 2]. The high oxygen vacancy concentrations - which are formed and stabilized *in situ* during the RMBE deposition process - lead to intrinsic resistivities as low as 300 $\mu\Omega$cm. We propose oxygen deficient hafnia thin films driven to the vicinity of the metal-insulator transition as a promising candidate for the functional layer of potentially forming-free and CMOS compatible resistive RAM devices.

[1] E. Hildebrandt, J. Kurian, M. M. Müller, T. Schroeder, H.-J. Kleebe, and L. Alff, Appl. Phys. Lett. **99**, 112902 (2011)

[2] E. Hildebrandt, J. Kurian, and L. Alff, J. Appl. Phys. **112**, 114112 (2012)

DS 32.5 Wed 16:00 CHE 89

Resistive switching of flash lamp crystallized $YMnO_3$ thin films prepared on Pt/Ti/SiO_2/Si substrates by low-temperature pulsed laser deposition — •Agnieszka Bogusz[1,2], Sławomir Prucnal[1], Wolfgang Skorupa[1], Daniel Blaschke[1], Barbara Abendroth[3], Hartmut Stöcker[3], Ilona Skorupa[1], Danilo Bürger[2], Oliver G. Schmidt[2,4], and Heidemarie Schmidt[2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — [2]Material Systems for Nanoelectronics, Chemnitz University of Technology — [3]Institute of Experimental Physics, TU Bergakademie Freiberg — [4]Institute for Integrative Nanosciences, IFW Dresden

Use of multiferroic oxides as a switching medium presents an opportunity to add the additional or novel functionalities into the switching device. Typically, the growth temperatures of such oxides are above 600 °C and so far CMOS compatibility has not been achieved. $YMnO_3$ exhibits unipolar resistive switching [1] however its high crystallization temperature (above 750°C) imposes difficulties in preparation of thin films on metal-coated substrates. This work presents the results of electrical and structural characterization of $YMnO_3$ thin films grown on $Pt/Ti/SiO_2/Si$ substrates by pulsed laser deposition at 400 °C and crystallized by flash lamp annealing (FLA). It is shown that the FLA process with optimized parameters allows the preparation of polycrystalline $YMnO_3$ films without deformation of the Pt/Ti electrode and interdiffusion processes in the $YMnO_3/Pt/Ti/SiO_2$ stack.

[1] A. Bogusz et al., IEEE Xplore (2013), DOI:10.1109/ISCDG.2013.656319

DS 32.6 Wed 16:15 CHE 89

Resistive Switching in TiO_2: Comparison of thermally oxidized and magnetron sputtered films — •Daniel Blaschke[1,2], Steffen Cornelius[1], Peter Zahn[1], Sibylle Gemming[1,2], Ilona Skorupa[1], Bernd Scheumann[1], Andrea Scholz[1], and Kay Potzger[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Chair of Scale-bridging Materials Modeling, Physics Department, Chemnitz University of Technology, Germany

Resistive RAM devices based on TiO_2 are promising candidates for the next generation memory storage devices. We compared TiO_2 thin films from two different preparation methods with respect to crystallinity and resistive switching behavior. While thermal oxidation of 100nm Ti on $Pt/Ti/SiO_2/Si$ substrates leads to polycrystalline rutile TiO_2 layers, dc-magnetron sputter deposition of films on Nb:STO substrates leads to epitaxial anatase TiO_2 structure. In case of the rutile films, unipolar switching occurred, which points to a filamentary mechanism based on the formation of Magnéli phases [1]. The epitaxial anatase films, however, showed bipolar switching, which we correlated with the modification of the metal/oxide interface due to the drift of oxygen vacancies in the applied electric field [2].

The project is funded by the Initiative and Networking Fund of the Helmholtz Association (VI MEMRIOX, VH-VI-422).

[1] Deok-Hwang Kwon et al., Nature Nanotechnology 5, 148 - 153 (2010)

[2] J. Joshua Yang et al., Nature Nanotechnology 3, 429 - 433 (2008)

DS 33: Focus session: Resistive Switching by Redox and Phase Change Phenomena IV (Kinetic in oxides and phase change)

Time: Wednesday 16:45–18:15 Location: CHE 89

DS 33.1 Wed 16:45 CHE 89

Evidence for power-dependent SET kinetics in valence change memories — •Stephan Menzel[1,2], Karsten Fleck[2,3], Ulrich Böttger[2,3], and Rainer Waser[1,2,3] — [1]Forschungszentrum Jülich GmbH, Jülich, Germany — [2]Institut für Werkstoffe der Elektrotechnik II, RWTH Aachen University, Germany — [3]JARA - Fundamentals of Future Information Technology, Jülich, Germany

Resistively switching thin oxide films based on the valence change mechanism (VCM) have attracted great attention for the potential use in future nonvolatile information storage. The oxide thin film resistance can be tuned by applying appropriate voltages, where the different resistance state encodes the digital information. The VCM cell stack typically consists of Metal-Insulator-Metal structure, whereas the I-layer is a thin oxide layer, e.g. TiOx, HfOx, TaOx or SrTiOx. The resistance change is initiated by migration of ions such as oxygen vacancies within the oxide layer and a subsequent valence change in the cation sublattice. It takes place locally along nanoscale filaments within the I-layer. VCM cells exhibit a highly nonlinear switching kinetics which origins in the temperature accelerated drift of oxygen vacancies. In this paper switching kinetics data of SrTiOx based devices at varying ambient temperature are presented that cover >10 orders of magnitude in switching time. The switching kinetics data is analyzed using a multidimensional electro-thermal simulation model. It is demonstrated that the switching kinetics are driven by the electric power rather than the applied voltage or electric field. The electric power is dissipated as Joule heat that accelerates the ion movement.

DS 33.2 Wed 17:00 CHE 89

Memristive tunnel junctions — •Mirko Hansen, Martin Ziegler, and Hermann Kohlstedt — Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel, Germany

We present results on a device concept which consists of a tunnel barrier and a thin titanium oxide layer in between two metal electrodes. In our device, oxygen vacancies are supposed to be confined between the tunnel barrier and the top electrode. This limits the distance of the oxygen vacancy drift under an applied electric field to the thickness of the titanium oxide. We discuss results on junctions with the layer sequence $Nb/Al/Al_2O_3/TiO_{2-x}/TE$ and the influence of different top electrode (TE) materials. First electrical measurements indicate a homogenous change in resistance without the formation of a conductive filament. These samples were prepared on 4″ wafers using standard optical lithography, (reactive) DC sputtering and reactive ion/wet etching.

DS 33.3 Wed 17:15 CHE 89

Doping and resistive switching effects induced by carrier injection in high temperature superconductors — •Irina Lazareva[1], Yilmaz Simsek[1], Yury Koval[1], Paul Müller[1], Sabine Wurmehl[2], Bernd Büchner[2], Tobias Stürzer[3], and Dirk Johrendt[3] — [1]Universität Erlangen-Nürnberg, Erlangen, Deutschland — [2]IFW, Dresden, Deutschland — [3]LMU, München, Deutschland

Doping by current injection was investigated in various high temperature superconductors. Only by injection of large currents along the c-axis we were able to change carrier concentration in $Bi_2Sr_2CaCu_2O_{8+\delta}$ cuprate as well as in $LaO_{1-x}F_xFeAs$ and $Ca_{10}(FeAs)_{10}(Pt_4As_8)$ pnictides. The doping effect is persistent and reversible resembling the resistive-memory switching phenomena observed in various oxides. The mutual influence of chemical doping and change of the charge carrier concentration by current injection is analyzed. The general tendency of carrier doping by trapped electrons is discussed.

DS 33.4 Wed 17:30 CHE 89

Optical and structural dynamics of the phase transition of GST phase change materials — •Lutz Waldecker[1], Timothy Miller[2], Roman Bertoni[1], Simon Wall[2], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]ICFO - Institut de Ciències Fotòniques, Castelldefels (Barcelona), Spain

The phase change material $Ge_2Sb_2Te_5$ (GST) exhibits large changes in its optical properties across the structural phase transition between its amorphous and crystalline phases. We investigate the transient behavior of the optical properties of GST after laser excitation below and above the threshold for persistent switching of the crystalline phase of the material by applying femtosecond transient reflectivity spectroscopy. In addition, we measure the electron-lattice coupling with time-resolved electron diffraction for separating electronic from structural contributions to the optical response. The combination of these two techniques allows for investigating the correlation between structure and function and addressing the question whether the phase transition is driven thermally or non-thermally.

DS 33.5 Wed 17:45 CHE 89

Ab initio molecular dynamics simulations of crystallization of AIST — •Wei Zhang[1], Ider Ronneberger[1], Peter Zalden[2,3], Martin Salinga[2], Matthias Wuttig[2,4], and Riccardo Mazzarello[1,4] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52056 Aachen, Germany — [2]I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany — [3]School of Medicine, Stanford University, Stanford, CA 94305, USA — [4]JARA, RWTH Aachen University, D-52056 Aachen, Germany

Chalcogenide phase change materials (PCMs) are of great interest for both industrial applications and fundamental research, owing to their remarkable properties. The ultrafast switching capability between amorphous and crystalline state together with the pronounced property contrast between the two states has led to applications in optical data storage as well as electronic non-volatile memories. In this work, we investigate the fast crystallization process of Ag, In-doped Sb2Te (AIST) using ab initio molecular dynamics (AIMD). We find a good match between the computed growth velocities and recent time-resolved reflectivity measurements at high temperature (550K-600K), while large deviations are present at lower temperature. We suggest that the large deviations are due to the different quenching rates and the high fragility of AIST in the supercooled phase. Besides, we identify the role of impurities (Ag/In) in the crystallization process of AIST at high temperature.

DS 33.6 Wed 18:00 CHE 89

Ab initio metadynamics simulation of phase change materials — •Ider Ronneberger, Wei Zhang, and Riccardo Mazzarello — Institute for Theoretical Solid State Physics, RWTH Aachen University

The microscopic description of the fast crystallization mechanism of phase change materials (PCMs) at elevated temperatures remains a challenge to both experimentalists and theorists. The computational limitation of ab initio Molecular Dynamics (AIMD) simulations in terms of system size and time scale can be partly overcome by the aid of enhanced sampling methods such as Metadynamics (MTD), which accelerates the exploration of the phase space and extracts estimations of the free energy changes involved in the process of interest. We study the crystallization of prototypical PCMs by means of AIMD and Well-Tempered MTD. MTD is used to enforce the formation of supercritical crystalline nuclei. The growth of the nuclei is subsequently investigated in unbiased AIMD runs.

DS 34: Focus Session: Resistive Switching by Redox and Phase Change Phenomena V (Structure, growth and general properties of PC materials)

Time: Wednesday 18:30–20:00 Location: CHE 89

Invited Talk DS 34.1 Wed 18:30 CHE 89

Materials engineering for phase change memory — •Simone Raoux[1] and Huai-Yu Cheng[2] — [1]IBM/Macronix PCRAM Joint Project, IBM T. J. Watson Research Center, P. O. Box 218, Yorktown Heights, NY 10598, USA — [2]IBM/Macronix PCRAM Joint Project, Macronix International Co., Ltd., Emerging Central Lab., 16 Li-Hsin Rd., Science Park, Hsinchu, Taiwan, ROC

Phase change memory is an emerging storage technology based on the unique combination of properties of phase change materials. Phase change materials exist an amorphous and a crystalline phase with distinctly different properties, and it is possible to switch the material repeatedly and rapidly between these two phases. The large difference in electrical resistance is used on phase change memory to store information. Phase change memory can have several potential applications such as storage class memory, embedded memory, replacement of DRAM (dynamic random access memory). We have explored various novel phase change materials and optimized their properties for specific applications. These materials include Ge-Sb-Te based alloys and Ga-Sb based alloys. A overview of the materials properties as function of composition is given with a focus on materials for high temperature applications, materials for high cyclability, and materials for ultra-fast switching.

DS 34.2 Wed 19:00 CHE 89

Application of the Mössbauer effect in Ge-Sb-Te and Sn-Sb-Te phase change materials — •Ronnie Ernst Simon[1,2], Ilya Sergueev[3], and Raphaël Pierre Hermann[1,2] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, Jara-FIT Forschungszentrum Jülich GmbH, D-52425 Jülich Germany — [2]Faculté des Sciences, Université de Liège, B-4000 Liège, Belgium — [3]Deutsches Elektronen-Synchrotron, D-22607 Hamburg, Germany

Phase change materials exhibit a significant change of the electrical resistivity upon crystallization which renders these materials promising candidates for resistive switches and non-volatile electronic memories. In order to understand the switching mechanism between the amorphous and crystalline phases a detailed knowledge of the structure on a microscopic scale is crucial. Mössbauer spectroscopy and nuclear forward scattering of synchrotron radiation which are both based on the application of the Mössbauer effect are suitable techniques for local structure investigations. We performed conventional ^{121}Sb Mössbauer spectroscopy and ^{73}Ge and ^{119}Sn nuclear forward scattering measurements in Ge-Sb-Te and Sn-Sb-Te phase change materials in order to study hyperfine interactions. Measurements were performed as a function of temperature, stoichiometry and crystallinity and reveal valence changes upon crystallization. The DESY (Petra III, P01) and ESRF (ID18) are acknowledged for the provision of beamtime.

DS 34.3 Wed 19:15 CHE 89

Atomic resolution investigation of defect structures in textured metastable $Ge_2Sb_2Te_5$ by aberration corrected high resolution STEM — •Ulrich Ross, Andriy Lotnyk, Erik Thelander, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e.V. Permoserstr. 15 D-04318 Leipzig

Local features in the structure of phase change materials (PCM) are of foremost importance for the characteristic phase transformation mechanics made use of in data storage applications. Specifically, distribution of vacancies as well as stabilization of an ordered sublattice in the amorphous and metastable phase are believed to significantly influence the performance of PCM-based devices. However, very few studies have been able to resolve the local nanostructure in an experimental setting.

We have employed a state of the art FEI Titan^3 G2 60-300kV probe aberration corrected transmission electron microscope in order to investigate the atomic structure of pulsed laser deposited metastable $Ge_2Sb_2Te_5$ (GST) with sub-angstrom resolution. Quantitative image simulations were carried out in order to evaluate local chemical information. The results of the investigation are discussed in the context of past and current structure models of metastable GST, and a brief outlook on the possibility of in-situ heating atomic resolution imaging experiments is given.

DS 34.4 Wed 19:30 CHE 89

Metal Organic Chemical Vapour Deposition of monocrystalline $Ge_1Sb_2Te_4$ (GST) and Sb_2Te_3 — •Martin Schuck[1,2], Sally Riess[1,2], Marcel Schreiber[1,2], Gregor Mussler[1,2], Toma Stoica[1,2], Hilde Hardtdegen[1,2], and Detlev Grützmacher[1,2] — [1]Peter Grünberg Institut 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technology

GST is considered as one of the most promising materials for non-volatile phase-change memories. The phase change between its amorphous and crystalline phase is switched by current pulses of different intensity and duration. For this application the alloys along the $GeTe-Sb_2Te_3$ pseudobinary are the most suitable, since they are characterized by fast switching speed and high scalability. Their crystallization characteristics are determined by their composition, which therefore needs to be controlled.

Here we present the MOCVD growth of $Ge_1Sb_2Te_4$ (GST) and Sb_2Te_3 on Si(111) substrates using triethylantimony (TESb), diethyltelluride (DETe) and digermane as precursors and pure N_2 as the carrier gas. A systematic variation of reactor pressure and growth temperature was carried out to obtain crystalline flat layers of only one composition. The deposited material was characterized by means of X-Ray Diffraction, Raman spectroscopy, atomic force and scanning electron microscopy. It was found that, depending on the growth temperature, at low reactor pressure only 2 alloys were found: $Ge_1Sb_2Te_4$ (GST) and Sb_2Te_3. The study on the influence of the growth parameters on material properties will be presented.

DS 34.5 Wed 19:45 CHE 89

Thermal annealing studies on GeSbTe alloy-films grown on Si(111) by Molecular Beam Epitaxy — •Valeria Bragaglia, Rui Ning Wang, Jos Boschker, and Raffaella Calarco — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Phase change materials are already a well established technology for data storage, in virtue of the strong optical and electrical contrast exhibited between the amorphous and the crystalline phase; additionally the switching between those two states can take place fast and reversibly. The study and comprehension of the crystallization process is then of fundamental importance. Effects of thermal crystallization on the structure of GST alloys have been widely studied. In general the films used in those investigations are produced by sputtering technique and grown on Si substrates with native SiO_2. The resulting crystalline phase is thus polycrystalline.

In this study we present the structural change upon annealing of amorphous and metastable-cubic GST films deposited on Si(111) by molecular beam epitaxy. High degree of ordering in the out-of-plane direction is achieved by annealing an amorphous GST film deposited on Si(111), as opposed to previous annealing experiments on GST deposited on non crystalline substrates. Additional annealing experiments were performed in order to find the best way to improve the quality of the GST films and find out a possible model of crystallization.

DS 35: Poster I: Application of thin films; Focus session: Sensoric micro and nano-systems; Focus Session: Sustainable photovoltaics with earth abundant materials; Graphen (joint session with TT; MA; HL; DY; O); Ion and electron beam induced processes; Layer properties: electrical, optical, and mechanical properties; Magnetic/organic interfaces, spins in organics and molecular magnetism; Micro- and nanopatterning (jointly with O); Organic electronics and photovoltaics (jointly with CPP, HL, O); Thermoelectric materials

Time: Wednesday 17:00–20:00 Location: P1

DS 35.1 Wed 17:00 P1

Preparation and Characterization of oxide Heterostructures for future Applications in Information Technology — •Markus Waschk, Alexander Weber, Markus Schmitz, Paul Zakalek, and Thomas Brückel — Jülich Center for Neutron Science JCNS and Peter Grünberg Institut PGI: Streumethoden, Forschungszentrum Jülich GmbH, 52428 Jülich, Germany

Nowadays the increased demand on highly efficient storage devices leads to the development of new materials for future devices. Promising candidates are multifunctional oxides that open a wide field of physical properties due to their correlated electron system. Especially the interface of two oxide thin films can exhibit different properties as found in bulk. For instance, the combination of the antiferromagnetic materials $LaMnO_3$ and $SrMnO_3$ in a thin film system leads to an interface with ferromagnetic behavior.

We want to present two state of the art preparation methods, which is the oxide molecular beam epitaxy on the one hand and the high oxygen pressure sputtering system on the other hand. These techniques provide the possibility to grow stoichiometric oxide thin films very precisely.

We identify the structural parameters of the films by using x-ray scattering and atomic force microscopy. Furthermore a SQUID magnetometer and a MOKE setup are used to determine the magnetic parameters of the samples. We use polarized neutron scattering to gain informations about the magnetic depth profile of our samples.

DS 35.2 Wed 17:00 P1

Ferromagnetic InMnAs prepared by Ion implantation and pulsed laser annealing — Ye Yuan[1], •Yutian Wang[1], Kun Gao[1], Muhammad Khalid[1], Eugen Weschke[2], Wolfgang Skorupa[1], Manfred Helm[1], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, P.O. Box 510119, 01314 Dresden, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Straße 15, D-12489 Berlin, Germany

Ferromagnetic InMnAs has been previously prepared by low temperature MBE. In this contribution, we present an alternative method what combines Mn ion implantation and pulsed laser annealing to achieve In1-xMnxAs (x = 0.04 and 0.08) [1], and to obtain a remarkably high Curie Temperature (TC) up to 80 K compared to InMnAs with the same Mn concentration as prepared by MBE. The advantage of pulsed laser annealing is its high process temperature within the nano-second range, eliminating n-type defects which can decrease its magnetization and TC. The saturation magnetization is ˜2.6μB / Mn by consideration of all implanted Mn ions. The out-of-plane [001] is the easy axis displaying a nearly square like hysteresis loop. Our results suggest that InMnAs prepared by ion implantation and pulsed laser annealing shows a promising prospect to get high TC DMS after optimizing the preparation parameters.

1) S. Zhou, et al. :Appl. Phys. Express 5 (2012) 093007

DS 35.3 Wed 17:00 P1

$BaTiO_3$ memristors for neuromorphic engineering circuits. — •Florian Hofmann[1], Savio Fabretti[2], Stefan Niehörster[2], Joachim Sterz[2], Andy Thomas[2], and Elisabetta Chicca[1] — [1]Technische Fakultät, Universität Bielefeld, Germany — [2]Fakultät für Physik, Universität Bielefeld, Germany

We investigated the memristive properties of Barium Titanate and its application in the field of Neuromorphic Engineering. It is suggested in [1] that memristive elements may be a perfect fit for replacing synaptic circuits in modelled neuronal networks. Therefore we sputtered thin BTO films and characterized them with X-ray defraction (XRD). We observed the required tetragonal stucture in the XRD spectra. Furthermore we measured first memristive i-v tunneling characteristic. Finally we plan to integrate memristive elements with a neuromorphic CMOS chip and discuss advantages over previous attempts.

[1] Giacomo Indiveri et al. “Integration of nanoscale memristor synapses in neuromorphic computing architectures”

DS 35.4 Wed 17:00 P1

LiPON electrolyte prepared by RF sputtering for solid state electrochromic and battery applications — •Yurong Su[1], Jane Falgenhauer[2], Matthias Geiss[3], Benedikt Kramm[1], Angelika Polity[1], and Bruno K. Meyer[1] — [1]I. Physics Institute, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Institute of Applied Physics, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [3]Institute of Physical Chemistry, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 58, 35392 Giessen, Germany

Lithium phosphorus oxynitride (LiPON) is one of the promising solid state electrolytes which can be used in lithium batteries as well as all solid state electrochromic (EC) devices due to their relatively high ionic conductivity and better durability among oxides.In the present study, amorphous LiPON films were prepared by radio frequency (RF) magnetron sputtering of a Li_3PO_4 target in N_2 atmosphere. The LiPON films were deposited by varying RF power and N_2 pressure in order to evaluate the best deposition conditions. The composition of films was determined by ICP-OES and EDX. The structural, optical and electrochemical properties were characterized by XRD, XPS, UV-visible and impedance spectroscopy, respectively. The highest ionic conductivity at room temperature observed in this study was about 3.6×10^{-6}Scm^{-1} with the activation energy of 0.47 eV. In addition the prepared LiPON films have good transparency in visible light region. This good performance of LiPON film may make it suitable both for solid state EC devices and battery applications.

DS 35.5 Wed 17:00 P1

Assisted ion beam interface investigation for highly reflective Cr/Sc multilayer mirrors — •Alexander Guggenmos[1,2], Stefan Radünz[1,2], Roman Rauhut[1,2], Bert Nickel[3], Sriram Venkatesan[4], Angela Wochnik[4], Christina Scheu[4], Eric M. Gullikson[5], Ferenc Krausz[1,2], and Ulf Kleineberg[1,2] — [1]LMU München, Fakultät für Physik, Garching, Germany — [2]MPQ, Garching, Germany — [3]CeNS, LMU München, München, Germany — [4]LMU München, Fakultät für Chemie, München, Germany — [5]CXRO, Lawrence Berkeley National Lab, Berkeley, USA

Extending single attosecond pulse technology from currently sub-200 eV to the water window spectral range may enable for the first time the unique investigation of ultrafast electronic processes within the core states of bio-molecules. The demand on highly reflective multilayer mirrors for spectral shaping or focusing attosecond pulses in the water window wavelength range, between the K-absorption edges of carbon and oxygen (2.3-4.4 nm), manifests itself due to the lack of sources with sufficient photon flux. Realizing this requisite utilizes interface optimized multilayer mirrors with almost perfect interfaces due to the huge loss in reflectivity which arises from boundary imperfections. We present our achievements in minimizing the interface roughness of ion-beam deposited Cr/Sc multilayer mirrors by optimizing the kinetic energy of the utilized Krypton ions both in the deposition and the interface polishing process. Experimental results from measurements using X-ray reflectometry, spectral ellipsometry and XUV reflectrometry as well as TEM cross section images are shown and discussed.

DS 35.6 Wed 17:00 P1

NIR-VUV Spectroscopic Study of $ZnFe_2O_4$, $CoFe_2O_4$ and $ZnCo_2O_4$ Thin Films — •Vitaly Zviagin[1], Peter Richter[2], Tammo Böntgen[1], Michael Lorenz[1], Dietrich R.T. Zahn[2], Georgeta Salvan[2], Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany — [2]Technische Universität Chemnitz, Semiconductor Physics, Reichenheinerstr. 70, Germany

We present optical and structural properties of $ZnFe_2O_4$, $CoFe_2O_4$, and $ZnCo_2O_4$ spinel oxides grown at different temperatures on MgO substrates by pulsed laser deposition. The optical properties were determined by spectroscopic ellipsometry in the range from 0.5 eV to 9.0 eV, and at temperatures from 10 K to 300 K. A model, consisting of Gauss and critical point functions located at the optical transition energies was developed to describe the measured dielectric function. The magneto-optical response of the dielectric tensor was measured by magneto-optical Kerr effect spectroscopy at room temperature.

The crystal structure of the films was determined from wide-angle X-ray diffraction. It was found that the temperature during the deposition induces a distinct shift in the observed transition energies as well as a change in the structural properties and surface topology of the thin films.

DS 35.7 Wed 17:00 P1

Generation of Hypersound Strain Pulses: Polyelectrolyte Nanolayers vs. Thin Metal Films — •Mathias Sander[1,2], Steffen Mitzscherling[1], Andre Bojahr[1], Daniel Schick[1], Peter Gaal[2], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam/Golm, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Wilhelm-Conrad-Röntgen Campus, Bessy II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

Ultrafast optical excitation of a thin transducer layer generates hypersound strain pulses that can be observed by pump-probe-spectroscopy. Typically, such transducers are realized by vacuum deposition of thin metal films. We demonstrate the generation of hypersound strain pulses by transducers composed of polyelectrolyte nanolayers that were grown by spin-assisted layer-by-layer deposition. Excitation of polyelectrolytes results in a several times higher strain compared to their metallic counterparts. We prepare samples with a reflecting interlayer, that allow for a direct comparison of both transducer materials. The measured phonon spectra are repoduced by theoretical simulations.

DS 35.8 Wed 17:00 P1

Homoepitaxial growth of single crystalline diamond — •Reinhard Remfort, Nicolas Wöhrl, and Volker Buck — University of Duisburg-Essen, Germany

Störstellen in Diamant stellen zentrale Elemente für eine Vielzahl von Anwendungen z.B. in der Quanteninformations- und Sensortechnologie dar. Diese Zentren, insbesondere das Stickstoff-Leerstellen (NV)-Zentrum werden daher seit einigen Jahren intensiv erforscht. Um die Eigenschaften dieser Zentren besser charakterisieren zu können und in größerem Maßstab nutzbar zu machen ist es nötig den Einfluss umliegender weiter Defekte zu minimieren. Ein erster Schritt hierbei ist die Erzeugung besonders reiner stickstoffarmer einkristalliener Diamantschichten. Das für diese Anforderungen am besten geeignete Verfahren bietet im Bereich der Niederdruckdiamantsynthese die MPCD (Microwave Plasma Chemical Vapor Deposition), da bei dieser Art der Diamantsynthese keine Elektroden für die Plasmaanregung erforderlich sind. Durch die zusätzliche Verwendung reiner Prozessgase ist es daher möglich sehr stickstoffarme Diamantschichten auf HPHT-Diamantsubstraten abzuscheiden. In einem weiteren Schritt können dann gezielt Stickstoffatome zur Erzeugung von (NV)-Zentren eingebracht werden. Dies kann entweder durch Ionenimplatation oder schon während des Syntheseprozesses durch die gezielte Beimischung sehr geringer Mengen Stickstoff geschehen.

DS 35.9 Wed 17:00 P1

rientation Dependent Enantioselective Adsorption of Homochiral Surface Mounted Metal Organic Framework — •Zhi-Gang Gu[1], Jochen Bürck[2], Jinxuan Liu[1], Xia Stammer[1], Zhengbang Wang[1], Peter Weidler[1], Anne Ulrich[2], Hartmut Gliemann[1], and Christof Wöll[1] — [1]Institute of Functional Interfaces, KIT — [2]Institute for Biological Interfaces 2, KIT

The research based on assembly of bulk crystal Metal-Organic Frameworks (MOFs) for nonlinear optics, enantioselective catalysis, and medicine has been extensively carried out1. However, the synthesis and properties of MOFs thin films on self-assembled monolayers (SURMOFs)are still a challenge. Up to now, MOFs (HKUST-1, MOF-2) formed by single ligand and other pillared-layer MOFs (MOF508a, [Cu2(bdc)2dabco]n and [Cu2(ndc)2dabco]n) constructed by mixed ligands on functionalized substrates by employing a step-by-step liquid-phase-epitaxy method (LPE) have been reported2. In previous works chiral linker were used to grow MOFs on substrate and the first example of chiral SURMOF [Cu2(+/-)Cam2dabco]n has been reported in 2012. In this work we grow another chiral SURMOFs [Cu2Cam2bipy]n with highly oriented and homogenous thin film via LPE method3. The potential of chiral SURMOFs for enantioselective adsorption of chiral molecules is studied by quartz crystal microbalance. 1.Shekhah, O.;Wöll, C.,et al. Chem. Soc. Rev. 2011, 40 (2), 1081-1106. 2.Shekhah O.,Wöll C.,et al. J. Am. Chem. Soc. 2007, 129 (15), 118-217. 3.Shekhah, O.; Woll, C.,et al. Nat. Mater. 2009, 8 (6), 481-484.

DS 35.10 Wed 17:00 P1

Spinel based magnetic tunnel junctions — •Torsten Hübner — Universität Bielefeld — Thin Films and Physics of Nanostructures

Using $MgAl_2O_4$ instead of MgO as barrier material in magnetic tunnel junctions has attracted some attention due to its small lattice mismatch of $\sim$1% with regard to standard ferromagnetic electrodes. The Δ_1 symmetry filter effect, which is responsible for the huge TMR effect in MgO based magnetic tunnel junctions, is also predicted for MgAl2O4 tunnel barriers[1]. Additionally, MAO barriers achieved a V_{half} twice as much as MgO ones, which makes them even more interesting for spintronic devices and applications[2]. We fabricated CoFeB/$MgAl_2O_4$/CoFeB exchange biased magnetic tunnel junctions via rf sputtering of a pure MAO target. A TMR effect of more than 30% was achieved reproducibly as well as a comparatively high area resistance product in the range of several k$\Omega\mu$m^2. In conclusion, MAO barriers require continuing research in order to take advantage of their potentially superior properties. [1]Zhang et al., Appl. Phys. Lett. 100, 222401 (2012) [2]Sukegawa et al., Appl. Phys. Lett. 96, 212505 (2010)

DS 35.11 Wed 17:00 P1

Dielectric constants of polycrystalline (Ba,Sr)TiO3 (BSTO) films — •Xueyong Yuan[1], Tiangui You[1], Varun John[1], Sabine Engelmann[1], Ilona Skorupa[1,2], Danilo Bürger[1], Heidemarie Schmidt[1], Daniel Grimm[1], and Oliver G. Schmidt[1,3] — [1]Material Systems for Nanoelectronics, Chemnitz University of Technology — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V — [3]IFW Dresden, Institute for Integrative Nanosciences

The dielectric constant for SrRuO3/30nm thick Ba1-xSrxTiO3/SrRuO3 all oxide capacitor was measured to be 550, which corresponds to an equivalent SiO2 thickness of 0.21 nm [1]. Although the leakage current of epitaxially-grown BSTO films is small compared to polycrystalline BSTO films, the low-cost polycrystalline capacitors are widely used in modern semiconductor technology. We studied the frequency dependent electrical polarization of polycrystalline BSTO films which have been grown by pulsed laser deposition (PLD) on large scale Pt bottom electrodes as a function of PLD growth conditions in the test frequency range from 100 Hz to 1 MHz. Most BSTO films reveal the expected constant bulk dielectric constant of around 20. Here the focus is on selected BSTO films which show a relatively high dielectric constant in the low frequency range up to 100 kHz. A model which considers the occupancy of bulk traps in insulators [2] is used to explain the frequency dependent capacitance of polycrystalline BSTO.

References [1] N. Fukushima et al. 493, 1997. [2] Y. Yuan et al. IEEE Trans. on Electron Devices, 59, 2012.

DS 35.12 Wed 17:00 P1

Low chromatic dispersion and high diffraction efficiency of zone plate for XUV and soft X-ray bandwidth — •Huaihai Pan[1,2], Christian Späth[3], Alexander Guggenmos[1,3], Jürgen Schmidt[3], Soo Hoon Chew[1,3], Quanzhong Zhao[2], and Ulf Kleineberg[1,3] — [1]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany — [2]State Key Laboratory of High Field Laser Physics, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Shanghai 201800, China — [3]Ludwig-Maximilians-Universität München, Fakultät für Physik, Am Coulombwall 1, 85748 Garching, Germany

Zone plate has a great potential in achieving high spatial resolution for the XUV and X-ray radiations [1]. However, due to strong chromatic dispersion [2] and low diffraction efficiency of the zone plate, the highest achievable spatial resolution is limited. Here we report the theoretical calculation based on the design of achromatic optics [3] which can potentially reduce chromatic dispersion and improve diffraction efficiency. Such optics is a combination of zone plate and lens, in which the positive dispersion induced by lens can compensate the negative dispersion induced by zone plate. An ultrafast laser pulse with a duration of 120 as and central wavelength at 13.5 nm is employed. The simulated results show that the intensity distribution of propagation is partially achromatic and the specific profile of zone plate can improve the diffraction efficiency at first order diffraction. [1] W. Chao, et al., Opt. Express 17, 17669 (2009).[2] J. Kirz., J. Opt. Soc. Am. 64, 301 (1974).[3] Y. Wang, et al., Nature 424, 50 (2003).

DS 35.13 Wed 17:00 P1

Nano Microphone — •Martin Bohrisch[1], Xianghui Zhang[2], Thomas Weimann[1], and Armin Gölzhäuser[2] — [1]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [2]Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

We plan to build and test a nano microphone that utilizes a 1 nm thick carbon nanomembrane (CNM) as a sensitive diaphragm. The CNM is made by electron induced crosslinking of aromatic self-assembled monolayers. To convert oscillations of the CNM into electrical signals, we have to integrate the molecular CNMs and electronic circuits into a functional nano electro- mechanical system (NEMS). The operation principle is based on a field effect transistor (FET). A freestanding conductive diaphragm is placed over the source-drain-channel of the FET and acts as flexible gate-electrode. Accordingly an oscillation of the membrane leads to an AC signal of the source-drain-current. Our objective is to build a prototype that will be used for sound measurements in air and water; it will be tested for spatially and timely resolved sound detection. The proof-of-concept experiments and first results of CNM-gated FETs will be presented.

DS 35.14 Wed 17:00 P1

Elastic Properties of Nickel Carbides — •Jeffrey Kelling[1,2], Peter Zahn[2], and Sibylle Gemming[1,2] — [1]Institute of Physics, TU Chemnitz, Chemnitz, Germany — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The nickel – carbon system has received increased attention over the past years due to the relevance of nickel as a catalyst for carbon nanotube growth and as a substrate for metal-induced crystallization of graphene and graphite. Nickel carbides as bulk materials are out of reach for experimental studies because of their meta-stability. Ab-initio studies are rare. We present our ab-initio – frozen phonon results for the elastic properties of Ni_3C, Ni_2C and NiC.

DS 35.15 Wed 17:00 P1

Carbon-Nickel Interface Dynamics During Physical Vapor Deposition — •Robert Wenisch[1], Matthias Krause[1,2], René Hübner[1], Sibylle Gemming[1,3], and Gintautas Abrasonis[1] — [1]Bautzner Landstraße 400, 01328 Dresden — [2]Mommsenstraße 9, 01069 Dresden — [3]Technische Universität Chemnitz, 09107 Chemnitz

Interface dynamics play a crucial role in Nickel catalyzed fabrication of carbon nanotubes, carbon nanowires and graphene. Interface dynamics are studied by deposition of atomic C on Ni at temperatures of 23–550°C. The obtained films are characterized by transition electron microscopy, Raman-spectroscopy, nuclear reaction analysis and X-ray photoelectron spectroscopy. Bulk diffusion and solubility are found negligible in the present experiments leaving surface diffusion as the main graphitization mechanism. The presented process may open new avenues for the fabrication of graphene on Ni at low temperatures ($< 300^\circ$C).

DS 35.16 Wed 17:00 P1

Spectroscopic Monitoring of Carbon Nanotube Dispersion Preparation — •Toni Hille[1,2,3], Thomas Blaudeck[1], Sascha Hermann[1], Christian von Borczyskowski[2], and Stefan E. Schulz[3] — [1]TU Chemnitz, Zentrum für Mikrotechnologien (ZfM), 09107 Chemnitz, Germany — [2]TU Chemnitz, Center for Nanostructured Materials and Analytics (nanoMA), 09107 Chemnitz, Germany — [3]Fraunhofer ENAS, 09126 Chemnitz, Germany

In this contribution, we introduce a systematic inspection tool for carbon nanotube dispersion preparation based UV-Vis-NIR-spectroscopy. Goal is the wafer-level integration of the CNTs by an electrokinetic deposition approach from an aqueous dispersion [1]. In order to estimate the dispersion quality during the preparation process, a microfluidic system with a quartz flow cell is built up. Related to the non-resonant and resonant features in the UV-Vis-NIR-spectra, the CNT concentration and degree of debundeling can be monitored and sonication paramters can be optimized [2]. It turns out that the degree of debundling is a function of both the absolute concentration of the CNTs and the relative concentration between the CNTs and the dispersion agents (sodiumlauryl sulfate, sodium deoxycholate, etc.)

[1] S. Hermann, H. Fiedler, H. B. Yu, S. Loschek, J. Bonitz, S. E. Schulz, T. Geßner, IEEE Proceedings Systems, Signals, and Devices (SSD), article ID 6198090 (5 pages) (2012).

[2] H. B. Yu, S. Hermann, S. E. Schulz, T. Geßner, Z. Dong, W. J. Li, Chemical Physics 408, 11-16 (2012).

DS 35.17 Wed 17:00 P1

Wafer-Level Functionalization of Carbon Nanomaterials with Metal Nanoparticles — •Thomas Blaudeck[1], David Adner[2], Sascha Hermann[1], Youwei Zhang[1,3], Stefan E. Schulz[4], Ran Liu[3], Heinrich Lang[2], and Thomas Gessner[1] — [1]TU Chemnitz, Zentrum für Mikrotechnologien (ZfM), 09107 Chemnitz, Germany — [2]TU Chemnitz, Inorganic Chemistry, 09107 Chemnitz, Germany — [3]Fudan University, School of Microelectronics, Fudan, P. R. China — [4]Fraunhofer ENAS, 09126 Chemnitz, Germany

We report about different technical approaches for an on-chip functionalization of single-walled carbon nanotubes (SWCNTs) with metal nanoparticles after electrokinetic deposition of individualized SWCNTs in the configuration of a CNT-based field effect transistor (CNT-FETs) for sensor applications. Based on a side-wall functionalization of the SWCNTs with (R-)oxocarbonylnitrene linkers according to Holzinger et al. [1] we extended the protocols towards long-chained ethylene glycol units for an effective deposition of nanoparticles. Characterization of the precursor included IR, Raman and NMR spectroscopy, the functionalized CNT-FETs were analyzed with morphological (AFM, Raman) and electric characterization . For the on-chip functionalization on silicon wafers (150 mm diameter), a microfluidic tool on a controlled heating stage was designed and applied on the integrated SWCNTs on a silicon wafer. Our experiments show that a selective functionalization of the SWCNTs with gold nanoparticles is possible. Results for other carbon-based nanomaterials are discussed.

[1] M. Holzinger et al., J. Am. Chem. Soc. 125, 8566-8580 (2003).

DS 35.18 Wed 17:00 P1

Integration von MOS-Transistoren als Wandler für mechanische Spannungen — •Michael Schramm[1], Sven Haas[2], Danny Reuter[2,3], Kay-Uwe Loebel[1], Steffen Heinz[1], Andreas Bertz[2], John Thomas Horstmann[1] und Thomas Gessner[2,3] — [1]Professur Elektronische Bauelemente der Mikro- und Nanotechnik, TU Chemnitz, 09107 Chemnitz — [2]Zentrum für Mikrotechnologien, TU Chemnitz, 09107 Chemnitz — [3]Fraunhofer Institut für Elektronische Nanosysteme, 09126 Chemnitz

Zur Wandlung einer mechanischen Spannung in ein elektrisches Signal finden häufig Piezowiderstände Anwendung. Um den Flächenbedarf zu reduzieren und die Kompatibilität zu CMOS-Prozessen zu erhöhen, ist es möglich, MOS-Transistoren als Wandlerelement einzusetzen. Die Wandlung einer mechanischen Spannung in ein elektrisches Signal erfolgt unter Ausnutzung des piezoresistiven Effekts. Im Fokus dieser Arbeit stehen die Simulation und Charakterisierung von MOS-Transistoren als Wandlerelement für mechanische Spannungen. Zur Erzeugung der mechanischen Spannung fanden dünne Siliziummembranen Anwendung. Um die Transistoren in den Gebieten der maximalen mechanischen Spannung zu platzieren, wurden die Membranen mit einer FEM-Software simuliert. Der Stresseinfluss auf das elektrische Verhalten der Transistoren ist mit einem angepassten BSIM3v3-

Modell simuliert worden. Die Skalierbarkeit wurde durch Simulationen von Halbleitertechnologien unterschiedlicher minimaler Strukturweiten nachgewiesen. Mit Hilfe der Messungen wurde der Stresseinfluss auf die Transistorkennlinien und Transistorparameter untersucht.

DS 35.19 Wed 17:00 P1

Laser induced changes in single-walled carbon nanotubes — •Jana Kalbacova, Raul D. Rodriguez, Honeyeh Matbaechi, and Dietrich R.T. Zahn — Semiconductor Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Carbon nanotubes (CNTs) are one of the materials of future technologies and already today they are finding their way into applications, such as in field effect transistors and photovoltaics. However, for the performance of the device, it is crucial to keep the ratio of metallic to semiconducting at minimum. To monitor this ratio, it is beneficial to use Raman spectroscopy where the so-called radial breathing mode (RBM) of CNTs is observed [1].

It was also shown that in order to induce defects in CNTs, high power laser can be employed. On the other hand, laser illumination was also proposed to eliminate carbonaceous contaminations without CNT destruction [1]. Thus predictably, with optimized laser power we can achieve changes within carbon nanotubes without their destruction. In this contribution, we show how optimized laser power can lead to changes in carbon nanotubes, while preserving the CNT integrity. Changes are observed mostly in the radial breathing mode region. We attribute these to the selective elimination of CNTs with certain chiralities. Simultaneously, by using spatially resolved Raman spectroscopy mapping, we show that the defective region is larger than expected, extending beyond the laser-illuminated spot. We will discuss the changes in the Raman spectra that originate from such defect gradient.

DS 35.20 Wed 17:00 P1

Interaction of gold nanoparticles with wafer-level integrated carbon nanotubes probed by Raman spectroscopy — •Raul D. Rodriguez[1], Jana Kalbacova[1], Thomas Blaudeck[2], Sascha Hermann[2], Parisa Bayat[1,2], David Adner[3], Heinrich Lang[3], Stefan E. Schulz[2,4], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [2]Center for Microtechnologies (ZfM), Technische Universität Chemnitz, 09107 Chemnitz, Germany — [3]Faculty of Natural Sciences, Institute of Chemistry, Inorganic Chemistry, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [4]Fraunhofer Institute for Electronic Nanosystems (ENAS), 09126 Chemnitz, Germany

By means of Raman spectroscopy we aim at determining the effect of gold nanoparticle decoration on single-walled carbon nanotubes (CNT) in a field effect transistor configuration (CNT-FET). The experiments were performed under green laser excitation (514.7 nm) focused by a 100x objective giving a power below 150 μW on the sample and spatial resolution below 500 nm. The spectral resolution allowed detecting changes in the Raman spectra with accuracy as low as 0.6 cm^{-1}. It was found from the analysis of the radial breathing mode (RBM) that small diameter CNT are preferentially affected by the decoration process while no significant increase in defect concentration was observed from the intensity ratio of the D and G bands. This suggests an optimal way of achieving functionalized CNT-FET devices without degrading its electronic properties but preserving the CNT crystallinity and sp^2 nature.

DS 35.21 Wed 17:00 P1

Nanomechanics of carbon nanotube-metal contacts investigated by molecular dynamics and validating experiments — •Steffen Hartmann[1], Ole Hölck[2], Sascha Hermann[1], Thomas Blaudeck[1], Stefan E. Schulz[1], Thomas Gessner[1], and Bernhard Wunderle[1] — [1]TU Chemnitz, Sachsen, Germany — [2]Fraunhofer IZM, Berlin, Germany

With this contribution we present our recent progress in understanding the mechanics of carbon nanotube-metal interfaces at the nano scale. A detailed understanding of the behaviour of a mechanically stressed CNT inside a metal support is of fundamental importance for thermo mechanical reliability predictions and failure-mechanistic treatment of future CNT devices. A simple test to study the reaction behavior of CNTs inside a metal support is the pull-out test. We simulated this pull-out test with molecular dynamics and varying parameters and conducted in-situ pull-out tests inside a scanning electron microscope. From our simulations we find that the ideal incommensurate interface between the lattices of chiral CNTs and metals leads to a behaviour that is independent on embedding length. On the other hand the CNT diameter is of significant importance. We report on predicted pull-out forces which were determined to be in the nN range. Further we explain the influence of defects on the pull-out forces. The results from our experiments are maximum forces between 20 and 35 nN. We compare our experimental findings with results of our numerical investigations and give interpretations for deviations according to material impurities or defects and their influence on the pull-out data.

DS 35.22 Wed 17:00 P1

MEMS based integration of nano scaled architectures manufactured by the rolled-up nanotech method — •Christian Helke[1], Tom Enderlein[1], Stefan M. Harazim[2], Jörg Nestler[1], Oliver G. Schmidt[2], Thomas Otto[3], and Thomas Gessner[1,3] — [1]TU Chemnitz, Zentrum für Mikrotechnologien, Reichenhainer Str. 70, 09126 Chemnitz, Germany — [2]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [3]Fraunhofer ENAS, Technologie-Campus 3, 09126 Chemnitz, Germany

In contrast to conventional laboratory based analysis methods Lab-on-a-Chip (LoC) systems reveal their advantage of performing complex bio-assays on very limited space right at the point of care. To fulfill these laboratory steps in a LoC system all necessary steps from sample preparation until evaluation have to be integrated within this smart system. For this approach rolled-up sensor elements based on the method of *rolled-up nanotech* have to be integrated. The possible integration techniques are limited regarding the sensor elements itself (architecture, material layer system and properties), the feasible functionalization on the inside wall of the sensor elements and the wafer level integration approach, which is aimed. Therefore a *dry* integration technique is favored, because of its not influencing of the inside wall functionalization and the aimed realizing at wafer level with standard CMOS microtechnologies. This system consists out of lithographically manufactured negative photoresist SU8 multilayered structures with microfluidic and integration layers for the rolled-up sensor elements.

DS 35.23 Wed 17:00 P1

Characterization of integrated single-walled carbon nanotubes by transmission electron microscopy — •Martin Hartmann[1], Sascha Hermann[1], and Stefan Schulz[1,2] — [1]TU Chemnitz, Center for Microtechnologies (ZfM), 09126 Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems (ENAS), 09126 Chemnitz, Germany

There is a strong interest in using single-walled carbon nanotube (SWCNTs) as ultrasensitive piezoresistive sensor element. For this kind of applications the knowledge of SWCNT properties and its environment are of crucial importance for understanding the device performance and for technology development. In our work we are particularly interested in effects of different process steps along a waferlevel technology for the fabrication of micro or nano electro mechanical devices (MEMS or NEMS) with integrated piezoresistive SWCNT sensors.

Therefore we present studies with a test structure which allows us to use transmission techniques such as transmission electron microscopy (TEM) to get profound information about chirality, defects and impurities introduced during the integration process of the SWCNTs. With a minimal invasive method, this test structure was dissected from a wafer-level processed sample with the focused ion beam (FIB) method. We present first results of a TEM investigation, which integrated SWCNTs between two electrodes of a MEMS structure. Moreover we present an approach for a systematic TEM characterization of a large amount of structures with integrated SWCNTs without using the time-consuming FIB method.

DS 35.24 Wed 17:00 P1

Laser based integration method of rolled-up nano membranes in polymer based LoC systems — •Tom Enderlein[1], Christian Helke[1], Stefan M. Harazim[2], Jörg Nestler[1], Oliver G. Schmidt[2], Thomas Otto[3], and Thomas Gessner[1,3] — [1]TU-Chemntiz, Zentrum für Mikrotechnologien, Reichenhainer Str. 70, 09126 Chemnitz, Germany — [2]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [3]Fraunhofer ENAS, Technologie-Campus 3, 09126 Chemnitz, Germany

The functionalities of Lab-on-a-Chip (LoC) systems today still become more and more complex and the degree of integration is further growing. Mostly driven by conventional MEMS technologies, the preparation for example of channels, pumps and valves is mainly realized in silicon and glass, but also in silicones like PDMS. In the case of LoC systems in the field of point of care diagnostics (PoC), those silicon based systems are barely applicable due to the high costs of the substrate materials for the large areas needed for the sample storage, preparation and so on. This is where polymer substrates reveal their advantage for those one-time-only LoC-cartridges and can well be processed by ultra-short pulse laser systems. Besides the laser structuring of channels and reservoirs, polymer welding is as well possible. The here demonstrated new approach shows on the one hand the integration of those functionalized rolled-up sensor elements by laser structured integration channels in the micrometer range. On the other hand this method uses laser micro-welding and the simultaneously melting of the surrounding material of the rolled-up membranes for their fixation.

DS 35.25 Wed 17:00 P1

A low-cost solution method to fabricate Cu$_2$ZnSn(S,Se)$_4$ solar cells — Chao Gao[1], Thomas Schnabel[2], •Christoph Krämmer[1], Erik Ahlswede[2], Michael Powalla[2,3], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany — [3]Light Technology Institute (LTI), Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Cu$_2$ZnSn(S,Se)$_4$ is a promising absorber material to fabricate high-efficiency environmentally friendly solar cells. Here a low-cost solution method has been developed to fabricate Cu$_2$ZnSn(S,Se)$_4$ solar cells. For the preparation, first SnS, CuS, and ZnS layers are successively deposited on a molybdenum/soda-lime glass substrate by chemical bath deposition, then the Cu$_2$ZnSn(S,Se)$_4$ thin films are obtained by a selenization process utilizing a graphite box in a tube furnace. The obtained Cu$_2$ZnSn(S,Se)$_4$ thin films show good crystallization and no obvious evidence for impurity phases except ZnSe is found in the selenized films. By optimizing the preparation process of the Cu$_2$ZnSn(S,Se)$_4$ thin films, Cu$_2$ZnSn(S,Se)$_4$ solar cells with efficiencies up to 3.2 % can be obtained. Current-voltage and quantum efficiency measurements imply that a barrier may exist at the Cu$_2$ZnSn(S,Se)$_4$/CdS interface that could be the limiting factor for the solar cell efficiency.

DS 35.26 Wed 17:00 P1

Cu$_2$ZnSnSe$_4$ layers and solar cells from selenized co-evaporated precursors — •Timo Musiol[1], Chao Gao[1], Thomas Schnabel[2], Mario Lang[1], Christoph Krämmer[1], Erik Ahlswede[2], Michael Powalla[2,3], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany — [3]Light Technology Institute, KIT

Cu(In,Ga)Se$_2$ (CIGS) is a well-established absorber material for thin-film solar cells and efficiencies up to 20.8% have been demonstrated. Due to its earth-abundant components, kesterite Cu$_2$ZnSn(S,Se)$_4$ is a very promising alternative. In this contribution we present results for Cu$_2$ZnSnSe$_4$ (CZTSe) layers fabricated by coevaporation of Cu, Zn, Sn, and Se, followed by a high-temperature selenization step. The layers are investigated with various techniques such as Raman spectroscopy, X-ray diffration, and photoluminescence spectroscopy. Based on CZTSe absorbers, solar cells have been processed and investigated. I–V data indicates that a conversion efficiency of up to 4.7% is achieved in these devices.

DS 35.27 Wed 17:00 P1

Polycrystalline Cu$_2$ZnSnSe$_4$ layers on GaAs(001) with a preferential grain orientation — •Johannes Sachs[1], Christoph Krämmer[1], Mario Lang[1], Chao Gao[1], Michael Powalla[2], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Light Technology Institute, KIT, and Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany

Due to its earth-abundant components the kesterite Cu$_2$ZnSnSe$_4$ (CZTSe) material system is a very promising alternative to Cu(In,Ga)Se$_2$. However, material properties such as the band structure or the impact of grain boundaries on solar cell performance are still poorly understood. In order to investigate these properties further, high-quality layers of CZTSe would be highly desirable. Towards this aim, we introduce a two-step fabrication approach which is based on the selenization of Sn/Cu/ZnSe(001) structures on GaAs(001) substrates. X-ray diffraction and Raman measurements do not only confirm the formation of the kesterite phase but also indicate a preferential orientation of the CZTSe grains in all three dimensions.

DS 35.28 Wed 17:00 P1

FDTD Simulations for Optimization of Light-Management in Thin-Film Solar Cells — •Benjamin Fries[1,2], Jonathan Lehr[1,2], Ruben Hünig[2], Heinz Kalt[1], Michael Powalla[2,3], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [3]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany

Thin-film solar cells made of Cu(In,Ga)Se2 (CIGS) have reached a high level of both energy conversion efficiency (20.8 %) and commercial cost-effectiveness. Yet a number of aspects remain to be understood and optimized. In this contribution we present a numerical model of a CIGS solar cell being developed in order to investigate the effects of minority carrier collection as well as light-management on the external quantum efficiency (EQE). Experimental data for the latter could be reproduced employing a finite-difference time-domain (FDTD) method. Surface-patterning of a solar cell lead to an experimentally observed increase in short-circuit current which could also be simulated successfully.

DS 35.29 Wed 17:00 P1

Temperature Dependent Electrical Charge Carrier Mobility and Concentration Measurements of Spin Coated Silicon Films — •Daniel Bülz, Michael Fronk, Ronny Fritzsche, Michael Mehring, Georgeta Salvan, and Dietrich R. T. Zahn — TU Chemnitz, 09126 Chemnitz, Germany

Nowadays many different methods for the production of silicon films are investigated. The main goal of these techniques is to lower the production costs and increase the production speed. For electronic applications the charge carrier mobility is a crucial parameter. This can be obtained from electrical Hall and conductivity measurements. Here a magneto-optical Oxford Spectromag Cryostat was upgraded with electrical wirings for electrical Hall and four point probe measurements in order to enable the determination of the charge carrier mobility and concentration. Furthermore, the Spectromag Cryostat offers the possibility of illuminating the sample to investigate the mobility of light induced charge carriers. The system is tested with an n-doped standard silicon wafer sample. Finally, the temperature dependent charge carrier mobility of silicon films is measured. For this purpose, the silicon films are prepared by spin coating of a Si-precursor (neopentasilane). After deposition the films are thermally treated to form amorphous silicon films.

DS 35.30 Wed 17:00 P1

Localisation and finite-size effects in graphene flakes — Clara González-Santander[1], Francisco Domínguez-Adame[1], •Michael Hilke[2], and Rudolf A. Römer[3] — [1]GISC, Departamento de Física de Materiales, Universidad Complutense - E-28040 Madrid, Spain — [2]Department of Physics, McGill University, Montréal (Québec) - H3A 2T8, Canada — [3]Department of Physics and Centre for Scientific Computing, University of Warwick - Coventry, CV4 7AL, UK

We show that electron states in disordered graphene, with an onsite potential that induces inter-valley scattering, are localised for all energies at disorder as small as 1/6 of the band width of clean graphene. We clarify that, in order for this Anderson-type localisation to be manifested, graphene flakes of size $\approx 200 \times 200$ nm^2 or larger are needed. For smaller samples, due to the surprisingly large extent of the electronic wave functions, a regime of apparently extended (or even critical) states is identified. Our results complement earlier studies of macroscopically large samples and can explain the divergence of results for finite-size graphene flakes.

DS 35.31 Wed 17:00 P1

Dry transfer method for CVD-graphene using hexagonal Boron Nitride — •Luca Banszerus[1], Michael Schmitz[1], Kenji Watanabe[2], Takashi Taniguchi[2], and Christoph Stampfer[3] — [1]JARA-FIT and II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan — [3]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich

Growing graphene on copper, using chemical vapor deposition is a promising technique allowing to produce high quality single crystals on large areas. However, recent results have shown that surface contamination by ionic substances and polymer residues substantially lower the quality of the grown graphene. In this work we present a novel transfer method where, in contrast to the common transfer technique, the graphene does not come into contact with any polymer or ionic substances. In a first step we grow graphene single crystals on copper with diameters of up to 400 μm. The graphene is then lifted off the copper with hexagonal boron nitride (hBN), using a van der Waals-pick up technique. Subsequently, the flakes are transferred to SiO_2 or hBN and are characterized using Raman spectroscopy. The Raman spectra show a low D-peak amplitude together with a ratio of G/2D of up to 10 and a G-Peak position around $1583cm^{-1}$ suggesting a high crystal quality and a low doping concentration. Our novel technique additionally allows us to transfer high quality CVD grown graphene from copper onto arbitrary substrates, which makes it potentially interesting for a number of scalable applications.

DS 35.32 Wed 17:00 P1

Raman Spectroscopy of Few-Layer Graphene after Oxygen Plasma Etching — •Mahsa Zoraghi, Jose Barzola-Quiquia, and Pablo Esquinazi — Division of Superconductivity and Magnetism, University of Leipzig, D-04103 Leipzig, Germany

The purpose of this study was to obtain few-layer graphene (FLG) samples of tens of nanometer thickness, from graphite flakes (GF) of 100 nm thickness. Rubbing process is used to prepare FLG samples on the top of isolating substrates. Using this method, GF and FLG samples can be produced without disorder according to Raman measurements. Oxygen plasma etching technique is used at room temperature to reduce the thickness of GF samples and also to study how obtained FLG samples are affected by etching process. Thickness variations can be measured by atomic force microscopy (AFM) after etching process. Raman spectroscopy was used to characterize the possible defects in FLG samples produced by oxygen plasma etching. As the Raman spectroscopy results indicated, we learned that by rubbing method, we do not produce defects in the GF sample however, oxygen plasma etching does. The temperature dependence of the electrical resistance of FLG samples before and after oxygen plasma treatment was also studied.

DS 35.33 Wed 17:00 P1

Charge transport in graphene and nitrogen-doped graphene — •Fabienne Musseau[1], Markus Rein[1], Nils Richter[1], Khaled Parvez[2], Hermann Sachdev[2], Mathias Kläui[1], and Klaus Müllen[2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Mainz, Germany — [2]Max Planck Institute for Polymer Research Mainz, Mainz, Germany

Graphene is a promising candidate for replacing silicon-based transistors due to its two-dimensional structure and high charge carrier mobilities. To this end it is necessary to engineer the band gap in this carbon-based material. One strategy to overcome this problem is the intentional doping of graphene.

Our work is based on a comparison between undoped and nitrogen-doped single graphene layer grown by chemical vapour deposition (CVD) on copper foils. First Raman spectroscopy was used to characterize the samples. Electrical measurements were performed at variable temperatures down to 2.3 K and at variable magnetic field perpendicular to the plane up to 8 T.

The behaviour of undoped samples is comparable to what was previously found in CVD grown graphene, including mobilities of around 1100 cm*/Vs and weak localisation at low temperatures. For the doped samples, the charge carrier concentration is significantly higher than in undoped cases, indicating an effective doping. Furthermore a negative magnetoresistance is observed in the range of -8 T to +8 T, which is not found for undoped graphene.

DS 35.34 Wed 17:00 P1

Hyperdoping Si with deep level impurities by ion implantation and short-time annealing — •Fang Liu, Slawomir Prucnal, Kun Gao, Muhammad Khalid, Wolfgang Skorupa, Manfred Helm, and Shengqiang Zhou — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, P.O. Box 510119, 01314 Dresden, Germany

It has been proposed that deep level impurities, such as Titanium (Ti) or chalcogens in Si, can induce an impurity band inside the bandgap at high enough doping concentration [1, 2]. The insertion of an impurity band can enhance the absorption at a broader wavelength range and leads to as applications in the so-called intermediate band solar cell [3]. In the present work, we are using ion implantation combined with short-time annealing to realize hyperdoping of Ti and chalcogens in Si. Our results show that the implanted Si layer can be recrystallized by both flashlamp and pulsed laser annealing. Ti ions mainly occupy the interstitial sites, while S and Se ions substitute the Si in the lattice. The consequent changes in electrical properties are also observed. [1] J. Olea, et al., J. Appl. Phys. 109, 063718 (2011). [2] B. P. Bob, et al., J. Aziz J. Appl. Phys. 107, 123506 (2010) [3] A. Luque and A. Martí, Phys. Rev. Lett. 78, 5014 (1997).

DS 35.35 Wed 17:00 P1

Analysis of lateral energy distribution for passive ion beam scattering element — Weiqi Han[1], •Constantin Csato[1], Florian Krippendorf[1], Michael Rüb[1], and Carsten Ronning[2] — [1]Ernst-Abbe-Fachhochschule Jena, Carl-Zeiss-Promenade 2, 07745 Jena — [2]Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

The task is to analyse the lateral energy distribution of ions passing through an energy filter. Details of the filter are given elsewhere [1]. Simulation with Geant4 [2] has shown that the lateral energy distribution of transmitted ions of an energy filter can be modified by the parameters ion energy, ion species, filter structure and material and filter - substrate distance. We present a tool for characterizing the lateral energy distribution experimentally. We demonstrate that our experimental approach is suitable to analyse the lateral energy distribution of transmitted ions. We implanted $7MeV$ Boron ions with a dose of $3 \cdot 10^{12}cm^{-2}$ through a silicon energy filter into a PMMA substrate. After implantation the PMMA is developed according to [3]. The developed structures are analysed by atomic force microscope and confocal microscope. The results confirm the dependency of the lateral energy distribution on filter-substrate distance.

[1] F. Krippendorf et al., Proceedings MikroSystemTechnik Kongress 2013, 14.-16. Oktober 2013, Aachen: VDE Verlag, 2013, 8.12, 662-665 [2] S. Agostinelli et al., Geant4 - a simulation toolkit, Nuclear Instruments and Methods section A, 2003, 506, 250-303 [3] F. Schrempel et al., Deep light ion lithography in PMMA - A parameter study, Nuclear Instruments and Methods section B, 1997, 3, 430 - 438

DS 35.36 Wed 17:00 P1

Determination of Fluorine dopants in Fused Silica by means of Nuclear Reaction Analysis (NRA) — •Emanuel Schmidt, Anne Nathanael, and Elke Wendler — Institut für Festkörperphysik Jena

Fluorine doped fused silica has plenty of applications, e.g. in modern optical systems or in the production of micro-electronic components. However the absolute determination of light elements, such as fluorine, in an substrate containing heavier atoms, such as fused silica, is a non-trivial task. Ion beam analysis provides therefore suitable methods, as they are independent of chemical processes and offers the possibility to measure absolute concentrations of light elements even for values smaller than 1ppm.

Therefore we used a proton-fluorine nuclear reaction ($^{19}\mathrm{F}(\mathrm{p}, \alpha_0)^{16}\mathrm{O}$) to measure absolute concentrations of fluorine atoms in fused silica. We have characterized the excitation-function of the nuclear reaction $^{19}\mathrm{F}(\mathrm{p}, \alpha_0)^{16}\mathrm{O}$ in our laboratory-system and could measure profiles of fluorine concentrations over sample depths and determine dopant concentrations within the SiO_2 matrix.

DS 35.37 Wed 17:00 P1

cAFM measurements of conductive ion tracks in ta-C — •Julian Alexander Amani[1], Johann Krauser[2], Hermann Rothard[3], Tristan Koppe[1], Ulrich Vetter[1], Hans Hofsäss[1], Serge Della-Negra[4], and Christina Trautmann[5] — [1]II. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Department of Automation and Computer Sciences, Harz University of Applied Sciences — [3]Centre de Recherche sur les Ions, les Matériaux et la Photonique Ganil, Caen — [4]Matière Nucléaire, Institute de Physique Nucléaire, Orsay — [5]Materialforschung, GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt

The passage of a swift heavy ion through tetrahedral amrophous carbon (ta-C), unlike through boron nitride (BN), leaves a conductive ion track behind. In this work three types of ion tracks were created: uninterrupted conductive ion tracks in ta-C only samples, tracks with a single, highly resistive barrier of BN and samples with two high-resistance BN barriers and a conductive island in the thin ta-C layer in between. The ta-C and BN layers were consecutively grown using mass selective ion beam deposition. The tracks were formed by irradiation with 30MeV C_{60}^{2+} fullerenes. The irradiated samples were analysed using conductive atomic force microscopy (cAFM) at room temperature. As a measure for the homogeneity of the created tracks, the distribution of track conductivities over a large-area of the sample is presented. Additionally, the current-voltage behaviour of the three variants of tracks will be shown.

DS 35.38 Wed 17:00 P1

Morphological heterogeneities of chemically exfoliated GaSe flakes and their impact on photoluminescence and Raman spectra — •Susanne Müller[1], Raul D. Rodriguez[1], Alexander Villabona[1,2], Tao Zhang[3], Ihsan Amin[3], Rainer Jordan[3], Santos A. Lopez-Rivera[2], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [2]Universidad de Los Andes, Applied Physics Lab, Merida 05101, Venezuela — [3]Professur für Makromolekulare Chemie, Department Chemie, Technische Universität Dresden, Mommsenstraße 4, 01069 Dresden, Germany

Gallium selenide (GaSe) is a two-dimensional material with a high anisotropy of the electrical and optical properties, which makes this material interesting for optoelectronic applications. We are interested in investigating the dependence of both Raman and photoluminescence (PL) spectra on the thickness and the morphology of GaSe flakes.

Therefore, we deposited chemically exfoliated GaSe flakes on highly oriented pyrolytic graphite. Raman spectra measured on GaSe flakes match bulk GaSe spectra, thus they were not modified by the preparation procedure. The thickness and morphology of the same flakes, where PL and Raman spectra were obtained, were determined by atomic force microscopy. We observed that the PL peak position varies for different flake thicknesses. We discuss the correlation of the flake orientation with respect to the polarization of incident light and the PL peak position. Furthermore, we can see that some of the typical bulk GaSe Raman modes vanish for some flakes.

DS 35.39 Wed 17:00 P1

Electronic properties and morphology of Cu-Phthalocyanine - C_{60} composite mixtures — •Friedrich Roth[1], Cosmin Lupulescu[2], Tiberiu Arion[1,3], Erik Darlatt[4], Alexander Gottwald[4], and Wolfgang Eberhardt[1,2] — [1]Center for Free-Electron Laser Science / DESY, Notkestraße 85, D-22607 Hamburg, Germany — [2]Inst. of Optics and Atomic Physics, TU Berlin, Straße des 17. Juni 135, D-10623 Berlin, Germany — [3]Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany — [4]Physikalisch-Technische Bundesanstalt (PTB), Abbestraße 2-12, D-10587 Berlin, Germany

Phthalocyanines in combination with C_{60} are benchmark materials for organic solar cells. Here we have studied the morphology and electronic properties of co-deposited mixtures (blends) of these materials forming a bulk heterojunction as a function of the concentration of the two constituents. For a concentration of 1:1 of CuPc:C_{60} a phase separation into about 100 nm size domains is observed, which results in electronic properties similar to layered systems. For low C_{60} concentrations (10:1 CuPc:C_{60}) the morphology, as indicated by Low-Energy Electron Microscopy (LEEM) images, suggests a growth mode characterized by (amorphous) domains of CuPC, whereby the domain boundaries are decorated with C_{60}. Despite of these markedly different growth modes, the electronic properties of the heterojunction films are essentially unchanged.

DS 35.40 Wed 17:00 P1

Work function measurements of sputtered TiO_2 in UHV ambience — •Sonja Urbahn, Rüdiger M. Schmidt, Alexandera Yatim, and Matthas Wuttig — I. Physikalisches Institut (IA), RWTH Aachen, 52056 Aachen

Titanium Dioxide (TiO_2) is a material with unique properties which have led to various applications such as anti-reflective coatings or self-cleaning surfaces. In particular, self-cleaning is possible by the high photocatalytic activity. However, the underlying process behind this attractive feature is still not understood in sufficient detail.

To improve the understanding of the correlation between the structural features of reactively sputtered TiO_2 with its photocatalytical activity we built a UHV Kelvin probe setup. Since self-cleaning implies the diffusion of photo generated charge carriers to the surface where they react with adsorbates, a change of the photocatalytic activity involves a change of the surface potential and thus of the work function. We show data measured with a Kelvin probe in UHV-ambience and link the behavior under UV illumination with structural properties. Although the Kelvin probe technique is very sensitive to the environment, the setup allows to measure data which show a correlation between the change in the work function under UV illumination and structural properties.

DS 35.41 Wed 17:00 P1

Electrical Properties of turbostratically disordered $[(\mathrm{SnSe})_{1.15}]_m(\mathrm{VSe}_2)_n$ misfit layer compounds — •Andreas Fiedler[1], Corinna Grosse[1], Ryan Atkins[2], David C. Johnson[2], and Saskia F. Fischer[1] — [1]Novel Materials, Department of Physics, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Chemistry, University of Oregon, Eugene OR 97401-3753, USA

Progress in materials science depends on the ability to discover novel materials and to investigate and understand their properties. The $[(\mathrm{SnSe})_{1+x}]_m[\mathrm{VSe}_2]_n$ ferecrystals are novel materials containing turbostratically disordered layers of SnSe and VSe_2. The aim of this study is to investigate the influence of the stacking sequence on the electrical properties. Therefore, these ferecrystals were electrically characterized by determining the in-plane resistivity and Hall coefficient between 4.2 K and 300 K, using the van der Pauw method. Assuming a single-band model, an increase in resistivity and a decrease in carrier concentration was observed for the $[(\mathrm{SnSe})_{1+x}]_m[\mathrm{VSe}_2]_1$ ferecrystals with $m = 1, 2, 3$ and 4, below an onset temperature between 100 K and 150 K. This is consistent with a localization of charge carriers, when, for example, a charge-density-wave (CDW) forms. The electrical measurements imply that it is possible to tailor the electrical properties of these ferecrystals by varying the stacking sequence, as the onset temperature increases with increasing m.

[1] Atkins, R. *et al.*: *J. Solid State Chem.* **202**, 128 – 133, (2013).

DS 35.42 Wed 17:00 P1

Characterization of $\mathrm{Zn}_x\mathrm{Mg}_{1-x}\mathrm{O}$:Al thin films deposited by RF sputtering — •Philipp Schurig, Marc Dietrich, Philipp Hering, Angelika Polity, and Bruno K. Meyer — Justus-Liebig-Universität Gießen, 1. Physikalisches Institut, Giessen, Deutschland

$\mathrm{Zn}_x\mathrm{Mg}_{1-x}\mathrm{O}$:Al is a transparent conductive oxide-semiconductor (TCO) with a tunable band gap which can be used for example as a photovoltaic electrode material. For this application a wide band gap as well as good conductivity is necessary. The thin films were deposited by RF sputtering on c-sapphire and float glass substrates. A ceramic ZnO target with two weight percent Al_2O_3 and mounted Mg-stripes was used. The band gap can be controlled through the magnesium content between 3.3 and 7.8 eV. The influences of the magnesium content on structural, optical and electrical properties are investigated using XRD-, SEM-, transmission- and Hall-measurements.

DS 35.43 Wed 17:00 P1

Stress Analysis on Copper Through Silicon Vias with Micro-Raman Spectroscopy — •Parisa Bayat[1], Dietmar Vogel[2], Raul D. Rodriguez[1], Evgeniya Sheremet[1], Sven Rzepka[2], Bernd Michel[2], and Dietrich R. T. Zahn[1] — [1]Technische Universität Chemnitz, Semiconductor Physics, D-09107 Germany — [2]Fraunhofer ENAS, Micro Materials Center, D-09126 Chemnitz, Germany

Most through silicon vias (TSVs) are filled with copper. The coefficient of thermal expansion of copper (c.a. 16-17 $\mathrm{x}10^{-6}$ /°C) is around six times higher than that of silicon (c.a. 2.7 $\mathrm{x}10^{-6}$ /°C). Therefore, temperature loadings on Cu-TSV lead to a very large local thermal expansion mismatch between copper and silicon/dielectric (e.g. SiO_2). This imposes very large stresses and strains in the vicinity of the interface region. The local strain/stress fields remaining after packaging processes can be high enough to introduce reliability issues in electronic devices. To evaluate the stress within the silicon surrounding of the TSV, micro-Raman spectroscopy is one of the most appropriate methods capable of providing local measurement of stress at high spatial resolution. We report on the analysis of the stress field in silicon adjacent to Cu-TSVs and the impact of thermal annealing in stress reduction.

DS 35.44 Wed 17:00 P1

Embedded Au nanoparticles in ZrO2 thin films for optical and electronical applications — •Sarah Seidel[1], Alex Sabelfeld[2], Tina Nestler[1], Ronald Otto[1], Johannes Heitmann[1], and Yvonne Joseph[2] — [1]TU Bergakademie Freiberg, Institut für Angewandte Physik, Leipziger Str. 23, 09599,Freiberg,Germany — [2]TU Bergakademie Freiberg, Institut für Elektronik- und Sensormaterialien, Gustav-Zeuner-Str. 3, 09599 Freiberg, Germany

The Au-nanoparticle (NP) was deposited via layer by layer self-assembly. The Au-nanoparticles are stabilized with dodecylamine and dissolved in toluene and have an average diameter of 4.5 nm. On the substrates an amin-terminated surface was prepared using (3-aminopropyl-)-triethoxysilan. We use the spin-coating technique for precipitation of the Au-NP. For the up-conversion a ZrO2 sol gel was doped with Er3+ und thin films were prepared using spin coating technique. We ascertained an optimum in the PL-signal for the 4I13/2-> 4I15/2 transition in Er3+ at 1536 nm with a doping concentration of 0.1 mol% Er3+ and 800°C annealing temperature. On top of the ZrO2 film we deposited a multilayer of Au-NP and analyzed the effect on the PL signal. For the nanofloating memory devices we deposited the Au-NC on a thin SiO2 tunnel oxide und use ZrO2 via electron beam evaporation as blocking oxid. The influence of tunnel oxide thickness on memory characteristics was investigated.

DS 35.45 Wed 17:00 P1

Transmission and optical properties of III-nitride multiple quantum wells and superlattices with disturbed periodicity — •Iglika Asenova and Evgenia Valcheva — Sofia University St. Kliment Ohridski, Faculty of Physics, 5 James Bourchier Blvd, 1164 Sofia, Bulgaria

The III-nitride semiconductors (AlN, GaN and InN) are object of a significant interest in the past years for they enable a wide range of innovative multiple layered nanosized systems and devices. Usually grown by MOCVD, the barrier periodic structures, such as superlattices and multiple quantum wells, sometimes exhibit a certain breach in their periodicity. In this study we will examine the 1 and 2 monolayer fluctuations in the barrier widths of III-nitride superlattices and multiple quantum wells and the effect the broken periodicity exerts upon the tunneling and the optical properties of the considered structures. Since in most cases the III-nitride structures are negatively doped, we restrain ourselves on examining the transmission coefficient in the conduction band only. Our calculations take account of the macroscopic internal polarization fields (spontaneous and piezoelectric) in the composing layers and the model we exploit is based on the envelope function approximation. Finally, we will compare our theoretical results with experimental data we have previously obtained.

DS 35.46 Wed 17:00 P1

Thin film stress evolution during deposition and interrupts: a thermodynamical assessment — •Amirmehdi Saedi and Marcel J. Rost — kamerlingh Onnes Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands

During Volmer-Weber thin film growth at conditions with sufficiently high atom mobility, the intrinsic film stress becomes compressive in the later stages. Moreover, upon deposition interruptions, the film reacts with a huge tensile jump, that surprisingly, is fully restored back to the original stress values before the interruption, if the deposition is switched on again.

Several mechanisms have been proposed to explain these phenomena, but none of them were able to explain all the details of the experimental results and they remain as mere hypotheses waiting for their proof to come. One suggestion is that the diffusion of adatoms into/out of the grain boundaries during the deposition/interruption would be responsible for the observed effects. There are some models, based on kinetic arguments, attempting to show that this mechanism is capable of reproducing the experimental observations. However all of these models suffer from a critical shortcoming as they do not take into account the thermodynamical aspects. These include e.g. relationships between the flux, adatom densities, chemical potentials of the surface and grain boundaries, and the elastic energy of the bulk. Here our aim is to check for the first time whether the adatom-GB theory can really survive the test of a rigorous thermodynamical analysis.

DS 35.47 Wed 17:00 P1

Organic lateral spin devices fabricated by trench technology — •Sreetama Banerjee[1,2], Peter Richter[1], Danny Reuter[2,3], Karla Hiller[2], Thomas Gessner[2,3], Dietrich R.T. Zahn[1], and Georgeta Salvan[1] — [1]Institute of Physics, Technische Universität Chemnitz, Germany — [2]Centre for Microtechnologies, Technische Universität Chemnitz, Germany — [3]Fraunhofer Institute ENAS, Chemnitz, Germany

Organic semiconductors are considered as attractive materials for spintronic applications. One of the current challenges in this field resides in the cost-effective fabrication of devices with laterally stacked electrodes and their integration at the wafer level. In this work lateral devices with electrodes separated by sub-100 nm gaps were fabricated using conventional UV lithography combined with semiconductor processing. Following a metallization step for the preparation of Au or Co electrodes, organic films were evaporated in high vacuum. Typically an average film thickness of 350 nm was required to form a nanomembrane that closes the gap between the electrodes. These structures allow the systematic investigation of electric and magnetoresistive properties of diamagnetic and paramagnetic organic semiconductor materials (in this case Alq_3 and cobalt phthalocyanine) as a function of the width of the electrode gap. These devices are intended to be used in magnetoresistive devices and molecular spintronics.

DS 35.48 Wed 17:00 P1

Characterisation of Terbium(III) Bis(phthalocyanine)/Cobalt Heterostructures by Ellipsometry and Magneto-optical Kerr Effect Spectroscopy — •Peter Robaschik[1], Michael Fronk[1], Svetlana Klyatskaya[2], Mario Ruben[2,3], Dietrich R.T. Zahn[1], and Georgeta Salvan[1] — [1]TU Chemnitz, 09126 Chemnitz, Germany — [2]KIT, 76344 Eggenstein-Leopoldshafen, Germany — [3]ICPMS, 67034 Strasbourg, France

The single molecule magnet (SMM) terbium(III) bis(phthalocyanine) is considered as a promising candidate for spintronic applications. In this work, films with thicknesses below 100 nm were deposited by organic molecular beam deposition on ferromagnetic, in-plane magnetized Co films. The (magneto-)optical properties were investigated by means of variable angle spectroscopic ellipsometry (VASE) and magneto-optical Kerr effect (MOKE) spectroscopy at room temperature. The molecular orientation was determined from the degree of uniaxial anisotropy of the optical constants and from the amplitude of the magneto-optical Voigt constant. The magnetic coupling of the molecules with the substrate is investigated by MOKE magnetometry in the temperature range from 4 K to 300 K.

DS 35.49 Wed 17:00 P1

Rigorous simulations and analysis of the optical response of silica sculptured thin films — •Eike Lennart Fricke[1], Christoph Grüner[2], Carsten Bundesmann[2], Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Universität Leipzig, Inst. für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e.V, Permoserstr. 15, 04318 Leipzig, Germany

We present full Mueller-matrix spectra of columnar silica sculptured thin films prepared by electron beam glancing angle deposition on silicon substrates in a wide spectral range from 0.5 to 6.5 eV. We analyse the data in two ways: (i) using anisotropic effective medium theory and (ii) using rigorous simulations based on the Rigorous Coupled Wave Approach.

The analysis by means of anisotropic Bruggeman effective medium approximation reproduces the measured data only qualitatively . Especially in the UV spectral range, where the long wavelength assumption of the Bruggeman EMA does no longer hold, the deviation drastically increases. As an alternative we employ the two-dimensional Fourier-Modal-Method, also known as Rigorous Coupled Wave Approach. The model takes the geometric parameters of the columns namely the inter-columnar distance, the radius and the inclination angle of the columns as well as their dielectric function as input parameters, that are optimised using non-linear regression.

A comparison of both methods highlights their different limitations for the analysis of complex surfaces.

DS 35.50 Wed 17:00 P1

Fabrication of sub-microstructures in solid copper surfaces by inverse laser microembossing — •Martin Ehrhardt, Pierre Lorenz, and Klaus Zimmer — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany

Both the ongoing miniaturization and integration of microdevices and the increasing complexity of microelectromechanical systems (MEMS) call for new machining and fabrication techniques. Laser microembossing is a manufacturing technology which enables the direct fabrication of three-dimensional microstructures in metal foils by replication of a master surface. In the present study a laser embossing process is employed which overcomes the traditional limitation of laser processing. A KrF excimer laser (wavelength $\lambda = 248$ nm, pulse duration $t_{pulse} = 25$ ns) was used to generate different kinds of 3D micro- and nanopatterns in metallic surfaces. The influence of the most important laser parameters on the embossing process with respect to the achieved quality of the generated surface pattern is presented. Therefore, the formed micro- and nanostructures were analyzed by scanning electron microscopy, atomic force microscopy, and white light interferometry. To investigate the material modification, e.g. defect formation and grain size changing due to the embossing process, cross section of the formed microstructures were analyzed by scanning electron microscopy.

DS 35.51 Wed 17:00 P1

Laser-based fabrication of MEMS structures on flexible polymeric substrates — Satish Panchani, •Pierre Lorenz, Martin Ehrhardt, and Klaus Zimmer — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04315 Leipzig, Germany

Silicon has been a primary material for fabrication of microelectromechanical systems (MEMS) for several decades. However, MEMS devices on flexible substrates are important for non-planar and non-rigid surface applications. To support the rapid advancements of non-silicon MEMS it is necessary to introduce innovative techniques to process-different MEMS material. Numbers of techniques for polymer-based microactuations have been demonstrated in recent years. One promising microactuation technique is based on the bimetallic effect which relies on the thermal coefficient of expansion mismatch between two components of sandwiched layers to provide displacement with change in temperature. In this study, the laser-based fabrication of MEMS on the example of the bimetal system Al/Mo on polyimide was studied. The temperature dependence of the system was measured by white light interference microscopy (WLIM) and verified by comparison with finite element studies. Furthermore, the resultant structures were investigated by scanning electron microscopy (SEM).

DS 35.52 Wed 17:00 P1

Topography-Controlled Alignment of DNA Origami Nanotubes on Nanopatterned Surfaces — •Bezuayehu Teshome[1,2], Stefan Facsko[1], and Adrian Keller[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Technische Universität Dresden, Mommsenstraße 13, 01069 Dresden, Germany

The controlled positioning of DNA nanostructures on technologically-relevant surfaces represents a major goal along the route toward the full-scale integration of DNA-based materials into nanoelectronic and sensoric devices. Previous attempts to arrange DNA nanostructures into defined arrays mostly relied on top-down lithographic patterning techniques combined with chemical surface functionalization.

Here we combine two bottom-up techniques for nanostructure fabrication, i.e., self-organized nanopattern formation and DNA origami self-assembly, in order to demonstrate the electrostatic self-alignment of DNA nanotubes on topographically patterned silicon surfaces. Self-organized nanoscale ripple patterns with periodicities ranging from 20 nm to 50 nm are fabricated by low-energy ion irradiation and serve as substrates for DNA origami adsorption. Electrostatic interactions with the charged surface oxide during adsorption direct the DNA origami nanotubes to the ripple valleys and align them parallel to the ripples. By optimizing the pattern dimensions and the Debye length of the adsorption buffer, we obtain an alignment yield of ˜ 70 %.

DS 35.53 Wed 17:00 P1

Investigation of metal nanoparticles formed by means of excimer laser irradiation of ion-exchanged glasses — •Maximilian Heinz[1], Manfred Dubiel[1], Jörg Meinertz[2], and Jürgen Ihlemann[2] — [1]Institute of Physics, Martin Luther University of Halle-Wittenberg, Halle, Germany — [2]Laser-Laboratorium Göttingen e. V., Göttingen, Germany

The localized formation of very small metal particles enables the generation of nanostructured materials, which are of interest for manifold applications in photonic and optoelectronic devices. This study investigates the space-selective precipitation of Ag and Ag/Au nanoparticles induced by 193 nm laser irradiation. The Ag and Au ions were introduced into the soda-lime silicate glass matrix by melt and ion exchange processes. The experimentally recorded spectra of optical spectroscopy demonstrated that the reduction of metal ions is due to defect generation, for example the generation electron hole centres. The sizes of nanoparticles, their distribution and their thermal stability were investigated as a function of the used laser parameters and the thermal treatments, respectively. Measurements of the optical density and experiments of small angle X-ray scattering (SAXS) allowed to identify the resulting surface plasmon resonance in correlation with the size and composition of formed nanoparticles.

DS 35.54 Wed 17:00 P1

Structuring of sub-wavelength Au nano-gratings — Christian Dull[1], •Gernot Goll[1], Silvia Diewald[1], Patrice Brenner[1], and Dmitry Strelnikov[2] — [1]DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Plasmon resonances of noble metal nanostructures are employed for developing sensors used for sensitive detection of molecules. We report on the structuring of arrays of sub-wavelength Au nano-gratings by electron-beam lithography on 20 x 20 mm^2 SiO$_2$ wafer pieces coated by a 64-nm thick PMMA resist layer. Sixteen grating arrays were exposed in one run, and the periodicity was varied between 100 nm and 1225 nm from array to array. A typical groove width of $W \approx 16$ nm was achieved. After development a 51-nm thick Au layer was evaporated. First measurements of the optical properties show a dip in the reflectance spectrum which moves from 600 to 1000 nm with increasing the periodicity from 400 to 700 nm. The polarization dependance was investigated as well by illuminating the grating with polarized light parallel and perpendicular to the direction of the lines. The result encourages the usage of such functionalized nano-grating surfaces for highly sensitive sensors.

DS 35.55 Wed 17:00 P1

Evolution of nanostructures induced by low energy ion sputtering on Si surfaces — •Kun Zhang, Hans Hofsäss, and Omar Bobes — II. Physikalisches Institut, Universität Göttingen, Göttingen, Germany

In order to study the allotropic effect on ripple formation on silicon surfaces induced by ion-beam sputter erosion, three types of silicon materials, single crystalline silicon, amorphous silicon grown with evaporation and amorphous silicon produced with ion irradiation, were irradiated with 1-keV Ar$^+$ ions at incidence angles from 30° to 87°. The ion fluence was 2 x 10^{17} /cm^2 for all irradiations. No ripples were formed for incidence angles smaller than 60° for all three materials, while perpendicular ripples occurred only in amorphous silicon at incidence angles between 82° and 85°. The presented results show, that ripple formation is influenced by the underlying silicon material, which reveal different atom densities depending on the growth of the Si substrate material.

DS 35.56 Wed 17:00 P1

Proton Beam Writing in p-GaAs and controlled subsequent electrochemical etching to create 3D structures for MEMS applications — •Charlotte Rothfuchs, Tristan Koppe, Ulrich Vetter, and Hans Hofsäss — 2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Recently, 3D structuring with Proton Beam Writing was demonstrated [1] and especially in combination with a variation of the irradiation fluence it has been shown to be a promising lithographic technique for semiconductors [2].

In order to create 3D structures with well-defined feature heights, we simulated the electrochemical etching process of irradiated p-GaAs with finite element simulations. The FEM simulations make use of Monte-Carlo simulations of the recoil distribution and implantation isolation data [3]. Based on those theoretical results it is possible to fabricate free-standing or undercutted structures in a controlled way. The fabrication is work in progress on which we are going to present latest results.

[1] J.A. van Kan et al., Appl. Phys. Lett. 83 (2003) 1629.

[2] M. Schulte-Borchers , U. Vetter, T. Koppe, H. Hofsäss, J. Micromech. Microeng. 22 (2012) 025011.

[3] H. Boudinov, A. V. P. Coelho, J. P. de Souza, Journal of Applied Physics 91(10) (2002) 6585

DS 35.57 Wed 17:00 P1

Self-organized nanopatterns on carbide surfaces by low energy ion irradiation with metal surfactants — •Omar Bobes, Kun Zhang, and Hans Hofsäss — II. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

We investigate the ripple pattern formation on tetrahedral amorphous carbon (ta-C) films during normal incidence ion beam erosion under simultaneous deposition of different metallic co-deposited surfactant atoms. We have irradiated ta-C films using 1 keV Ar ions under continuous deposition of titanium, tungsten, Molybdenum and Platinum surfactants. The co-deposition of small amounts of Ti, W and Mo leads to the steady state formation of a TiC, WC or MoC nanocomposite surface layer of few nm thickness. This has a tremendous impact on the evolution of nanoscale surface patterns on ta-C. While the surface keeps always flat under co-deposition of Pt-atoms, where there is no possibility for phase separation, ripple pattern are observed under co-deposition of Ti-atoms. The results confirm that the phase separation is the major driving force for the pattern formation in the case of irradiation with normal incident beam.

DS 35.58 Wed 17:00 P1

Influence of dipoles on the recombination in organic photovoltaic devices — •Jędrzej Szmytkowski — Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gdańsk, Poland

Although organic compounds are promising materials to use them in photovoltaic devices, the efficiencies of organic solar cells are still lower in comparison to inorganic photocells. The recombination of charge carriers leads to the loss of photocurrent, therefore a detailed theoretical description of this process is required. In the present work, an influence of interface dipoles on the recombination process is discussed. We show how electrical dipoles cause the reduction of nongeminate recombination in organic bulk heterojunction solar cells.

DS 35.59 Wed 17:00 P1

The degradation process of spin coated and flexo printed polytriarylamine thin films studied by IR ellipsometry — •Michael Sendner, Jens Trollmann, and Annemarie Pucci — Kirchhoff-Institut für Physik der Universität Heidelberg

Due to their potential in a roll-to-roll printing process, solution processed organic semiconductor thin films require basic research on the production-related properties. Especially, the knowledge of the degradation processes in organic devices consisting of such thin films is of importance for the application. Therefore, spin coated and flexo printed thin films of polytriarylamine (PTAA) that is used in p-type organic field effect transistors were degraded in a controlled manner by heat and high humidity (65°C, 85% r.h.) over a period of 60 days. The changes of vibrational modes of PTAA during the degradation process were studied in the mid infrared region by IR ellipsometry. Additionally, changes in film morphology were investigated with atomic force microscopy. Our work contributes to a better understanding of the degradation processes and helps to prevent aging of organic devices. Funding by BMBF (Polytos) is gratefully acknowledged.

DS 35.60 Wed 17:00 P1

Studying the contacts of organic solar cells — •Tobias Jenne[1,2], Felix Schell[1,2], Michael Scherer[1,3], Robert Lovrincic[1,3], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab GmbH, Speyerer Str. 4, 69115 Heidelberg, Germany — [2]University of Heidelberg, Kirchhoff-Institute for Physics, INF 227, 69120 Heidelberg, Germany — [3]TU Braunschweig, Institute for High-Frequency Technology, Schleinitzstr. 22, 38106 Braunschweig, Germany

During the last two decades, the power conversion efficiencies of organic solar cells (OCSs) substantially improved due to new materials and more complex device structures. For further optimization, a deeper understanding of the electric potential within OSCs is necessary. To achieve this, we perform in situ scanning Kelvin probe microscopy (SKPM) [1] measurements in high vacuum on cross sections of OSCs with different active layers and contact materials. These SKPM measurements are accompanied by IV characterization and linked with simulations to gain deeper insights into the fundamentals of complete OSC devices.

[1] Saive et al.: Imaging the Electric Potential within Organic Solar Cells, Adv. Funct. Mater. 2013, DOI: 10.1002/adfm.201301315

DS 35.61 Wed 17:00 P1

Impact of PC[60]BM on the Photo-Degradation of PCPDTBT — •Ulf Dettinger[1], Heiko Peisert[1], Hans-Joachim Egelhaaf[2], and Thomas Chassé[1] — [1]Eberhard-Karls-University, Institute for Physical and Theoretical Chemistry, Auf der Morgenstelle 18, D-72076 Tübingen, Germany — [2]Belectric OPV GmbH, Landgrabenstr. 94, D-90443 Nürnberg, Germany

Organic photovoltaic (OPV) offer a promising low-cost technology for the increasing energy demand of the future. Although higher device efficiencies are still required, the stability of the device materials remains an important factor for organic solar cells. It was shown, that the electron acceptor (EA) in bulk-heterojunction solar cells can affect the stability of electron donor materials in different ways, significantly [1], [2]. The impact of the commonly used EA material PC[60]BM on the Photo-Degradation of the Low-Band-Gap Polymer (LGB) PCPDTBT, as well as its own degradation under irradiation of standard Air Mass 1.5 conditions are studied. The Photo-Degradation of the materials was observed using UV/VIS and FTIR transmission spectroscopy. Basically PCPDTBT exhibits an enhanced stability compared to its blend with PC[60]BM. In particular, IR spectroscopy allows the discussion of the influence of PC[60]BM on the stability of the LBG polymer PCPDTBT.

[1] A. Dupuis et al. Eur. Phys. J. Appl. Phys. 2011, 56, 34104

[2] A. Distler et al. Chem. Mater. 2012, 24, 4397

DS 35.62 Wed 17:00 P1

Infrared spectroscopic study of molecular orientation and interaction in emitter systems for blue organic light emitting diodes — •David Gerbert[1,2,3], Tobias Glaser[1,2], Sebastian Beck[1,2], Christian Lennartz[1,4], and Annemarie Pucci[1,2,5] — [1]Kirchhoff-Institut für Physik, Heidelberg, Germany — [2]InnovationLab GmbH, Heidelberg, Germany — [3]Institut für Physikalische Chemie, Heidelberg, Germany — [4]BASF SE, Ludwigshafen, Germany — [5]Center of Advanced Materials, Heidelberg, Germany

In this study, two emitter systems for blue phosphorescent organic light emitting diodes were investigated by means of infrared spectroscopy. Thin layers of the single materials as well as doped layers have been achieved by evaporation under ultrahigh vacuum conditions. By performing angle-dependant measurements, a preferred molecular orientation has been found for the pure layer of the blue phosphorescent emitter material Ir(dbfmic)3. Such a preferred orientation could not be observed in thin films of the related emitter material Ir(dpbic)3, which can be explained by mutual screening of possible hydrogen bonds by the molecules' ligands themselves. Doping thin films of the matrix material SiDBF with different amounts of Ir(dbfmic)3 leads to small changes in the vibrational spectra with respect to the spectra of the single materials. These spectral changes are probably arising due to van-der-Waals forces and serve as a measure for the interface area between SiDBF and Ir(dbfmic)3 in the doped layers.

DS 35.63 Wed 17:00 P1

Morphology of Small Molecule Vacuum Deposited Organic Solar Cells from Analytical Transmission Electron Microscopy — •Felix Schell[1,2], Tobias Jenne[1,2], Diana Nanova[1,2,3], Anne Katrin Kast[1,2,4], Michael Scherer[1,3], Robert Lovrincic[1,3], Rasmus R. Schröder[1,4], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab GmbH, Heidelberg, Germany — [2]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [3]Institute for High-Frequency Technology, TU Braunschweig, Germany — [4]CellNetworks, BioQuant, Heidelberg University, Germany

For efficient charge generation and extraction in bulk heterojunction (BHJ) organic solar cells a suitable morphology of the active layer is crucial. However, most imaging techniques cannot distinguish among typical donor/acceptor systems used in BHJs, as these have similar characteristics. It has been shown that spectral information obtained by electron energy loss spectroscopy (EELS) and electron spectroscopic imaging (ESI) can be combined with multivariate statistics and machine learning to yield contrast between the two materials of the interpenetrating network of polymer solar cells. We extend these techniques to small molecule co-evaporated devices using fluorinated zinc phthalocyanine (F_4ZnPc) as donor and the fullerene C_{60} as acceptor. F_4ZnPc exhibits strong optical absorption features in EELS. Vacuum deposition of materials allows better control of morphology compared to solution processing, making it possible to directly correlate microstructural with electrical properties and ultimately with the performance of photovoltaic devices.

DS 35.64 Wed 17:00 P1

Charge Transport in Organic Solar Cells studied by (Photo-) CELIV — •Lars Müller[1,2], Diana Nanova[1,2,3], Norman Mechau[1,4,5], Robert Lovrincic[1,2,3], Uli Lemmer[1,2,4,5], Rasmus R. Schröder[6], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab GmbH, Heidelberg, Germany — [2]University of Heidelberg, Kirchhoff-Institute for Physics, Germany — [3]TU Braunschweig, Institute for High-Frequency Technology, Germany — [4]Karlsruhe Institute of Technology, Light Technology Institute, Germany — [5]Karlsruhe Institute of Technology, Institute of Microstructure Technology, Germany — [6]CellNetworks, BioQuant, University of Heidelberg, Germany

The efficiency of organic solar cells is determined by certain factors such as the materials themselves or the morphology. Parameters like thermal treatment or the processing technique highly influence some of these factors. Therefore, investigations on working devices are of utmost importance to deepen the already achieved understanding. We study this relationship between processes, materials, and intrinsic properties with the CELIV- and Photo-CELIV-technique (Photoinduced Charge Extraction by Linearly Increasing Voltage). Parameters such as overall device performance and morphology are linked to the CELIV-measured intrinsic properties charge carrier mobility and density. We investigate fully working solar cells with varying materials, processes and treatments. Additionally, charge-transport-studies on P3HT with different molecular weights are performed and compared to morphological changes, measured with analytical TEM and AFM.

DS 35.65 Wed 17:00 P1

Highly conductive vapor phase deposition of poly-3,4-ethylenedioxythiophene (PEDOT) as transparent electrode in organic devices — •Jakob Holfeld, Jan Ludwig Bormann, Lars Müller-Meskamp, and Karl Leo — Institut für Angewandte Photophysik - Technische Universität Dresden, Dresden, Deutschland

Highly conductive poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) is a promising alternative to the brittle and expensive indium tin oxide (ITO) as transparent electrode in organic solar cells. However, since PSS is highly acidic and hygroscopic, residual PSS can harm the devices after integration.

We investigate a PSS and water free deposition of PEDOT by introducing its monomer via vapor phase. This was carried out in different ways: In a process with iron-(III)-tosylate as pre-spin-coated oxidant, the addition of pyridine as base inhibitor or an amphiphilic block-copolymer as structure directing additive can lead to an dramatic improvement in conductivity (we achieved over 1100 S/cm) and makes PEDOT competitive to ITO. An all-gas-phase PEDOT layer growth with Fe(III)Cl as oxidant agent was also carried out, offering excellent possibilities on solvent sensitive and rough surfaces. Furthermore, planarization of silver nanowires by the use of vapor phase PEDOT, increasing their integrability into organic devices, was tested.

DS 35.66 Wed 17:00 P1

Solution-processed small molecule absorber layer for organic photovoltaics — •Matthias Saalfrank, Ludwig Bormann, Christian Körner, Lars Müller-Meskamp, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Straße 1, 01069 Dresden, Deutschland

Organic solar cells (OSCs) based on small molecules are commonly processed by vacuum deposition, while for polymer OSCs solution-processing (e.g. spin-coating) is the means of choice. Since the latter technique is also more promising for processing of small molecules in terms of low-cost mass production of organic photovoltaics, it is investigated in this work.

As a first step towards all-solution-processed small molecule OSC we deposit the active layer materials by spin-coating the donor-acceptor blend from solution onto ITO-coated glass substrates covered with an insoluble metal oxide transport layer (MoO_3 as hole transport layer for normal pin structures, TiO_2 as electron transport layer for inverted nip structures). Subsequently, the transport layer and aluminium electrode are deposited by vacuum evaporation. As the small-molecule donor we use an oligothiophene derivative with butyl side chains (DCV6T-Bu) and the commonly used acceptor PCBM. The solution-processed DCV6T-Bu:PCBM bulk heterojunction cells are compared with a corresponding vacuum-deposited DCV6T-Bu:C_{60} reference cell.

DS 35.67 Wed 17:00 P1

Atomistic calculation of thermoelectric properties of Si nanowires — Igor Bejenari and •Peter Kratzer — Fakultät für Physik and Center for Nanointegration (CeNIDE), Universität Duisburg-Essen, Duisburg, Germany

In contrast to the bulk materials conventionally used in thermoelectrics, nanostructured materials offer the possibility to design thermoelectric devices with improved efficiency by exploiting the quantum confinement of electrons and phonons on the nanoscale. In this case, a fully atomistic simulation considering both the electron and phonon band structures as well as electron-phonon interaction is required to estimate thermoelectric properties.

We study thermoelectric properties of Si square nanowires with <100> crystalline orientation taking into account atomistic electron-phonon interaction. In our model, facets <010> and <001> are passivated by hydrogen and there are Si dimers on the nanowire surface. The electronic structure was calculated by using the sp3-spin-orbit-coupled atomistic second-nearest-neighbor tight-binding model. The phonon dispersion and density of states were calculated in framework of Brenner's model. Based on Fermi's golden rule, the electron-phonon scattering rate was obtained by combining the electron and phonon eigenstates. Both elastic and inelastic scattering processes are taken into consideration. We used a solution of linearized Boltzmann transport equation to calculate transport characteristics. For the Si nanowire with a thickness of 1.6 nm at room temperature, the electron mobility is 422 $cm^2V^{-1}s^{-1}$ and ZT=0.8 at $n = 10^{20}$ cm^{-3}.

DS 35.68 Wed 17:00 P1

Bor-dotierte nanokristalline Diamantschichten für thermoelektrische Anwendungen — •Regina Berendakova, Nicolas Wöhrl und Volker Buck — Universität Duisburg-Essen und CENIDE, Fakultät für Physik, Lotharstr. 1, 47057 Duisburg, Deutschland.

Nanokristalline Diamantschichten werden durch Mikrowellenplasma unterstützte CVD aus einem $Ar/H_2/CH_4$ Plasma mit Zusatz von Trialkylboran $B(C_3H_7)_3$ p-dotiert erzeugt. In vorhergehenden Arbeiten wurde gezeigt, dass sich Bor-dotierte Nanodiamantschichten gut für thermoelektrische Anwendungen eignen. Dabei wurde eine thermische Leitfähigkeit niedriger als 10 W/mK und ein Seebeck-Koeffizient höher als 200 μV/K erreicht. Das Ziel der vorliegenden Arbeit ist die unabhängige Variation von Kristallitgröße (entscheidend für die thermische Leitfähigkeit) und Dotierstoffkonzentration (entscheidend für elektrische Leitfähigkeit).

DS 35.69 Wed 17:00 P1

Phase separation in the (Ti,Zr,Hf)CoSb$_{0.8}$Sn$_{0.2}$ system for improved thermoelectric properties — •Elisabeth Rausch[1], Benjamin Balke[1], and Claudia Felser[1,2] — [1]Institut für Anorganische und Analytische Chemie, Johannes Gutenberg-Universität Mainz — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

Heusler compounds with $C1_b$ structure are very promising materials for high-temperature thermoelectric applications. Their advantages are excellent electronic properties reflected in high power factors and high mechanical stability. However, disadvantage is their relatively high thermal conductivity. To overcome this obstacle the fabrication process of state-of-the-art p-type materials based on the TiCoSb system all involve a nano structuration via ball-milling. We herein present an alternative approach for the improvement of the thermoelectric properties. The effect of an intrinsic phase separation caused by isoelectronic alloying of Ti with Zr and Hf was investigated in the system $Y\mathrm{CoSb}_{0.8}\mathrm{Sn}_{0.2}$ (Y = Ti, Zr, Hf, $Ti_{0.5}Hf_{0.5}$, $Zr_{0.5}Hf_{0.5}$, $Ti_{0.5}Hf_{0.5}$, $Ti_{0.3}Zr_{0.35}Hf_{0.35}$). Upon this we achieved a thermal conductivity as low as 3.1 mW/K and a maximum figure of merit ZT of 0.9 at 979 K with a simple arc melting fabrication process.

DS 35.70 Wed 17:00 P1

Tailored thermoelectric efficiencies by controlling disorder — •Stefan Jakobs[1], Felix Lange[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

Thermoelectric materials require high complexity in material tailoring since both electrical and thermal transport properties play a significant role for their energy conversion efficiency.

A relatively high electrical conductivity as well as a low thermal conductivity is described by the phonon glass-electron crystal (PGEC) concept.

One approach is the concerted variation of stoichiometry (e.g. doping) to enhance the power factor or embedding 'rattling atoms' to reduce the lattice thermal conductivity.

Another approach is the controlled use of disorder. Sittner *et al.* have shown recently that disorder in pseudo-binary $(\mathrm{GeTe})_x(\mathrm{Sb_2Te_3})_{1-x}$ phase-change materials (PCM) can be tuned to obtain moderate thermoelectric efficiencies up to $zT = 0.7$ at 120 °C[1].

Here we explore the potential of concerted doping of pseudo-binary PCM with SnTe to further enhance thermoelectric properties.

[1] E.-R. Sittner *et al.*, Phys Status Solidi **A**, 210 (2013)

DS 36: Focus Session: Unconventional Spin Structures (jointly with MA)

Organizer: J. Fassbender (HZDR)

Time: Thursday 9:30–12:45 Location: BEY 118

Topical Talk DS 36.1 Thu 9:30 BEY 118

Topological Effects in Nanomagnetism - From Perpendicular Recording to Monopoles — •Hans-Benjamin Braun — University College Dublin

Similar to knots in a rope, the magnetization in a material can form particularly robust configurations. Such topologically stable structures include domain walls, vortices and skyrmions which are not just attractive candidates for future data storage applications but are also of fundamental importance to current memory technology. For example, the creation of soliton pairs of opposite chirality delimits the thermal stability of bits in current high anisotropy perpendicular recording media. After an introduction into various types of topological defects and their implications for current data storage it will be discussed how vortices can be robustly implemented in a system of nanoislands, a system that is in principle scaleable to the smallest length scales. It will then be shown how magnetic monopoles emerge as topological defects in densely packed arrays of nanoislands, a system also known as artificial spin ice. In contrast to conventional thin films, where magnetization reversal occurs via nucleation and extensive domain growth, magnetization reversal in 2D artificial spin ice is restricted to an avalanche-type formation of 1D strings. These objects can be viewed as classical versions of Dirac strings that feed magnetic flux into the emergent magnetic monopoles. It is demonstrated how the motion of these magnetic charges can be individually controlled experimentally and used to perform simple logic operations.

Topical Talk DS 36.2 Thu 10:00 BEY 118

Topology and Origin of Effective Spin Meron Pairs in Ferromagnetic Multilayer Elements — •Sebastian Wintz — Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Topological spin textures, such as vortices or skyrmions, are attracting significant attention because of their intriguing fundamental properties as well as their promising applicability in memory devices or spin torque oscillators. A particular topological texture that was theoretically predicted is the two-dimensional hedgehog state, also known as a 'Spin Meron'. It had been unclear, however, whether this kind of highly divergent magnetization structure can exist in real continuum systems. Only recently, evidence for the occurrence of meron-like states was reported for trilayer elements consisting of two ferromagnetic layers and a non-ferromagnetic interlayer [1]. On this background we now present a direct proof for the existence of meron-like states in trilayer elements via direct magnetic imaging. We also show that in the presence of biquadratic interlayer exchange coupling, such meron-like pair states may even represent the magnetic ground state of the system. Interestingly, the highly divergent magnetization distribution induces an additional, three-dimensional torus vortex that in-turn causes a symmetry break for the allowed topological pair configurations. [1] C. Phatak et al., Phys. Rev. Lett. 108, 067205 (2012). [2] S. Wintz et al., Phys. Rev. Lett. 110, 177201 (2013).

Topical Talk DS 36.3 Thu 10:30 BEY 118

Symmetry breaking in the formation of magnetic vortex states in a permalloy nanodisk — •Peter Fischer[1], Mi-Young Im[1], Keisuke Yamada[2], Tomonori Sato[3], Shinya Kasai[4], Yoshinobu Nakatani[3], and Teruo Ono[2] — [1]CXRO, LBNL, Berkeley CA USA — [2]Inst. f.Chem. Res., Kyoto University Japan — [3]U of Electro-Comm., Chofu, Japan — [4]Spintronics Group, Magn. Mat Center, NIMS, Tsukuba, Japan

Mesoscale phenomena will transform nanomagnetism research to the next level [1], as they add complexity and functionality, which are essential to meet future challenges of spin driven devices.

A priori, one would assume that the formation of magnetic vortex states should exhibit a perfect symmetry, because the magnetic vortex has four degenerate states. We report on the direct observation of an asymmetric phenomenon in the formation process of vortex states in a permalloy nanodisk by magnetic full field transmission soft x-ray microscopy [2]. Micromagnetic simulations confirm that an intrinsic Dzyaloshinskii*Moriya interaction is decisive for the asymmetric formation of vortex states.

Supported by the U.S. Department of Energy (# DE-AC02-05-CH11231) and by the Leading Foreign Research Institute Recruitment Program (# 2012K1A4A3053565) through the NRF of Korea funded by the Ministry of Education, Science and Technology.

[1] R. Service, Science 335 1167 (2012) [2] M.-Y. Im, P. Fischer, Y. Keisuke, T. Sato, S. Kasai, Y. Nakatani, T. Ono, Nature Communications 3 983 (2012)

15 min. break

Topical Talk DS 36.4 Thu 11:15 BEY 118

Commensurability and chaos in magnetic vortex oscillations — •Joo-Von Kim[1], Sébastien Petit-Watelot[1], Antonio Ruotolo[2,3], Rubén Otxoa[1], Karim Bouzehouane[2], Julie Grollier[2], Arne Vansteenkiste[4], Ben Van de Wiele[5], Vincent Cros[2], and Thibaut Devolder[1] — [1]Institut d'Electronique Fondamentale, UMR CNRS 8622, Univ. Paris-Sud, 91405 Orsay, France — [2]Unité Mixte de Physique CNRS/Thales and Univ. Paris-Sud, 1 av. A. Fresnel, 91767 Palaiseau, France — [3]Department of Physics and Materials Science, City University of Hong Kong, Kowloon, Hong Kong — [4]Department of Solid State Sciences, Ghent University, Krijgslaan 281-S1, B-9000 Ghent, Belgium — [5]Department of Electrical Energy, Systems and Automation, Ghent University, Sint-Pietersnieuwstraat 41, B-9000 Ghent, Belgium

In spin-torque driven vortex oscillations in small nanocontacts, periodic reversal of the vortex core appear above a critical current and results in a self-modulation phenomenon involving gyration and relaxation oscillations. By tuning the ratio between the gyration frequency and the rate of core reversal, we show that commensurate phase-locked and incommensurate chaotic states are possible, resulting in Devil's staircases with driving currents. This represents a novel dynamical regime for vortex dynamics in which the gyrotropic dynamics is self-modulated by the periodic core reversal.

Topical Talk DS 36.5 Thu 11:45 BEY 118

Dynamic ordering of vortex cores in interacting mesomagnets — •Valentyn Novosad — Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA

Manipulation of the magnetization is a key problem in applied magnetism. In this talk a novel method of controlling the ground state using two interacting vortices as a model system will be presented. A spin vortex consists of an in-plane and out-of-plane (core) regions of magnetization. Control of an in-plane magnetization has been demonstrated previously, whereas manipulation of the vortex cores remain challenging. In our work this is achieved by driving the system from the linear regime of constant vortex gyrations to the non-linear regime of vortex-core reversals at a fixed excitation frequency of one of the coupled modes. Subsequently reducing the excitation field to the linear regime, stabilizes the system to a polarity combination whose resonant frequency is decoupled from the initialization frequency [2]. The transition of the state from one polarity combination to the other is clearly evident from the contrast in the microwave absorption amplitude obtained by gradually increasing the rf-field to higher magnitudes at the resonant frequency of one of the modes and subsequently decreasing it. The results of this work may benefit future advancement of dynamically controlled spintronic devices, such as magnonic crystals, spin-torque oscillators, and magnetic memories.

[1] S. Jain, et al., Applied Physics Letters, 102, 052401 (2013).

[2] S. Jain et al., Nature Comm., DOI: 10.1038/ncomms2331 (2012).

Topical Talk DS 36.6 Thu 12:15 BEY 118

Magnetic Vortex Core Reversal by Excitation of Spin Waves — •Hermann Stoll[1], Matthias Kammerer[1], Matthias Noske[1], Markus Sproll[1], Georg Dieterle[1], Ajay Gangwar[1,2], Markus Weigand[1], Manfred Fähnle[1], Georg Woltersdorf[2], Christian H. Back[2], and Gisela Schütz[1] — [1]MPI for Intelligent Systems, Stuttgart, Germany — [2]University of Regensburg, Germany

Essential progress in the understanding of nonlinear magnetic vortex dynamics was achieved when low-field vortex core reversal by (sub-GHz) excitation of the vortex gyromode was observed using time-resolved scanning transmission X-ray microscopy [1]. This switching scheme, based on the creation and subsequent annihilation of a vortex-antivortex pair [1,2], has been proved to be universal and independent of the type of excitation, e.g., pulsed magnetic fields or spin transfer torque (STT).

Magnetic vortex structures possess azimuthal spin wave modes showing eigenfrequencies in the multi-GHz range. We could demonstrate [3-5] by experiments and micromagnetic simulations that even much faster unidirectional vortex core reversal can be achieved by exciting these spin wave modes with (multi-GHz) rotating magnetic fields. In that way we have been able to switch vortex cores selectively within less than 100 ps.

[1] B. Van Waeyenberge et al., Nature 444, 462 (2006) [2] A. Vansteenkiste et al., Nature Physics 5, 332 (2009) [3] M. Kammerer et al., Nature Communications 2, 279 (2011) [4] M. Kammerer et al., PRB 86, 134426 (2012) [5] M. Kammerer et al., APL 102, 012404 (2013)

DS 37: Focus Session: Sustainable Photovoltaics with Earth Abundant Materials I

Energy conversion technologies, especially photovoltaics, exibit enormous growth aiming at extremely high power capacities per year. Therefore nontoxicity, low energy footprint and abundance of the materials used for photovoltaic devices are among the key requirements to a sustainable photovoltaic technology. Binary and ternary oxides and related materials are promising as the key materials to reach these goals. From this point of view copper and zinc based materials like ZnO, ZnS, Cu_2O, $ZnSnN_2$, Cu_2S, Zn_3P_2, Cu(In,Ga)Se_2, $Cu_2ZnSn(S,Se)_4$ are of special interest. For instance, the combination of ZnO and Cu_2O has been shown to be one of the promising approaches for next generation photovoltaics. Theoretical predictions promise efficiencies of such solar cells of up to 18%. Recently a breakthrough has been reported demonstrating of ZnO/Cu_2O thin film solar cell with efficiency of ca. 5%. Nevertheless, the fabricated devices are still far from commercial application. Further fundamental investigations are needed in order to understand the relevant materials and device physics in detail and to improve the efficiency of the cells. Progress on the growth of thin films, heterostructures and nanostructures, as well as new fabrication approaches will be discussed. Special attention will be given to the effect of the materials properties on the device efficiency, phenomena at interfaces, band gap alignment and surface passivation. This topical session aims to give an overview over the latest developments in the dynamic field of sustainable photovoltaics with earth abundant materials. (Organizers: Andrey Bakin and Andreas Waag, Technische Universität Braunschweig)

Time: Thursday 9:30–12:45 Location: CHE 91

Invited Talk DS 37.1 Thu 9:30 CHE 91
Photovoltaics with Copper Oxides — •Bruno Meyer — 1. Physikalisches Institut, JLU Giessen

The p-type conducting Copper-oxide compound semiconductors (Cu2O, Cu4O3 and CuO) provide a unique possibility to tune the band gap energies from 2.1 eV to the infrared at 1.40 eV into the middle of the efficiency maximum for solar cell applications. They appear to be an attractive alternative absorber material in terms of abundance, sustainability, and non-toxicity of the elements. Heterostructures with n-type AlGaN and MgZnO will be the basis of the solar cells. We present experimental results on the band offsets between the three copper oxides and the transparent conducting oxides and nitrides. Based on these finding various combinations of thin-film solar-cells are fabricated and compared to each other. The role of intrinsic defects and interface properties are discussed.

Invited Talk DS 37.2 Thu 10:00 CHE 91
Energy band alignment at interfaces of polycrystalline semiconductors for thin film solar cells — •Andreas Klein — Technische Universität Darmstadt, Germany

Thin film solar cells utilizing CdTe or Cu(In,Ga)Se_2 chalcogenide semiconductors have reached conversion efficiencies close to or even above 20%, respectively. The device structure of these cells is characterized by a sequence of an ohmic back contact, an unintentionally doped medium-gap chalcogenide as light absorber, a wide-gap chalcogenide buffer layer, and a transparent conducting oxide (TCO) front contact. Critical for high conversion efficiencies of such heterojunction devices is the energy band alignment at the various interfaces, which enable or block current transport. Historically, suitable interface properties have been achieved mainly by empirical device optimization. Photoelectron spectroscopy (PES) can provide detailed information on the chemical and electronic interface properties. This contribution introduces the experimental approach of interface analysis using PES and reviews available experimental data and understanding of interfaces for various thin film solar cells. In addition to interface properties of CdTe, Cu(In,Ga)Se_2, metallic back contacts, and TCO front contacts, the challenge of finding new absorber materials and device structures will be particularly addressed.

Invited Talk DS 37.3 Thu 10:30 CHE 91
Use of doped oxides for enhanced performance solar cells — •Judith MacManus-Driscoll — Dept. Materials Science, University of Cambridge, U.K.

ZnO and TiO2 are two of the most commonly used n-type metal oxide semiconductors in new generation solar cells due to their abundance, low-cost and stability. ZnO and TiO2 can be used as active layers, photoanodes, buffer layers, transparent conducting oxides, hole-blocking layers and intermediate layers. Doping is essential to tailor the materials properties for each application. The dopants used and their impact in hybrid solar cells and all inorganic solar cells are presented. In addition, the advantages, disadvantages and commercial potential of the various low energy fabrication methods of these oxides are presented.

Coffee break (15 min)

Invited Talk DS 37.4 Thu 11:15 CHE 91
Nanowire device concepts for thin film photovoltaics — •Silke Christiansen — Helmholtz Zentrum für Materialien und Energie, Berlin — Max-Planck-Institute for the Science of Light, Erlangen

Aligned silicon nanowire (SiNW) arrays to aim for power conversation efficiencies >>15% are fabricated on multi-crystalline Si layers on glass substrates using reactive ion etching with prior lithographic patterning using densely packed polystyrene (PS) spheres. Diameter, length, density and shape of SiNWs can be controlled and tuned for highest absorptions (close to 90%). Cell concepts with SiNWs are realized: (i) a hybrid organic/inorganic cell using SiNWs as absorber and PEDOT:PSS as a hole conducting polymer; (ii) a semiconductor-insulator-semiconductor (SIS) cell with SiNWs as absorbers, oxide (few Å thick Al2O3 by atomic layer deposition-ALD)) tunneling barriers for charge carrier separation and a transparent conductive oxide (TCO here: Al:ZnO, by ALD). Initial thin film solar cell prototypes reached open-circuit voltages of > 680 mV, short-circuit current densities of even > 35 mA/cm2 and efficiencies >13%. Advanced analytics to improve materials and cells are: (i) electron beam induced current (EBIC) to study charge carrier distributions; (ii) electron backscatter diffraction (EBSD) to study structural quality of the multi-crystalline Si layer; (iii) integrating sphere measurements to study optical properties and (iv) 4-point nano-probing to study electrical properties. Alternative electrodes such as graphene or silver nanowire webs are studied to even further improve the cells.

Invited Talk DS 37.5 Thu 11:45 CHE 91

Core shell ZnO nanowire heterostructures for solar cells — •Vincent Consonni — Laboratoire des Matériaux et du Génie Physique, Grenoble INP - CNRS, Minatec, 3 parvis Louis Néel 38016 Grenoble, France

ZnO nanowires (NWs) have received increasing interest due to their potential applications for instance in photovoltaic devices via core shell heterostructures. The core can be composed of ZnO NWs as electron transporting layer and the shell can comprise an absorbing layer such as a direct band gap semiconductor or a chemical dye in order to form type II heterostructures [1,2]. In this work, the structural properties and electron scattering mechanisms are investigated for SnO2:F thin films acting as front electrodes in nanostructured solar cells made from ZnO NW heterostructures [3]. A special emphasis is made on the formation mechanisms of ZnO NWs in solution by specifically focusing on polarity and crystal orientation effects [4]. Also, the light absorption properties of core shell ZnO NW heterostructures are studied by rigorous coupled wave analysis in order to design nanostructured solar cells. Eventually, several types of solar cells made from core shell ZnO NW heterostructures are fabricated by using different types of absorbing layers and their photovoltaic performances are tested under dark and AM 1.5G standard illumination conditions [1,2].

[1] V. Consonni et al., Appl. Phys. Lett. 98, 111906 (2011). [2] E. Puyoo et al., J. Phys. Chem. C 116, 18117 (2012). [3] V. Consonni et al., Acta Mater. 61, 22 (2013). [4] S. Guillemin et al., J. Phys. Chem. C 117, 20738 (2013).

Invited Talk DS 37.6 Thu 12:15 CHE 91

Potential and challenges of kesterite-type materials for thin film solar cells — •Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie

$Cu_2ZnSn(S,Se)_4$ thin film semiconductors have attracted much interest recently because of their potential application as absorber layers in thin-film solar cells. These kesterite-type materials can be derived from the chalcopyrite semiconductor $CuInSe_2$ by replacing the relatively rare element indium alternatingly with the more abundant elements tin and zinc, which would allow sustainable deployment of this technology on the terawatt scale. The close relation of their crystal structures raises the hope that also for the kesterite materials the excellent optoelectronic properties of their chalcopyrite cousins can be achieved. Although conversion efficiencies of 12% have now been demonstrated for kesterite-type solar cells, this value is still substantially lower than the record efficiencies above 20% for $Cu(In,Ga)Se_2$. One major challenge with kesterite materials lies in the control over defects and secondary phases imposed by the quartenary nature of this semiconductor. Interestingly, solution-based synthesis methods so far have yielded electronically superior material compared to vacuum-based deposition methods, in contrast to previous experience with the synthesis of almost any other inorganic semiconductor.

DS 38: Focus Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale VI (jointly with O)

Time: Thursday 10:30–13:15 Location: TRE Ma

Topical Talk DS 38.1 Thu 10:30 TRE Ma

Localization at the edge of 2D topological insulator by Kondo impurities — •Boris Altshuler[1], Igor Aleiner[1], and Vladimir Yudson[2] — [1]Physics Department, Columbia University, New York, NY 10027, USA — [2]Institute for Spectroscopy, Russian Academy of Sciences,Troitsk, Moscow 142190, Russia

Recent interest to the topological insulators [1] is inspired by the fact that their boundaries host gapless electronic excitations, which are extended and make the system conductive even in the presence of a potential disorder. 1D edge of a 2D topological insulator is predicted to have perfect conductance (2e2/h): right and left moving electrons carry opposite spins and potential disorder cannot flip spins and thus causes neither back-scattering nor the usual 1D localization.

What if there are localized spins coupled to the edge electrons? It turns out that the conductivity is still perfect provided that this coupling conserves the z-projection of the total spin of the impurities and electrons. Magnetic anisotropy violates this conservation and causes the backscattering even at T=0, i.e. an arbitrary small density of the spins with arbitrary weak anisotropy of the coupling leads to Anderson localization of the edge states in long enough samples [3]. The conclusion follows from the mapping of the electron-spin coupling to the well-studied problem [2] of disordered Luttinger liquid.

1. M.Z. Hasan and C.L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
2. T.Giamarchi and H.J.Schulz, Phys. Rev. B 37, 325 (1988).
3. B.L.Altshuler, I.L.Aleiner, V.I. Yudson Phys. Rev. Lett 111, 086401 (2013)

DS 38.2 Thu 11:00 TRE Ma

Multiple Exciton Generation in Si and Ge Nanoparticles with high pressure core structures — •Stefan Wippermann[1], Marton Vörös[2], Dario Rocca[3], Adam Gali[4], Gergely Zimanyi[2], and Giulia Galli[2] — [1]Max-Planck-Institute for Iron Research, Düsseldorf — [2]University of California, Davis — [3]Universite de Lorraine, Nancy — [4]Budapest University of Technology and Economics

Multiple exciton generation (MEG) in semiconductor nanoparticles (NPs) is a promising path towards surpassing the Shockley-Queisser limit in solar energy conversion efficiency. Recent studies demonstrate MEG to be more efficient in NPs than in the bulk, including Si. However, the increased efficiency is observed only on a relative energy scale in units of the gap: quantum confinement (QC) effects believed to be responsible for efficient MEG in NPs, also increase their optical gap, swiftly shifting the MEG threshold beyond the solar spectrum.

We present density functional and many body perturbation theory calculations of the electronic, optical, and impact ionization properties of Si and Ge nanoparticles (NPs) with core structures based on high-pressure bulk Si and Ge phases. Si and Ge particles with a BC8 or ST12 core structure exhibit significantly lower optical gaps and multiple exciton generation (MEG) thresholds, and an order of magnitude higher MEG rate than diamondlike ones of the same size (1).

(1) S. Wippermann et al., Phys. Rev. Lett. 110, 046804 (2013)

DS 38.3 Thu 11:15 TRE Ma

Advanced time-evolution method for optical absorption spectra calculations — •Tobias Sander and Georg Kresse — Computational Materials Physics, University of Vienna, Sensengasse 8/12, 1090 Vienna, Austria

The Green's function formalism from many-body perturbation theory gives access to electronic structure calculation within the quasiparticle picture, as well as provides for calculating optical absorption spectra. Within the traditional ansatz [1], a Bethe-Salpeter like equation for the polarizability is solved. This requires to diagonalize an in general non-hermitian and complex matrix (BSE matrix). Usually, the off-diagonal elements of the BSE matrix are neglected and this is referred to as Tamm-Dancoff approximation. The computational effort can be reduced by using the time-evolution ansatz [2] which avoids the matrix diagonalization. We present a method based on the time-evolution algorithm, that finally avoids storing and diagonalizing the BSE matrix. This leads to a reduction of the scaling w.r.t the system size N from N^5 to N^3. Finally, we present first results for typical systems.

[1] S. Albrecht, L. Reining, R. Del Sole, G. Onida, PRL 80, 4510 (1998)
[2] W. G. Schmidt, S. Glutsch, P. H. Hahn, F. Bechstedt, PRB 67, 085307 (2003)

DS 38.4 Thu 11:30 TRE Ma

New starting point for the calculation of optical properties — •Igor Reshetnyak[1,2] and Lucia Reining[1,2] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, F-91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF)

The Bethe-Salpeter Equation based on Hedin's GW approximation to the self-energy is a powerful approach for describing electron-hole interactions in optical properties and photo-absorption spectra. However, in its current formulation it is both computationally heavy and displays cancellation effects not accounted for analytically. We discuss the sources of these cancellations and the possibility of putting them forward explicitly. We furthermore assess alternative formulations and sets of approximations to the BSE. For each of them we examine its behavior on model systems as well as their computational applicability. Finally we suggest possible directions for further investigations.

DS 38.5 Thu 11:45 TRE Ma

Electron-Energy Loss and Inelastic X-ray Scattering of CuO from First Principles — •Claudia Rödl, Francesco Sottile, Matteo Gatti, and Lucia Reining — Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau cedex, France and European Theoretical Spectroscopy Facility (ETSF)

Even though the strongly correlated transition-metal oxide CuO has many fields of application (potential absorber material in photovoltaic devices, pigment in glass and ceramics, building block of cuprate superconductors,...), surprisingly little is known about its electronic excitations from a theoretical point of view. The band gap and all electronic excitations in its vicinity are governed by the intricate interplay between itinerant O $2p$ and localized Cu $3d$ electrons. Complex many-body effects, that are still not well understood nowadays, determine the screening of the electron-electron interaction.

Electron-energy loss and inelastic x-ray scattering experiments yield direct access to the wave-vector- and frequency-dependent loss function $-\mathrm{Im}\,\varepsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega)$, and, hence, to the screened Coulomb interaction W. We use time-dependent density-functional theory (TDDFT) to calculate the loss spectrum of CuO and discuss the occurring *d-d* and plasmon excitations. This allows us, by comparing theory and experiment, to assess the quality of the screened Coulomb interaction which is a key quantity for many-body approaches, for instance, *GW* and Bethe-Salpeter calculations.

DS 38.6 Thu 12:00 TRE Ma

Optical Spectra from Molecules to Solids: Insight from Many-Body Perturbation Theory — •Caterina Cocchi and Claudia Draxl — Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

The spurious long-range behavior of time-dependent (TD) density functional theory (DFT) is a well known source of error in describing bound excitons in solids. Remarkably, TD-DFT is often able to capture the optical features of isolated systems, even with the most simple exchange-correlation kernels, like the TD local density approximation. With the example of molecular crystals, we aim at solving the puzzle when and why TD-DFT can be relied on. We answer this question by confronting TD-DFT with many-body perturbation theory (GW and Bethe-Salpeter equation), which is the most accurate methodology to describe optical excitations in solids. Our results are obtained with the all-electron code "exciting" (http://exciting-code.org), where all the quantities entering the two formalisms are treated on the same footing [1]. In-depth analysis allows us to identify the shortcomings of TD-DFT in predicting the excitonic spectra of extended systems and to understand when this methodology is capable of providing correct results.

[1] S. Sagmeister and C. Draxl, Phys. Chem. Chem. Phys. 11, 4451 (2009)

DS 38.7 Thu 12:15 TRE Ma

Relativistic Solar Cells — •Paolo Umari[1], Edoardo Mosconi[2], and Filippo De Angelis[2] — [1]Dipartimento di Fisica e Astronomia, Università di Padova, via Marzolo 8, I-35131 Padova, Italy — [2]Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), CNR-ISTM, Via Elce di Sotto 8, I-06123, Perugia, Italy

Hybrid AMX$_3$ perovskites (A=Cs, CH$_3$NH$_3$; M=Sn, Pb; X=halide) have revolutionized the scenario of emerging photovoltaic technologies. Indeed, a rapid evolution led, very recently, up to 15% efficient solar cells. CH$_3$NH$_3$PbI$_3$ has so far dominated the field, while the similar CH$_3$NH$_3$SnI$_3$ has not been explored for photovoltaic applications, despite the reduced band-gap. Replacement of Pb by the more environment-friendly Sn would facilitate the large uptake of perovskite-based photovoltaics. Despite the extremely fast progress, the materials electronic properties which are key to the photovoltaic performance are relatively little understood. Here we develop an effective GW method incorporating spin-orbit coupling which allows us to accurately model the electronic, optical and transport properties of CH$_3$NH$_3$SnI$_3$ and CH$_3$NH$_3$PbI$_3$, opening the way to new materials design. The different CH$_3$NH$_3$SnI$_3$ and CH$_3$NH$_3$PbI$_3$ properties are discussed in light of their exploitation for solar cells, and found to be entirely due to relativistic effects.

DS 38.8 Thu 12:30 TRE Ma

Solar nanocomposites with complementary charge extraction pathways for electrons and holes: Si embedded in ZnS — •Stefan Wippermann[1], Marton Vörös[2], Adam Gali[3], Francois Gygi[2], Gergely Zimanyi[2], and Giulia Galli[2] — [1]Max-Planck-Institute for Iron Research, Düsseldorf — [2]University of California, Davis — [3]Budapest University of Technology and Economics

We propose that embedding silicon nanoparticles (NP) into amorphous, non-stoichiometric ZnS leads to promising nanocomposites for solar energy conversion. Using ab initio molecular dynamics simulations we show that upon high temperature amorphization of the host chalcogenide, sulfur atoms are drawn to the NP surface. We found that the sulfur content may be engineered to form a type II heterojunction, with complementary charge transport channels for electrons and holes, and that sulfur capping is beneficial to lower the nanoparticle gap, with respect to that of NPs embedded in oxide matrices. Our analysis was conducted using density functional theory with local and hybrid functionals and many body perturbation theory at the GW level.

DS 38.9 Thu 12:45 TRE Ma

Ultraviolet photo-emission spectroscopies from Koopmans-compliant functionals — •Ngoc Linh Nguyen[1], Giovanni Borghi[1], Andrea Ferretti[2], Ismaila Dabo[3], and Nicola Marzari[1] — [1]Theory and Simulations of Materials, École Polytechnique Fédérale de Lausanne, Station 12, 1015 Lausanne, Switzerland. — [2]Centro S3, CNR-Istituto Nanoscienze, I-41125 Modena, Italy — [3]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, USA.

We study the photo-electron properties of organic photovoltaic molecules using Koopmans-compliant functionals [1] as well as the Perdew-Zunger self-interaction correction (PZ-SIC) [2] to density-functional theory. A simple method for simulating ultraviolet photo-emission spectra (UPS) of molecules has been implemented. It is based on a plane-wave approximation for the final states to account for the spectra intensities. Our calculations show that Koopmans-compliant functionals provide ionization potentials and electron affinities closely comparable with those obtained by many-body perturbation theory (GW). In addition, we find that UPS spectra computed imposing the Koopmans' condition on the PZ-SIC functional are in remarkable agreement with experimental results.

Refs: [1] I. Dabo, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, and M. Cococcioni, Phys. Rev. B 82, 115121 (2010); [2] J. P. Perdew and A. Zunger, Phys. Rev. B 23, 5048 (1981).

DS 38.10 Thu 13:00 TRE Ma

Self-consistent dynamical embedding in real space — •Wael Chibani[1], Xinguo Ren[1,2], Patrick Rinke[1], and Matthias Scheffler[1] — [1]*Fritz Haber Institute of the Max Planck Society, Berlin, Germany* — [2]*Key Laboratory of Quantum Information, USTC, Hefei, China*

Density-functional theory with its local-density (LDA) and generalized gradient approximations (GGA) is known to fail for localized states. To extend *ab initio* approaches to this domain, we have devised an embedding scheme that facilitates the treatment of the physically important part of a system with electronic structure methods, that are computationally too expensive for periodic systems, whereas the rest of the periodic system is treated with computationally less demanding approaches, i.e. LDA/GGA, in a self-consistent manner. Our scheme is based on the concept of dynamical mean-field theory (DMFT) [1]. However, in contrast to the original DMFT formulation for correlated model Hamiltonians, we consider here the unit cell as embedded cluster in an *ab initio* way, that includes all electronic degrees of freedom. The performance of our scheme is demonstrated by treating the embedded region with hybrid functionals for simple bulk systems, e.g. Si or NiO. The total energy and the density of states converge rapidly with respect to the computational parameters and approach their bulk limit with increasing cluster size. By treating the embedded region with *GW* we were able to improve the band gap using only a small cluster. The effect of self-consistency in *GW* for the embedded region will also be addressed. [1] A. Georges *et al.*, Rev. Mod. Phys. **68**,14 (2006)

DS 39: Focus Session: Resistive Switching by Redox and Phase Change Phenomena VI (Kinetics and Transport in PC materials)

Time: Thursday 9:30–11:15 Location: CHE 89

Invited Talk DS 39.1 Thu 9:30 CHE 89

Switching kinetics in phase change materials — •Martin Salinga — RWTH Aachen, Sommerfeldstrasse 14, 52074 Aachen, Germany

Phase change materials are essential ingredients for next-generation electronic memory devices and reconfigurable electronics for their ability to be switched between states with very different resistivity within nanoseconds upon electrical excitation, while being stable over many years otherwise. It is these materials' characteristic combination of electronic excitability of their amorphous phase and their unconventional structural transformations that makes this seeming contradiction possible. Thorough experimental investigations of both phenomena allowed us to gain deeper insights into the fundamental properties of this family of materials. Recently the crystallization kinetics could be traced back to an extremely high fragility of the undercooled liquid phase. A comprehensive model including the quenching rate dependence of the glass formation and relaxation processes in the glass managed to explain the different experimental observations reported in literature. Our investigations of transient effects in electrical excitation of phase change materials concentrate on the changes around the threshold for resistivity breakdown in the amorphous phase. The results from both studies are discussed to give guidance to experimentalists and theoreticians aiming for a fundamental understanding of the physics of phase change materials.

DS 39.2 Thu 10:00 CHE 89

Growth of GeTe/Sb_2Te_3 Superlattices by Molecular Beam Epitaxy — •Rui Ning Wang[1], Jos Boschker[1], Raffaella Calarco[1], Jamo Momand[2], and Bart Kooi[2] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Zernike Institute for Advanced Materials, Groningen, Netherlands

For their ability to be reversibly switched between a crystalline and a stable amorphous phase, drastically changing their optical and electrical properties, GeTe and GeSbTe alloys (GST) have already been used in optical data storage applications for more than a decade. These materials are also serious candidates in electrical data storage devices because of non-volatility and high scalability. Simpson *et al.* have demonstrated that arranging GeTe and Sb_2Te_3 into a superlattice (SL) structure enables an analogous crystalline ↔ crystalline switching mechanism that greatly reduces the switching energy while improving the cyclability and switching speed [1].

In the work presented here, GeTe/Sb_2Te_3 SLs were grown on Si(111) substrates by molecular beam epitaxy. The epi-structures showed an out-of-plane Si $\langle 111\rangle \parallel$ SL $\langle 0001\rangle$ orientation and in-plane Si $\langle 11\bar{2}\rangle \parallel$ SL $\langle 10\bar{1}0\rangle$ orientation. An effort has been made to reduce the layer thickness of each constituent down to 1 nm for GeTe and to 2 nm for Sb_2Te_3, and improve surface and interface roughness. These state of the art superlattices provide a clear platform for fundamental studies of the switching mechanism in such structures.

[1] R. Simpson *et al.*, Nature nanotechnology, vol. 6, pp. 501-5, 2011.

DS 39.3 Thu 10:15 CHE 89

Phase-Change Materials: Impact of Disorder on Thermal and Electrical Transport — •Karl Simon Siegert[1], Felix Lange[1], and Matthias Wuttig[1,2] — [1]1.Physikalisches Institut (IA), RWTH Aachen University — [2]JARA - Fundamentals of Information Technology, RWTH Aachen University, 52056 Aachen, Germany

Disorder plays a vital role in crystalline phase-change compositions along the pseudo-binary line between GeTe and Sb_2Te_3 (GSTs). Many of these compounds crystallize in a rocksalt-like structure where one sublattice is fully occupied by Te atoms, while a random distribution of Ge, Sb and vacancies populates the second sublattice. This gives rise to pronounced configurational disorder which impacts charge transport by localizing electrons [1].

A thorough investigation of GST stoichiometries and measurements of thermal conductivity by the 3ω method towards low temperatures (50 K) demonstrate that thermal transport is affected by disorder as well. Especially disordered vacancies act as efficient point scattering sources and disrupt phonon heat transport. Hence, thermal and electrical conductivities are affected by the same mechanism, albeit on different scales. This finding opens up a pathway to manipulate electrical and thermal transport properties in GSTs through the degree of disorder. Such transport engineering is not only crucial for future data storage devices based on resistance switching, but should be highly valuable for thermoelectrics as well.

[1] T. Siegrist *et al.*, Nat. Mater. 2011, 10, 202-208.

DS 39.4 Thu 10:30 CHE 89

Drift of the voltage dependence of resistance in melt-quenched phase change memory cells — •Martin Wimmer, Matthias Kaes, and Martin Salinga — 1. Physikalisches Institut (IA), RWTH Aachen

Phase change materials are the essential ingredients for promising novel non-volatile electronic memory devices. The materials have the ability to be switched upon electrical excitations within nanoseconds between two otherwise stable phases, which show large contrast in electrical resistivity. One approach to improve the information density of such a phase change memory device is to store several logic bits in one physical cell by distinguishing between different states of partial crystallization (multilevel storage). For such a device it is important that the resistance is stable over many orders of magnitude in time. While for the crystalline phase this requirement is sufficiently fulfilled, the amorphous phase shows a strong time dependence of the resistance, the so-called resistance drift. In literature this effect is often ascribed to structural relaxation effects, which, as a consequence, lead to changes of electronic defect states and thereby altering the electronic properties, e.g. the conductivity, of the material. In this work, we study the effect of drift on the voltage dependence of the resistance in phase change memory devices on a time scale starting only microseconds after melt-quenching. Our experimental findings are interpreted within the common drift theories, e.g. the Poole-Frenkel model for conduction in the sub-threshold regime.

DS 39.5 Thu 10:45 CHE 89

Structure and Transport Properties of Pseudo Ternary SnTe, GeTe, Sb_2Te_3 Chalcogenides — •Felix R. L. Lange[1], Stefan Jakobs[1], Tim Labohm[1], Jan Kirchhof[1], Tobias Schäfer[1], K. Simon Siegert[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA - Fundamentals of Information Technology, RWTH Aachen University, 52056 Aachen, Germany

Ternary chalcogenides along the line between GeTe and Sb_2Te_3 have caught interest due to their high degree of disorder in the crystalline phase. Only recently Siegrist *et al.* reported an insulator-to-metal transition in the crystalline phase [1]. Depending on the annealing temperature of the thin films the electrical resistivity is either thermally activated or develops metallic at elevated temperatures. While little change is noticed on the carrier concentration the electrical resistance spans over six orders of magnitude at room temperature. Based on DFT calculations Zhang *et al.* identified clusters of vacancies to localize the wave functions responsible for charge transport in the early meta-stable cubic phase [2]. Dissolution of these clusters upon annealing then leads to a delocalization of the corresponding wave functions concomitant with the transition to the metallic state. Here we explore pseudo ternary alloys of SnTe, GeTe and Sb_2Te_3 in order to utilize both, stoichiometry and annealing condition to adjust the degree of disorder concomitant with tailored transport properties.

[1] T. Siegrist *et al.*, Nat. Mater. **10**, 202-208 (2011)
[2] W. Zhang *et al.*, Nat. Mater. **11**, 952-956 (2012)

DS 39.6 Thu 11:00 CHE 89

Disorder Induced Localization in Crystalline Phase Change Materials: $Sn_1Sb_2Te_4$ as a Model System — •Tobias Schäfer[1], Hanno Volker[1], Felix vom Bruch[1], Artur Romanov[1], Stefan Jakobs[1], Felix Lange[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA FIT, RWTH Aachen University

The electrical resistivity of the crystalline phase of many phase-change materials (PCMs) can be reduced by several orders of magnitude via annealing. This annealing effect can be attributed to the reduction of disorder in the material, which is initially exceptionally high in most PCMs and therefore dominating the transport. Disorder-dominated transport is a key feature of most PCMs due to their low electron correlation, while most other semiconductors and semimetals feature both disorder and correlation effects (Mott-Anderson-physics).

While previous studies on disorder-dominated transport in PCMs have been mostly conducted on $Ge_1Sb_2Te_4$ and other materials on the pseudobinary line between GeTe and Sb_2Te_3 [1,2], this study focuses on the isoelectronically replaced $Sn_1Sb_2Te_4$ to emphasize the universality of disorder-dominated transport in PCMs. Low-temperature transport and magneto-transport measurements are utilized to analyze the influence of disorder in PCMs.

[1] T. Siegrist et al., Nat. Mater. 10, 202 (2011)

[2] N.P. Breznay et al., Phys. Rev. B 86, 205302 (2012)

DS 40: Focus Session: Resistive Switching by Redox and Phase Change Phenomena VII (Optical properties and theory of PC materials)

Time: Thursday 11:30–13:00 Location: CHE 89

DS 40.1 Thu 11:30 CHE 89

Near-field optical investigation of Sb_2Te_3 hexagonal platelets in the mid-infrared — Benedikt Hauer[1], Tobias Saltzmann[2], Ulrich Simon[2], and •Thomas Taubner[1] — [1]Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]Institute of Inorganic Chemistry (IAC), RWTH Aachen University, 52056 Aachen, Germany

Antimony telluride (Sb_2Te_3) has gained attention as a candidate for phase-change memory applications, thermoelectric devices, and as a three-dimensional topological insulator. We imaged Sb_2Te_3 hexagonal platelets grown by hydrothermal synthesis using scattering-type scanning near-field optical microscopy (s-SNOM).

In the mid-infrared spectral range between 5.5 μm and 11 μm we find a highly symmetric and very sharp pattern in both optical amplitude and phase images. This optical pattern is correlated to a growth spiral and extends over the entire platelet. We assume domains with different surface-densities of charge carriers to be the origin of the optical contrast. These domains could be caused by growth twins in the crystal lattice. On epitactically grown Sb_2Te_3 samples we did not observe any comparable pattern.

This contribution demonstrates the unique potential of s-SNOM to visualize fundamental material properties that are hard to address with any other method.

DS 40.2 Thu 11:45 CHE 89

Large area optical tuning of mid-infrared resonant nanostructures by using low-loss phase-change materials — Ann-Katrin Michel[1], Peter Zalden[2,3], •Dmitry Chigrin[1], Aaron Lindenberg[2,3,4], and Thomas Taubner[1] — [1]Institute of Physics 1A, RWTH Aachen University, Aachen, Germany — [2]Stanford Institute of Materials and Energy Physics, SLAC, Menlo Park, USA — [3]PULSE Institute, SLAC, Menlo Park, USA — [4]Department of Materials Science and Engineering, Stanford University, Stanford, USA

Phase-change materials (PCMs) are stable in at least an amorphous and a crystalline phase. This structural contrast of PCMs is accompanied by a huge difference of the refractive index n.

So-called metallic nanoantennas are able to produce significantly enhanced and confined electromagnetic fields. By varying the fabrication parameters, such as antenna material, geometry and substrate their resonance frequency can be tuned over a wide range. If these nanoantennas are embedded in PCMs, the variation in n can be used for tuning of the resonance. To minimize any damping due to a high absorption of PCMs, we chose Ge3Sb2Te6 as an example with a very small imaginary part $\epsilon 2$ of the dielectric function $\epsilon(\nu)$ in the MIR [1].

Since reversible switching of the antenna resonances would allow for interesting applications e.g. in the field of plasmonics, we investigated the use of femtosecond laser pulses for reversible switching, where the huge benefit lies in the switching of several antenna arrays at the same time (total diameter ca. 270 μm2). [1] Michel et al. Nano Lett. 13 (8), 2013.

DS 40.3 Thu 12:00 CHE 89

Understanding Stability Trends at Clean and Oxidized GeTe Surfaces — •Volker Deringer[1] and Richard Dronskowski[1,2] — [1]Institute of Inorganic Chemistry, RWTH Aachen University, 52056 Aachen, Germany — [2]Jülich–Aachen Research Alliance (JARA)

Phase-change memory devices are becoming smaller and smaller, necessarily so. In turn, the surfaces of phase-change materials surely deserve increased attention: the surface–volume ratio rises dramatically on the nanoscale, and surface oxidation (detrimental to long-term switching capability) becomes important. Here, we present comprehensive DFT computations for the prototypical germanium telluride (GeTe) surfaces. We have simulated freshly cleaved and reconstructed surfaces, as well as molecular O_2 adsorption and higher oxygen coverage.

The predicted stability trends are then investigated and rationalized at the hand of chemical-bonding analysis: by partitioning the electronic structure into bonding (stabilizing) and antibonding contributions, we offer a straightforward explanation for why one type of surface termination is favorable while the other is not. This model can be directly extended to surface oxidation: more stable surfaces are rather inert whereas others readily react with oxygen, thereby reducing unfavorable antibonding interactions at the surface. Our simulations of oxidized GeTe surfaces agree well with previous XPS measurements, and the atom-resolved and chemical-bonding techniques provide a worthwhile additional viewpoint.

DS 40.4 Thu 12:15 CHE 89

Vibrational Properties of Layered Tellurides from First-Principles Calculations — •Ralf Stoffel[1] and Richard Dronskowski[1,2] — [1]Institute of Inorganic Chemistry, RWTH Aachen University, 52056 Aachen — [2]Jülich–Aachen Research Alliance (JARA)

We present recent results of density-functional theory (DFT) based calculations of the vibrational properties of layered tellurides, such as Sb_2Te_3 and several $Ge_xSb_yTe_z$ (GST) compounds, using the ab initio force-constant method. The latter compounds are well-known phase-change materials on the pseudo-binary tieline GeTe–Sb_2Te_3, and they can be switched easily between amorphous and crystalline phases which significantly differ in their optical and electrical properties. Here, we discuss the thermodynamically stable hexagonal polymorphs of those GST phases. Common DFT approaches are known to fail in describing the weak, non-covalent Te–Te interactions within these layered structures. For that reason, we investigate the influence of dispersion-corrected DFT on the calculated properties. We discuss phonon properties such as band structures and densities of states as well as thermochemical data such as Gibbs free energies or heat capacities. Other derived properties will also be presented, for example Grüneisen and atomic displacement parameters. The reliability of the results is verified by comparing the theoretical data with experimental references obtained from nuclear inelastic scattering (NIS). Finally, we show how our results help to interpret experimental data, and also give a more detailed insight into the theoretical background.

DS 40.5 Thu 12:30 CHE 89

Structural phase transitions in thin films under elastic and microstructural constraints — •Stefan Wagner and Astrid Pundt — Institut für Materialphysik, Universität Göttingen

Palladium hydrogen (PdH) thin films are used as a model system to investigate the impact of elastic and microstructural constraints on structural phase transitions. Mechanical stress arises both from thin film clamping on the substrate and at coherent interfaces in phase mixtures. It changes chemical potentials, modifying phase stabilities regarding phase boundaries and enthalpies of formation. Mechanical stress is superimposed by microstructural constraints, channeling stress relaxation mechanisms such as the formation of misfit dislocations.

In this paper hydrogen absorption and hydride formation in PdH thin films with different microstructure and clamping conditions are investigated [1]. Hydrogen solubilities and phase stabilities are quantitatively related to the hydrogens' chemical potential by in-situ XRD as well as stress and electromotive force (EMF) measurement [2]. They differ for films with coherent interfaces and films where stress relaxation is possible. [1] S. Wagner, A. Pundt, Acta Mat. 59 (2011) 1862. [2] S. Wagner, M. Moser, A. Pundt et al., Int. J. Hydr. Energy 38 (2013) 13822.

DS 40.6 Thu 12:45 CHE 89

Reducing the number of domain orientations of Sb_2Te_3 on Si(111) by surface engineering — •Jos Boschker[1], Jamo Momand[2], Bart Kooi[2], and Raffaella Calarco[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

The epitaxy of interfacial phase change memory [1] requires a detailed understanding of the stacking of van der Waals solids (Sb_2Te_3) with 3-dimensional solids (GeTe). Here we use to growth of Sb_2Te_3 on Si(111) as a model system for studying this kind of epitaxy. We show that Sb_2Te_3 grown on Si(111)-(7x7) exhibits ten different domain orientations, even though only one is expected based on the symmetries of the two materials. We show that the in-plane rotations are due to the formation of a coincidence lattice between Sb_2Te_3 and the dangling bonds on the Si(111)-(7x7) surface. Furthermore, we demonstrate that the number of domain orientations can be reduced to two when Sb_2Te_3 is grown on Si(111)-($\sqrt{3}$x$\sqrt{3}$)R30°-Sb or Si(111)-(1x1)-H. Finally, in-plane rotations of ultrathin Sb_2Te_3 layers on Si(111)-(7x7) and Si(111)-($\sqrt{3}$x$\sqrt{3}$)R30°-Sb are determined using angular resolved RHEED. This detailed understanding of the epitaxy of Sb_2Te_3 on Si(111) is important for the growth of Sb_2Te_3/GeTe superlattices and thus for the optimization of interfacial phase change memory.

[1] R. E. Simpson, P. Fons, A. V. Kolobov, T. Fukaya, M. Krbal, T. Yagi, and J. Tominaga, Interfacial phase-change memory, Nat. Nanotechnol., vol. 6, pp. 501-5, Aug. 2011.

DS 41: Focus Session: Sustainable Photovoltaics with Earth Abundant Materials II

Time: Thursday 15:00–17:30 Location: CHE 91

DS 41.1 Thu 15:00 CHE 91

Electroless deposition of porous zinc oxide films on sheets of aluminium — •Stephanie Künze and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Metal foils, wires or metalized polymer fibres are of interest as substrate electrodes for porous wide band-gap semiconductors in dye-sensitized solar cells (DSC) if protected against corrosion by a passivating oxide layer. Here, aluminium sheets were used to deposit porous zinc oxide for DSC. For the deposition of ZnO, the natural insulating Al_2O_3 layer on Al was removed by chemical etching in hydrochloric acid (HCl). A subsequent treatment in alkaline zinc hydroxide (zincate stain) was used to grow Zn in order to protect the metal and to provide a reactive surface for the deposition of ZnO. Porous ZnO films were then prepared by electroless deposition without any electrical connections on such pre-treated Al substrates from aqueous $ZnCl_2$ saturated with O_2. The xanthene dye *EosinY* was used to form pores in the growing crystalline ZnO. The film thickness of porous ZnO and the coverage of the metal surface increase with the deposition time and with the amount of Zn from the pre-treatment. These results were contrasted with the results from electrochemical depositions at an applied potential under otherwise identical conditions. For comparison purposes, depositions of porous zinc oxide on etched sheets of Zn were analyzed to provide a virtually unlimited supply of Zn. Al and Zn unlike other elements often used in photovoltaics offer the chance of large-scale applications since both are abundant on earth.

DS 41.2 Thu 15:15 CHE 91

Copper oxide for photovoltaic applications — Alexander Wagner, Nikolai Ehrhardt, Mathieu Stahl, Andreas Fahl, Johannes Ledig, Lorenzo Caccamo, Andreas Waag, and •Andrey Bakin — Institute of Semiconductor Technology, Technische Universität Braunschweig, Hans-Sommer-Strasse 66, 38106 Braunschweig, Germany

Oxides and related materials are extremely promising materials for sustainable photovoltaics providing abundance and nontoxicity. For an all-oxide solar cell p-type Cu2O is a promising absorber material with a high absorption coefficient and 2.1 eV band gap. Theoretically predicted efficiencies of Cu2O based solar cells are up to 20% but till now the devices on the base of copper oxide show significantly lower efficiencies. Further fundamental investigations are needed in order to understand in depth the physics behind the devices on the base of these materials and to improve the efficiency of the cells. Influence of different buffer layers on the performance of an all oxide solar cell is discussed. Controllably grown Cu2O layers are also prerequisites for fabrication of high efficiency solar cells and vapor phase epitaxial growth of Cu2O is presented.

DS 41.3 Thu 15:30 CHE 91

The effect of hydrogen in RF-sputtered copper oxide thin films — •Philipp Hering, Benedikt Kramm, Julian Benz, Peter Klar, and Bruno Meyer — 1. phys. Inst., JLU Giessen, Deutschland

Cuprous oxide (Cu2O), despite its band gap of 2.17 eV, is a promising material for photovoltaic applications, due to its high absorption coefficient, non-toxicity and the abundance of its composing elements. While recently more attention has been paid to heterojunctions, highest efficiencies were reached by employing copper sheets, which were oxidized and annealed at high temperatures. For technological applicability, a thin film deposition process with mass production capabilities, which provides decent film properties at low temperatures, has to be established. Such thin films however suffer from low carrier mobilities and lifetimes, due to their polycrystalline nature. It has been reported that post treatments with hydrogen can passivate grain boundaries. Copper oxide thin films were deposited from a metallic copper target via reactive radio frequency magnetron sputtering, utilizing gaseous argon and oxygen under the addition of hydrogen. The films were characterized and the influence of hydrogen was investigated via X-ray diffraction, X-ray photoelectron spectroscopy, Raman spectroscopy, photoluminescence and Hall effect.

DS 41.4 Thu 15:45 CHE 91

Improved Anchoring of Indoline Dyes for the Sensitization of *ZnO* — Felix Fiehler[1], •Jane Falgenhauer[1], Melanie Rudolph[1], Christoph Richter[1], Hidetoshi Miura[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. — [2]Chemicrea Inc, Iwaki, Fukushima, Japan.

D149 is a well-established indoline dye for the sensitization of ZnO. Although high efficiencies can be obtained, the dye partly desorbs from the ZnO surface in contact with the redox electrolytes in dye-sensitized solar cells. Similar indoline dyes with a second carboxylic binding group at the molecule to attach to the ZnO surface showed higher stability [1]. In this work, sandwich-cells were built with electrodeposited ZnO on conductive glass as the working electrode which was sensitized with D149 or D149-derivatives DN91, DN216 and DN285 having two binding groups of different length of a hydrocarbon spacer. Current-voltage curves and dynamic measurements like electrical impedance spectroscopy at AM1.5 illumination and intensity-modulated photovoltage/photocurrent spectroscopy (IMVS/IMPS) were performed. The observed shift of effective band positions, the recombination resistance and the observed lifetime of the excited state were found to be comparable for the different sensitizers. DN216, however, showed higher photocurrent densities than the D149 reference and the cell characteristics were more reproducible. Implications for the future development of dye-sensitized solar cells based on solution-processed ZnO will be discussed. [1] J. Falgenhauer, C. Richter, H. Miura, D. Schlettwein *Chem.Phys.Chem.*, 13, 2893-2897 (2012).

DS 41.5 Thu 16:00 CHE 91

Silver nanowire networks for ITO replacement — •Julian Reindl and Lukas Schmidt-Mende — Department of Physics, University of Konstanz, Germany

Indium-tin oxide (ITO) is the state-of-the-art material for transparent electrodes in optoelectronic devices such as solar cells. However, Indium is a very scarce material and the increasing demand for transparent conductors drives the need for alternative materials.

Here we present networks of silver nanowires which are embedded in a matrix of the doped polymer PEDOT:PSS. This system enables a good conductivity through the metallic pathways, supported by the polymer. The latter also provides a good light transmission in the visible range.

DS 41.6 Thu 16:15 CHE 91

Study of the Crystalline Fraction Dependent Microstructure Characteristics of $\mu c - SiOx : H$ for Micromorph Solar Cells — •Max Klingsporn[1], Simon Kirner[2], Ioan Costina[1], and Daniel Abou-Ras[3] — [1]IHP, im Technologiepark 25, Frankfurt (Oder), Germany — [2]PVcomB, Schwarzschildstr. 3, 12489 Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Since some years $\mu c - SiOx : H$ attracted attention as a wide band gap material for the use in silicon based thin film solar cells. With material parameters tunable over wide ranges it qualifies for several applications. One of the most popular today is the use as an intermediate reflector layer in tandem solar cells. In the present work a SiOx sample series with a fixed elemental composition and a crystalline fraction (Fc) varied between 10 and 60 % was studied by X-ray photoelectron spectroscopy and scanning transmission electron microscopy combined with electron energy loss spectroscopy. The analysis reveals a transition from an amorphous phase of silicon suboxides to a two-phase system of silicon nanofilaments embedded in a SiO_2 matrix. A consistent correlation between Fc and electrical properties is found.

Keywords: $\mu c - SiOx : H$, STEM, EELS, Plasmon Imaging, XPS, ESCA, Raman, IRL, Micromorph, Solar Cells, Silicon Filaments

DS 41.7 Thu 16:30 CHE 91

High Vapour Pressure Selenization and Grain Growth Mechanisms of Sulfide-CZTS Precursors — •Justus Just[1], Steffen Kretzschmar[1], Stephan van Duren[1], Roland Mainz[1], Claudia Coughlan[2], Kevin Ryan[2], and Thomas Unold[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie — [2]University of Limerick, Irland

We report about the fundamental growth mechanisms and properties of CZTS,Se absorber layers, produced by selenization of various different precursors at high selenium partial pressures deposited in vacuum as well as in non-vacuum processes. We will compare the selenization and growth mechanisms of precursors consisting of PVD-deposited CZTS at low temperature, CZTS nanoparticles and wurzite CZTS nanorods. Samples are characterized by scanning electron microscopy, depth resolved elemental analysis (energy dispersive X-ray fluorescence) and X-ray diffraction. In order to estimate the electronic quality of the selenized material, photoluminescence measurements are carried out additionally. While the selenization is similar depending on the temperature and selenium partial pressure for different types of precursors, the grain growth mechanisms are found to be substantially different, as the grain growth is depending on nucleation and interdiffusion of cations.

DS 41.8 Thu 16:45 CHE 91

Growth and characterization of polycrystalline $Cu_2ZnSnSe_4$ layers with a preferential grain orientation — •Christoph Krämmer[1], Johannes Sachs[1], Mario Lang[1], Chao Gao[1], Sabine Schuster[1], Michael Powalla[2], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Light Technology Institute, KIT, and Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany

The absence of the technologically relevant metals indium and gallium makes the kesterite $Cu_2ZnSnSe_4$ (CZTSe) material system a promising alternative to the established Cu(In,Ga)Se_2. Hiqh-quality CZTSe layers on GaAs would be highly desirable for the study of basic material properties such as the band structure. We use selenization of a Sn/Cu/ZnSe(001) structure on GaAs(001) substrate in order to fabricate polycrystalline CZTSe layers with preferential grain orientation. In this contribution we present a detailed investigation of those layers by means of X-ray diffraction and Raman spectroscopy. These measurements prove that a highly preferential grain orientation in all three dimensions is indeed obtained in the formed CZTSe film.

DS 41.9 Thu 17:00 CHE 91

Raman investigation of $Cu_2ZnSnSe_4$ layers with and without preferential grain orientation — •Mario Lang[1], Christoph Krämmer[1], Johannes Sachs[1], Chao Gao[1], Sabine Schuster[1], Michael Powalla[2], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Light Technology Institute, KIT, and Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany

$Cu_2ZnSnSe_4$ (CZTSe) is attracting more and more attention as an alternative to the well-established Cu(In,Ga)Se_2 material system for thin-film photovoltaics due to its composition of earth-abundant elements. Raman spectroscopy is a powerful technique to detect secondary phases in the thin-film absorber layers. Futhermore, using polarization-dependent measurements it is possible to gain information on the crystal orientation when performed on samples with a preferential grain orientation. We present a comparative study of polycrystalline absorber layers with and without a preferential grain orientation. The results are analyzed using theoretical modeling of the Raman line intensities.

DS 41.10 Thu 17:15 CHE 91

Radiative recombination in Cu2ZnGeSe4 single crystals — •Sergiu Levcenko[1], Maxim Guc[2], Steffen Kretzschmar[1], Ernest Arushanov[2], and Thomas Unold[1] — [1]Helmholtz Zentrum Berlin für Materialien und Energie, 14109 Berlin,Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, MD 2028 Chisinau, Moldova

Cu2ZnGeSe4 (CZGSe) is considered as a promising absorber material for thin film solar cells, owing to its high absorption coefficient and its optimum band gap for the sunlight spectrum. While structure and optical properties of CZGSe are studied, little is known about its electronic structure. To reveal intrinsic defect properties of this semiconductor we carried out photoluminescence spectroscopy on the CZGSe single crystals grown by chemical vapour transport. At low temperature two defect related transitions at about 1.2 and 1.3eV were observed. These transitions are systematically investigated by means of temperature and excitation dependent measurements and the defect recombination model has been proposed.

DS 42: Thermoelectric Materials

Time: Thursday 15:00–19:00 Location: CHE 89

DS 42.1 Thu 15:00 CHE 89

Thermoelectric Property Modification in Hybrid Semiconducting/Metal Superlattices and Local Characterization by SThM — •Guodong Li[1,2], Daniel Grimm[1,2], and Oliver. G Schmidt[1,2] — [1]Institute for Integrative Nanosciences, IFW Dresden, Germany — [2]Technische Universität Chemnitz, Material Systems for Nanoelectronics, Germany

Nanostructured materials show great promising applications in thermoelectric industry not only owing to their intrinsic quantum confinement effects but also related to the enhanced boundary or interface scattering to phonon transport. The ideal modified thermoelectric structures should have much decreased thermal conductivity while keeping thermal power unaffected or even enhanced. Here, we combine the self-rolling and compressing technique to demonstrate a straight forward route to make hybrid superlattices consisting of a large number of nanomembranes that are mechanically stacked on top of each other. Depending on what kind of material we choose as the interfacial layer, we have successfully fabricated superlattices composed of different kinds of hybrid interfaces. Together with conventional time-domain thermoreflectance (TDTR) method that shows the cross-plane thermal conductivity of as-fabricated superlattice being nearly two orders of magnitude smaller than the thin film, we also characterize the local thermal transport property by using scanning thermal microscopy (SThM) technique. By taking the standard thermal samples as references, we are purposing to develop a quantitative model to characterize the cross-plane thermal transport property of fabricated superlattices.

DS 42.2 Thu 15:15 CHE 89

Thermoelectric properties of meso-porous thin films from laser-assisted wet-chemically doped group-IV nanoparticles — •Anton Greppmair[1], Benedikt Stoib[1], Tim Langmann[1], Nils Petermann[2], Hartmut Wiggers[2], Martin Stutzmann[1], and Martin S. Brandt[1] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching — [2]Institut für Verbrennung und Gasdynamik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg

We present recent studies on the morphology and the thermoelectric properties of thin films of laser-sintered group-IV nanoparticles. The structure size of the meso-porous network can be controlled by the laser fluence used for sintering, doping is achieved by immersing the nanoparticle film in a liquid containing the dopants prior to sintering. Conductivity and thermopower measurements provide insight into the doping efficiency and confirm n- and p-type doping. For the doping with group-V elements we find a threshold concentration, above which the conductivity can be increased by several orders of magnitude using different dopant concentrations in the dopant solution. Adsorption of the dopant atoms to the nanoparticles is the limiting process for the doping efficiency. The doping process was successfully transferred to various SiGe alloy compositions ranging from pure Ge to pure Si. Thermal properties were also investigated by microscopic infrared thermography.

[1] B. Stoib et al., Physica Status Solidi A **210**, 153 (2012)

DS 42.3 Thu 15:30 CHE 89

Thermoelectric transport in Sb_2Te_3 thin films — •Nicki F. Hinsche[1], Florian Rittweger[2], Tomáš Rauch[1], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, DE-06120 Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, DE-06120 Halle

Bulk chalcogenides, e.g. Bi_2Te_3 and Sb_2Te_3, as well as related heterostructures and ternary alloys are well known as efficient thermoelectric materials [1,2]. Today these chalcogenides are known to be strong topological insulators, i.e. their bulk is insulating, while their surface is metallic due to the presence of robust gapless surface states [3]. While the spin structure and the low-temperature electrical transport gained much attention, the physics at room temperature and the thermoelectric transport is still under debate. To contribute on this, we studied the electronic structure of Sb_2Te_3 thin films, with 3-36nm thickness, with a fully relativistic screened Korringa-Kohn-Rostoker Green's function method. The thermoelectric transport properties were calculated within the relaxation time approximation of the Boltzmann theory. The influence of thickness, temperature and doping on the thermoelectric transport properties of the surface states were analysed in detail.

[1] T. M. Tritt *et al.*, MRS bulletin **31**, 188 (2006); [2] N. F. Hinsche *et al.*, Phys. Rev. B **86**, 085323 (2012); [3] H. Zhang *et al.*, Nature Phys. **5**, 438 (2009);

DS 42.4 Thu 15:45 CHE 89

Reduction of Thermal Conductivity in Si-Isotope-Multilayers — •Michael Bachmann, Michael Czerner, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

The electronic parameters of Silicon show that Silicon is a promising thermoelectric material. The only drawback of using Silicon as a thermoelectric material is its high lattice thermal conductivity. One idea to reduce the lattice thermal conductivity is the manufacturing of Si-isotope-multilayers. It is expected, that in such structures the phonon-phonon scattering is enhanced due to the mass change at the interfaces between the layers, whereas the electronic transport is unaffected. We present phonon transport calculations based on an atomistic Greens function method [1] for $^{28}Si/^{29}Si$ and $^{28}Si/^{30}Si$ isotope-multilayer. These results show that a periodic arrangement of the layer-system cannot decrease the phonon thermal conductivity substantially, whereas a random arrangement of the layer-system can lead to a strong decrease in the phonon conductivity. We also show that small deviations from the periodic arrangement are enough to end up in the random regime.

[1] W. Fisher, T.Mingo, N.Numerical Heat Transfer, Part B: 2007, 51, 333

DS 42.5 Thu 16:00 CHE 89

Full ZT and Crystallographic Characterization of Individual Bismuth Telluride 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]AG Neue Materialien, Humboldt-Universität zu Berlin, D-10099 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

Thermoelectrical properties of nanowires (NWs) have been investigated because of their potential in energy conversion. In order to determine the thermoelectric figure of merit ZT of NWs, individual electrochemically grown bismuth telluride (Bi_2Te_3) NWs [1] are transferred to a micro device (TNCP)[2] and contacted using electron beam induced deposition (EBID) of platinum. The TNCP design allows a complete thermoelectric characterization and structural and compositional analysis by transmission electron microscopy (TEM) for the same NW. We measured the electrical and thermal conductivity λ (3ω-method) as well as the Seebeck coefficient for an individual Bi_2Te_3 NW at room temperature. These measurements give $\lambda = 0.8$ W/(mK) and $ZT \approx 0.1$. TEM measurements reveal a textured crystal orientation preserved along the whole NW and a rough surface morphology.

[1] W. Töllner *et al.*, Adv. Func. Mater. **22**, 151 (2012)

[2] Z. Wang *et al.*, IEEE 26th Intern. Conf. on MEMS 2013, pp. 508.

DS 42.6 Thu 16:15 CHE 89

Full thermoelectric characterization and Lorenz number of individual metallic nanowires — •Rüdiger Mitdank[1], Danny Kojda[1], Zhi Wang[2], Michael Kröner[2], Peter Woias[2], and Saskia F. Fischer[1] — [1]AG Neue Materialien, Humboldt-Universität zu Berlin, D-12489 Berlin, Newtonstr. 15 — [2]Laboratory for Design of Microsystems, University of Freiburg , IMTEK, D-79110 Freiburg

A full characterization of the thermo electrical properties of nanowires (NWs) needs information about Seebeck coefficient as well as electrical and thermal conductivity. In order to determine the thermoelectric figure of merit of NWs, individual NWs are transferred to a micro machined measurement platform (TNCP) [1] and contacted by electron beam induced deposition (EBID) with platinum. A special issue of such measurements consists in the determination of the thermal conductivity (3-Omega-method). The compliance with boundary conditions and the presence of thermal contact resistances are discussed.

Especially, we present a technique to determine the Lorenz number L from the ratio of two voltages. We observed a Lorenz number L smaller than the Sommerfeld value Ls. This difference increased with decreasing temperature. The deviation of L from Ls is compared with different models.

[1] Z. Wang et al., IEEE 26th Intern. Conf. on MEMS 2013, pp. 508.

DS 42.7 Thu 16:30 CHE 89

Phonon thermal conductivity in cross-section modulated Si wires: A transition from nano- to microscale regime — Alexandr I. Cocemasov[1], Denis L. Nika[1], •Vladimir M. Fomin[2], Daniel Grimm[2,3], and Oliver G. Schmidt[2,3] — [1]E. Pokatilov Lab., Dep. Theor. Phys., Moldova State University, Chisinau MD-2009, Rep. of Moldova — [2]Institute for Integrative Nanosciences, IFW-Dresden, D-01069 Dresden, Germany — [3]Material Systems for Nanoelectronics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Periodically modulated nanowires are perspective for thermoelectric applications due to low values of phonon thermal conductivity [1-2]. At present, modulated profiles can be fabricated at the scale of tens and hundreds nm. We have studied a transition of phonon thermal transport in cross-section modulated Si wires from nano- to microscale regime, considering phonon spectra for modulated nanowires obtained within an atomistic model of lattice dynamics and scattering of bulk Si phonons on external faces of the modulated segments for microstructures. For a Si wire of a square cross-section with side d, modulation depth of $d/10$, modulated segment width of $d/4$ and distance between neighboring modulated segments of $3d/4$, the transition from the nano- to microscale transport regime at room temperature occurs at $\sim$ 100 nm. The work was supported by Moldova State Projects 11.817.05.10F and 12.819.05.18F. A.I.C. acknowledges the support by DAAD.

[1] D. L. Nika, A. I. Cocemasov, C. I. Isacova, A. A. Balandin, V. M. Fomin, O. G. Schmidt, PRB 85, 205439 (2012). [2] D. L. Nika, A. I. Cocemasov, D. V. Crismari, A. A. Balandin, APL 102, 213109 (2013).

DS 42.8 Thu 16:45 CHE 89

Phonon processes in silicon crystalline quantum wires with amorphous surface — Dmitrii V. Crismari[1], Denis L. Nika[1], •Vladimir M. Fomin[2], Daniel Grimm[2,3], and Oliver G. Schmidt[2,3] — [1]E. Pokatilov Lab., Dep. Theor. Phys., Moldova State University, MD-2009 Chisinau, Republic of Moldova — [2]Institute for Integrative Nanosciences, IFW-Dresden, D-01069 Dresden, Germany — [3]Material Systems for Nanoelectronics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Advancements in high-tech fabrication have attracted interest to the investigation of amorphous microstructures, e.g., Si-based microtubes and radial superlattices with amorphous silica layers [1]. We study phonons in crystalline Si quantum wires with amorphous surface using the Valence Force Field approach with stochastic parameters of interatomic interactions. The phonon thermal conductivity (PTC) is calculated taking into account the phonon-phonon and phonon-surface scattering. Non-zero-velocity phonons, which penetrate amorphous coating, are strongly scattered there and removed from the heat transport. A considerable suppression of the PTC is revealed for experimentally feasible structures. Even for wide (cross-section sizes of 0.5 to 1 μm) quantum wires with amorphous surface, the PTC is suppressed by a factor of 1.5 to 2 as compared with fully crystalline ones. The suppression significantly increases in quantum wires of smaller cross-section. The work was supported by Moldova State Project 11.817.05.10F. D.V.C. acknowledges the support by DAAD. [1] R. Songmuang, A. Rastelli, S. Mendach, and O. G. Schmidt, APL 90, 091905 (2007).

Coffee break (15 min)

DS 42.9 Thu 17:15 CHE 89

Half Heusler compounds as high performance thermoelectric materials — •J Schmitt[1,2], Z Gibbs[2], J Snyder[2], and C Felser[1,3] — [1]Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg-University, Mainz, Germany — [2]Materials Science, California Institute of Technology, Pasadena, USA — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Half Heusler compounds with the general formula XNiSn crystalize in a C1$_b$ cubic structure. They are considered to be promising thermoelectric materials because of their low costs and they consist of environmentally friendly elements. Those with 18 valence electrons are expected to be narrow band gap semiconductors. Numerous compounds have been studied focusing on their high thermoelectric properties. The majority of these materials in the class of XNiSn-systems are n-type thermoelectrics. In this study we investigated the thermoelectric behavior of the Zr$_{1-x}$Sc$_x$NiSn (x¡0.15) solid solutions, a p-type counterpart of the high zT n-type ZrNiSn family. Measurements of the carrier concentration, Hall mobility, electrical resistivity, thermal diffusivity and thermopower were measured up to 850K. The substitution of Zirconium by Scandium, which possesses one valence electron less, lead to a domination of holes as charge carriers changing the sign for the Seebeck coefficient and the Hall carrier concentration. From the Hall measurements lower mobilities as expected were observed. This observation can be understood within the model of mixed conduction, leading to a depression of the thermopower or bipolar effects in thermal transport measurements.

DS 42.10 Thu 17:30 CHE 89

Simulation Study on Thermoelectric Half Heusler Materials — •Heiko G. Schoberth, Heike Emmerich, and Thomas Gruhn — Material- und Prozesssimulation, Universität Bayreuth, 95447 Bayreuth, Germany

One major task in the development of new thermoelectric materials is to increase the figure of merit by lowering the thermal lattice conductivity. This can be achieved with nanostructured thermoelectrics, in which the phonons are damped at the cluster interfaces. Of special technological interest of thermoelectric materials are CoSb- or NiSn-based half Heusler compounds, in which a complex domain structure forms by partial demixing of the material during the production process [T. Graf et. al., Scripta Mater. 63, 625 (2010)]. We have studied the miscibility of (Ti,Z)CoSb with Z=Cr,Fe,Mn,V,Sc and (Ti,Zr,Hf)NiSn with the help of ab initio calculations. On the one hand, (Ti,Z)CoSb does not show a miscibility gap in the equilibrium state. Therefore, domain structures found in the experiments must result from the preparation method. On the other hand, demixing is found for (Ti,Zr)NiSn and (Ti,Hf)NiSn, while (Zr,Hf)NiSn mixes. We have used a cluster expansion method which provides pseudo-hamiltonians from the first-principles calculations. They are used to perform Monte Carlo Simulations to analyze statistical properties and the phase diagram of the systems, as well as the structure of the domain boundaries. The results will enter later on into phase field simulation to cover the full range from atomistic to micrometer length scale.

DS 42.11 Thu 17:45 CHE 89

Long term stability of Half Heusler compounds at high temperatures — •Julia Krez[1,2], Benjamin Balke[1], and Claudia Felser[1,3] — [1]Johannes Gutenberg University Mainz, Mainz, Germany — [2]Graduate School of Excellence MAINZ, Mainz, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Half-Heusler compounds attracted much attention to be a promising materials for thermoelectric applications in a medium temperature range (470 - 770 K). The recovery of waste heat from e.g. automotive and industrial devices requires not only powerful materials in a particular temperature range but also long term stability regarding to a commercial success. Recent works have shown approaches for an up-scaling of the material synthesis and first constructions for thermoelectric modules with Half-Heusler. This work presents the latest results on a long term stability study of Half-Heusler compounds in a temperature range from room temperature up to 873K. The thermoelectric properties of n- and p-type materials were measured in a cycle test after 50, 100 and 500 cycles.

DS 42.12 Thu 18:00 CHE 89

Phase separation as the key to thermoelectric highly efficient Heusler compounds — •Benjamin Balke — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany

The Half-Heusler compounds are one of the most promising candidates among the high-temperature thermoelectric materials being investigated for automotive and industrial waste heat recovery applications. For n- as well as p-type materials ZT values with peak values larger than one have been published recently and first modules have been built. In this talk, we will give an overview about our recent investigations about phase separation in the thermoelectric Heusler compounds. We will present the most recent results on our studies on the phase separations in the quasi-ternary system TiNiSn-ZrNiSn-HfNiSn. Studying patents and publications the last two years carefully one could read a lot about not-single phase samples inside of the TiNiSn-ZrNiSn-HfNiSn system. Furthermore, we will show how we adapted this knowledge to design a p-type Heusler compound which led to a ZT increase of 50% compared to the best published bulk p-type Heusler compound in the literature. This results strongly underline the importance of phase separations as an important tool in the design of highly thermoelectric efficient materials which fulfill the industrial demands for a thermoelectric converter. In the end, I will briefly discuss the most recent development of thermoelectric modules using Heusler compounds.

DS 42.13 Thu 18:15 CHE 89

Reduced thermal conductivity in Half-Heusler superlattices — •Paulina Holuj[1], Tino Jaeger[1], Benjamin Balke[2], Sascha Populoh[3], Anke Weidenkaff[3], Claudia Felser[2], and Gerhard Jakob[1] — [1]Institute of Physics, University of Mainz, Germany — [2]Institute of Inorganic and Analytical Chemistry, University of Mainz, Germany — [3]EMPA, Ueberlandstrasse 129, 8600 Duebendorf, Switzerland

Research on thermoelectric materials has strongly increased in recent years due to their high application potential in production of a clean energy from wasted heat. Despite many advantages, their weakness is the limited efficiency, that is related to the dimensionless figure of merit $ZT = \alpha^2\sigma\kappa^{-1}T$. One of the approaches to enhance ZT is the reduction of the thermal conductivity by phonon scattering at the interfaces of a superlattice (SL), keeping electrical parameters $(\alpha^2\sigma)$ unchanged.

The ability to produce good quality SLs made out of Half-Heusler compounds is demonstrated by a clearly visible satellite peaks in X-ray diffractograms. Additionally, measured data are in good agreement with simulated patterns. Expected reduction of the thermal conductivity of $\mathrm{TiNiSn/Zr_{0.5}Hf_{0.5}NiSn}$ SLs has been obtained by the differential 3ω method. High temperature measurements of the Seebeck coefficient show a reversible behavior up to 550 K, revealing the stability of SLs up to this temperature range.

Currently HfNiSn, another member of the family of Half-Heusler materials is under investigation, where the ratio of interface scattering to atomic disorder scattering is enhanced.

DS 42.14 Thu 18:30 CHE 89

Thermal conductivity of nano-structured thermoelectric materials — •Chandan Bera[1], Lasse Bjerg[2], Ankita Katre[1], Georg K. H. Madsen[1], and Ralf Drautz[1] — [1]Department of Atomistic Modelling and Simulation, ICAMS, Ruhr-Univesität Bochum, Germany — [2]Center for Materials Crystallography, Department of Chemistry & iNANO, Aarhus University, Denmark

Manipulating the thermal properties of materials by nano-structuring is new successful route to improve the performance of thermoelectric materials. We present a new parameter free model to predict anharmonic scattering in bulk and nanoscale materials. Velocities and anharmonic scattering rates are calculated from the Grüneisen parameter of the full phonon dispersions and used to calculate the lattice thermal conductivity using the phonon Boltzmann transport equation in the relaxation time approximation. We find good agreement with experiments for a range of materials. Furthermore, we show that our model, as opposed to simple models based on only the acoustic bands, finds the correct trend in the thermal conductivity of Mg2Si, Mg2Ge and Mg2Sn. We also examine thermal transport in more complex materials like Type-I Si clathrates and zinc-antimonides. Finally, discuss how nano-structure and disorder effect the thermal conductivity.

DS 42.15 Thu 18:45 CHE 89

Phonon drag effect in $\mathrm{FeGa_3}$ — Maik Wagner-Reetz[1], •Deepa Kasinathan[1], Walter Schnelle[1], Raul Cardoso-Gil[1], Helge Rosner[1], Peter Gille[2], and Yuri Grin[1] — [1]MPI CPfS, Dresden, Germany — [2]LMU Munich, Germany

The thermoelectric properties of single and polycrystalline $\mathrm{FeGa_3}$ are systematically investigated over a wide temperature range. At low temperatures, below 20 K, pronounced peaks in the thermal conductivity $(\approx 800\,\mathrm{W\,K^{-1}\,m^{-1}})$ with corresponding maxima in the thermopower $(\approx 16000\,\mu\mathrm{V/K})$ were found. Such large values have previously not been reported in $\mathrm{FeGa_3}$. Measurements along [100] and [001] directions indicate only a slight anisotropy in both the electrical and thermal transport coefficients. From susceptibility and heat capacity measurements, a structural or magnetic phase transition as a possible reason for the low temperature enhancement in thermopower and thermal conductivity can be exculded. After careful considerations, we assign the peaks in the thermopower as a manifestation of the phonon-drag effect. Using density functional theory based calculations, we have revisited the electronic structure of $\mathrm{FeGa_3}$ and compared the magnetic (including correlations) and non-magnetic electronic structure. Thermopower at fixed carrier concentrations are calculated using semi-classical Boltzmann transport theory and the calculated results match fairly with our experimental data.

D.K. and H. R. acknowledge funding by the DFG within SPP 1386.

DS 43: Poster II: Organic thin films; Atomic layer deposition, Thin film characterization: Structure analysis and composition (XRD, TEM, XPS, SIMS, RBS, ...)

Time: Thursday 16:00–19:00 Location: P1

DS 43.1 Thu 16:00 P1

Influence of surface energetics on perylene thin film growth — •Cathy Jodocy, Daniel Mokros, Mathias Cornelissen, Christian Effertz, Carolin C. Jacobi, and Matthias Wuttig — I. Institute of Physics (1A), RWTH Aachen University, D-52056 Aachen, Germany

In recent years, organic semiconductors have received considerable interest. Promising applications include organic field effect transistors (OFETs), organic light-emitting devices (OLEDs) and photovoltaic cells. These devices have in common that they are based on organic thin films, and that they are very sensitive to the order of these films. An understanding of thin film growth is crucial to tailor surface morphologies and organic film properties suitable for specific applications.

The molecule-substrate interaction plays a significant role for resulting film structure. Therefore, the evolution of the growth of perylene thin-films on substrates, which were deposited on self-assembled monolayers (SAMs), was investigated.

In this study, perylene has been used as an organic semiconductor material, which has been deposited both on surfaces treated with SAMs and on clean silicon dioxide. Atomic Force Microscopy (AFM) has been employed to investigate the surface morphology and X-Ray Diffraction (XRD) has been used to determine the crystalline structure of the thin perylene films.

DS 43.2 Thu 16:00 P1

Growth Study of Organic Thin Films - Perylene derivatives on DTC-modified noble metals — •Janina Felter, Daniel Mokros, Dominik Meyer, Ingolf Segger, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, D-52056 Aachen, Germany

Perylene derivatives, such as N,N'-dimethyl-3,4,9,10-perylenetetracarboxylic diimide (DiMe-PTCDI), are high potential organic semiconductors for thin film applications like organic solar cells (OSC), organic light emitting diodes (OLED) and organic thin film transistors (OTFT). In order to access the full potential of these molecules the structural and electronic thin film properties have to be optimized. To achieve this goal, an in-depth understanding of the molecular ordering is necessary. In recent works, it has been shown that the application of self-assembling monolayers of Dithiocarbamate (DTC) molecules leads to a significant downshift of the work function of Au by 2 eV, which enhances the electron injection from the metal to the active organic layer of an OTFT. In this work, films of perylene derivatives have been deposited by molecular beam deposition (MBD) on smooth noble metal surfaces, which are modified by DTC monolayers. Additionally to their influence on the electronic structure examined by Ultraviolet and X-ray Photoemission Spectroscopy (XPS/UPS), we investigate the molecular orientation by Fourier Transform Infrared Spectroscopy (FTIR). The surface morphology is investigated by Atomic Force Microscopy (AFM), while crystallinity and texture are determined by X-ray Diffractometry (XRD).

DS 43.3 Thu 16:00 P1

Influence of Surface Energetics on Thin Film Evolution —

•Daniel Mokros, Christian Effertz, Cathy Jodocy, Mathias Cornelissen, Ingolf Segger, Dominik Meyer, and Carolin Jacobi — I. Institute of Physics (IA), RWTH Aachen University, D-52056 Aachen, Germany

The evolution of the growth of perylene thin-films on substrates, which were energetically modified by polymeric dielectrics such as PDMS and PMMA, was investigated by atomic force microscopy (AFM). Thin-film evolution from a few monolayers to thick films in the case of perylene is a three step process: Initial growth is dominated by the formation of high isolated islands, which show an average height significantly higher than the nominal film thickness. This growth phase is influenced by a significant post-growth behavior. In the second step, the evolution of thin-films undergoes a transition to a more lateral growth mode. In the final growth phase, with increasing amount of deposited material the growing islands coalesce. At the contact point of two islands dislocations can occur. In the case of PDMS modified substrates, the regime of coalescence is accompanied by a pronounced spiral growth. Additionally the PDMS modified substrates show a high crystalline order, which was confirmed by x-ray diffraction (XRD) measurements. By combining measurements of the surface free energy of the differently modified substrates with the scaling relationship of nucleation, we were able to predict a profound influence of the dielectric on thin-film growth kinetics.

DS 43.4 Thu 16:00 P1

Manipulating the Electronic Properties of Manganese Phthalocyanine Thin Films by Potassium Intercalation — •Francisc Haidu[1], Lars Smykalla[2], Michael Hietschold[2], and Dietrich R. T. Zahn[1] — [1]Technische Universität Chemnitz, Semiconductor Physics Department, D-09107 Chemnitz, Germany — [2]Technische Universität Chemnitz, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

Manganese phthalocyanine (MnPc) presents great promise towards molecular spintronics due to its high spin state of $S=3/2$ which can be lowered to $S=1/2$ by reaction with molecular oxygen [1] or even increased to $S=5/2$ by doping with alkali metals [2], which promotes 3 stable n-doped phases [3]. Within this work the changes of the occupied and unoccupied electronic states of K intercalated MnPc were investigated by combined UPS, IPS, XPS, and NEXAFS techniques. MnPc films of 10 nm thickness were prepared by organic molecular beam deposition onto Co foils and consecutively doped by K evaporation from a getter source in UHV conditions. The amount of K was determined by XPS while the NEXAFS Mn L edge branching ratio provides information on the spin states of $S=3/2$ and $S=5/2$ for pristine and fully doped MnPc, respectively. Finally, from the UP and IP spectra the evolution of the transport band gap upon K intercalation was revealed.

[1] R. Friedrich *et al.*, J. Chem. Phys. 136, 064704 (2012)
[2] Y. Taguchi *et al.*, J. Am. Chem. Soc. 128, 3313 (2006)
[3] B. Mahns *et al.*, J. Chem. Phys. 134, 194504 (2011)

DS 43.5 Thu 16:00 P1

FePc and CoPc on Ni(111) and graphene/Ni(111): Influence of the central metal atom — •Johannes Uihlein, Heiko Peisert, Hilmar Adler, Mathias Glaser, Małgorzata Polek, and Thomas Chassé — Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen, Germany

The interactions at interfaces between transition metal phthalocyanines (TMPCs) and metal substrates play an important role for charge transport across the interfaces, which may become important for possible future spintronic devices. Molecule-substrate interactions may influence the local charge and thus the spin state of the central metal atom within the first molecular adlayer. This will be especially important for metal atoms possessing an open shell structure. For cobalt phthalocyanine (CoPc) on Ni(111) it has recently been shown, that a graphene buffer layer preserves a charge transfer from the Ni substrate to the molecules metal atom, but changes the detailed electronic situation at the molecule substrate interface [1]. To reveal the effect of the central metal atom of the Pc on interactions at these interfaces we studied iron phthalocyanine on Ni(111) and graphene/Ni(111) using X-ray absorption and photoemission spectroscopies. The comparison to CoPc reveals significant differences.

[1] J. Uihlein et al., *J. Chem. Phys.* **2013**, 138, 081101.

DS 43.6 Thu 16:00 P1

Impact of plasmonic nanostructures on the optical properties of fluorinated ZnPc thin films — •Verena Kolb[1], Michael Brendel[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilians University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

By adjusting the localized surface plasmon resonance (LSPR) of defined metal nanostructures either the absorption or photoluminescence of organic layers can be enhanced and thus might be an interesting approach for improving both organic solar cells and LEDs. This enhancement is caused by an increase of the near-field component of the electromagnetic field and in the case of absorption the scattering of light. In this contribution gold nanostructures were fabricated via shadow nanosphere lithography and optically and morphologically characterized. Complementary, finite difference time domain simulations were used to determine their LSPR. Finally, their impact on the optical properties of fluorinated Zn-Phthalocyanines (ZNPc), which prove to be interesting candidates for organic electronics, was investigated. Financial support by the Solar Technologies go Hybrid project is gratefully acknowledged.

DS 43.7 Thu 16:00 P1

Growth Study of Thermally Evaporated Metal Thin Films on PTCDI-C13 — •Matthias M. Dück, Carolin C. Jacobi, Juri Banchewski, Cathy Jodocy, Christian Effertz, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

Optoelectronic devices based on organic thin films have gained more and more interest over the last few years. The performance of such devices depends critically on the interfaces between the different layers, e.g. the organic layer and the metal electrodes. Especially during the evaporation of metals onto organic thin films various effects can occur, such as thermally induced stress, or diffusion of metal atoms into the organic layer. This is our motivation to study the interface between organic and metallic thin films, in order to be able to optimize functionality of future devices.

Its high electron mobility makes N,N'- ditridecyl-3,4,9,10-perylenetetracarboxylic diimide (PTCDI-C13) a promising n-type material for organic field effect transistors (OFETs). In this work, thin films of various metals have been deposited by thermal evaporation on 30 nm PTCDI-C13 films produced with Organic Molecular Beam Deposition (OMBD). The surface morphology has been investigated by atomic force microscopy (AFM) and scanning electron microscopy (SEM), whereas the crystallinity was determined by x-ray diffractometry (XRD).

DS 43.8 Thu 16:00 P1

Investigation of electronic and structural properties of vanadyl phthalocyanine on graphene interlayers on Ni(111) — •Hilmar Adler, Heiko Peisert, Mateusz Paszkiewicz, Johannes Uihlein, Małgorzata Polek, and Thomas Chassé — Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen, Germany

In previous years, transition metal phthalocyanines (TMPcs) gained increasing attention due to their tunable properties, resulting in various applications based on these materials such as light-emitting diodes, field-effect transistors and solar cells and, most recently, the interface between TMPcs and metal substrates raised additional interest due their important role in spintronic nanodevices. In the case of TMPcs, molecule-substrate interactions can drastically influence both electronic and magnetic properties of the first layer of the organic semiconductor. The interface properties however can be tuned by the insertion of a buffer layer [1]. Graphene with its exciting electronic properties is an ideal candidate for such layers. Vanadyl phthalocyanine as a polar and non-planar TMPc is in particular suited for the tuning of electronic properties of interfaces. Charge transfer processes depending on the adsorption geometry on Ni(111) and graphene/Ni(111) were investigated using scanning tunneling microscopy, X-ray photoelectron spectroscopy and X-ray absorption spectroscopy.

[1] J. Uihlein, H. Peisert, M. Glaser, M. Polek, H. Adler, F. Petraki, R. Ovsyannikov, M. Bauer, T. Chassé J.Chem.Phys. 138 (2013) 081101.

DS 43.9 Thu 16:00 P1

AlClPc on silver: Influence of substrate surface. — •Małgorzata Polek[1], Tamara V. Basova[2], Fotini Petraki[1], Florian Latteyer[1], Heiko Peisert[1], and Thomas Chassé[1] — [1]University of Tuebingen, Institute of Physical and Theoretical Chemistry, Auf der Morgenstelle 18, 72076 Tuebingen, Germany — [2]Nikolaev Institute of Inorganic Chemistry, Lavrentiev Pr. 3, Novosibirsk, 630090, Russia

Phthalocyanines (Pcs) are promising materials for various applications such as organic solar cells, field effect transistors and light emmitting diodes. To improve the efficiency of the aforementioned opto-electronic devices, one needs to adjust the properties and understand better the interactions between the building blocks. Due to its permanent dipole moment and the chemical reactivity, AlClPc is in particular suited for the tuning of the interface properties. We investigated electronic properties and chemical interactions of AlClPc with polycrystalline Ag foil and Ag(100) using photoelectron spectroscopy (XPS, UPS) and low energy electron diffraction (LEED). Clear indications for a chemical interactions were found for both substrates. In addition, charge transfer processes to the macrocycle of the Pc were observed, indicated by the appearance of an interface-related peak at E_F, which can be explained as a partial filling of the former LUMO at the interface.

DS 43.10 Thu 16:00 P1

PS-b-PMMA block copolymer films: Self-assembly and dielectric properties on different substrates — •Riitta Savikoski[1,2], Guillaume Fleury[2], Andrea Gassmann[1], Georges Hadziioannou[2], and Heinz von Seggern[1] — [1]Electronic Materials Division, Institute of Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Str. 2 , 64287 Darmstadt, Germany — [2]Laboratoire de Chimie des Polymères Organiques, Université Bordeaux 1, Bât 8, Avenue des Facultés, 33405 Talence cedex, France

The self-assembly of block copolymers (BCPs) on Si-substrates has been widely investigated. The present work aims using self-assembled BCP films as gate dielectric in bottom gate organic field-effect transistors and evaluating in how far the morphology of the film influences the performance of the device. Nowadays silicon is not the material of choice for the gate electrode any more. Instead, metals or ITO are common materials. The BCP under investigation is polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA). PS-b-PMMAs, with molar ratios of 1:1 and 2:1, were self-assembled on different gate electrode materials, including gold, silver, ITO and Si-substrates as a reference. A vertical orientation of BCP films was achieved on oxidized Si-substrates by adding a brush layer of random BCP (PS-r-PMMA). However, this vertical orientation can also be achieved through a nanometer scale surface roughness. The success of self-assembly was studied for spin coated films using atomic force microscopy (AFM). Furthermore, dielectric properties of the films were investigated by impedance measurements.

DS 43.11 Thu 16:00 P1

Influence of the short interaction range of C_{60} on nucleation and step-edge barrier during growth — •Sebastian Bommel[1,2], Nicola Kleppmann[3], Sabine H.L. Klapp[3], and Stefan Kowarik[2] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany — [3]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

Atoms, molecules and colloids show different growth phenomena attributed to their different phase diagrams, particle sizes and interaction ranges. Here, we report on the influence of the short interaction range of the fullerene C_{60} on nucleation and step-edge barrier [1]. Quantitative agreement between real-time x-ray scattering experiments during molecular growth with kinetic Monte Carlo (KMC) simulations allow us to analyze the particle-resolved dynamics of C_{60} on the surface. Compared to atoms, we find relatively long surface diffusion times before the molecules are immobilized at islands. We attribute these to the colloid-like, short-ranged character of C_{60}-interactions [2]. However, the step-edge barrier of C_{60} differs from colloids in that it is not a pseudo-step-edge barrier arising from lower diffusion probability at a step-edge, but a true energetic barrier as is observed for atoms. Thus, our findings will help to gain insight into nucleation and surface growth processes between the scales of atomic and colloidal systems.

[1] S. Bommel, N. Kleppmann et al., submitted [2] S. P. Tewari et al., Int. J. Mod. Phys. B 24, 4281 (2010)

DS 43.12 Thu 16:00 P1

Theoretical analysis of the Anthracene NEXAFS signature — •Michael Klues[1], Klaus Hermann[2], and Gregor Witte[1] — [1]Physics Department, Phillipps Uni. Marburg, 35032 Marburg — [2]Theory Department, Fritz Haber Institute, 14195 Berlin

NEXAFS is a powerful technique that is experiencing a renewed interest owing to the recent success in the field of organic electronics, as it provides detailed information on electronic properties and orientational ordering in such molecular materials. However, to fully exploit the potential of this technique, a precise and reliable identification and assignment of spectral features within the NEXAFS spectra is needed. In the present work, we have calculated the NEXAFS spectra of Anthracene in the frame of density functional theory by using the StoBe code. Comparison to experimental data shows excellent agreement and points out the high precision StoBe reaches in predicting energies of excitations with errors less than 300meV. The key to such accurate values without any subsequent, empirical energy shift is to handle excited electronic configurations. By matching spectra resulting from excited states with different localized excitation centers we carve out the influence of chemical shifts and core hole effects. Furthermore it is possible to label the numerous resonances occurring in the NEXAFS spectrum. The detailed calculation also enables a visualization of final states like for example Rydberg states using the fully relaxed excited electronic structure. These illustrations point out the influence of initial and final states on the intensity and energetic shift of the individual partial NEXAFS resonances of the various excitation centers.

DS 43.13 Thu 16:00 P1

Optical anisotropy in picene thin films — •Johannes Dieterle, Katharina Broch, Alexander Gerlach, and Frank Schreiber — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

The organic semiconductor picene has attracted significant interest due to reports on its excellent charge-transport properties and O_2 gas sensing ability in organic field-effect transistors (OFETs) [1,2]. In thin films picene grows in high columnar islands depending on substrate temperature and growth rate and exhibits uniaxial anisotropic optical properties. For a complete characterization of the system a knowledge of the in-plane as well as the out-of-plane optical properties is fundamental [3,4]. We investigate thin picene films using optical spectroscopy including variable angle spectroscopic ellipsometry in an energy range of 1.5 to 5 eV at different preparation conditions. Due to the complexity of the system only the in-plane component of the system has been reported so far [5]. We discuss results of different growth conditions.

[1] R. Mitsuhashi et al., Nature, 464 (2010), [2] H. Okamoto. et al., Am. Chem. Soc., 130 (2008), [3] T. Hosokai et al., Chem. Phys. Lett., 544 (2012), [4] M. Dressel et al., Opt Express., 16 (2008), [5] S. Fanetti et al. J. Chem. Phys., 137 (2012)

DS 43.14 Thu 16:00 P1

Hydration effects of chitosan on silicon. — •Marcelo Cisternas[1], Maria J. Retamal[1], Sebastan Gutierrez[2], Mark Busch[3], Patrick Huber[3], Tomas Perez-Acle[2], Ulrich Volkmann[1], and Michael Kappl[4] — [1]P. Universidad Catolica de Chile, Santiago, Chile — [2]Fundacion Ciencia y Vida, Santiago, Chile — [3]Tech. Univ. Hamburg-Harburg, Hamburg, Germany — [4]MPI for Polymer Research, Mainz, Germany

Chitosan (CH) is a polysaccharide obtained by the deacetylation of chitin, a component of the exoskeleton of crustaceans. Among its most important features we can mention that it is biocompatible, non-toxic and biodegradable. Therefore, it has been used both in the field of agriculture, as well as in medicine. Chitosan appears to be very interesting for biological applications, both as a macro-and micro-scale material. We are interested in CH deposited on a planar silicon substrate (with a native SiO2 surface) as a possible support for hydration of artificial biological membranes (phospholipids), which form the base for different biosensors. We prepare CH islands and layers of different thickness in a solvent free environment and control with high resolution ellipsometry the layer thickness during formation as well as before and after hydration. The film topography is studied with AFM at room temperature and during heating cycles. The CH-layer capability for water storing is tested with ellipsometry during heating cycles from room temperature to 370 K. We observed that CH does not wet the SiO2 surface when deposited from the gas phase. It forms spontaneously semi-spheres. This behavior favors the capability of the structure for water storage.

DS 43.15 Thu 16:00 P1

Growth of Gold on P(VDF-TrFE) During RF-Sputter Deposition — •Alexander Hinz[1], Oleksandr Polonskyi[1], Thomas Strunskus[1], Matthias Schwartzkopf[2], Gonzalo Santoro[2], Jan Perlich[2], Ezzeldin Metwalli[3], Yuan Yao[3], Franz Faupel[1], Stephan Roth[2], and Peter Müller-Buschbaum[3] — [1]CAU zu Kiel, Technische Fakultät, LS Materialverbunde, Kaiserstr. 2, 24143 Kiel — [2]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607

Hamburg, — [3]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Metallization of organic surfaces via sputtering is well established in industry and important for many applications. However, in contrast to metal evaporation, the basic mechanisms determining the final microstructure are not well understood due to the complex deposition process involving collisions with gas molecules and defect generation on the sensitive organic surface by energetic ions. The complex nature of the sputter process calls for in-situ measurements. Here we use in-situ grazing incidence small angle scattering (GISAXS) to obtain structural information with high spatial and temporal resolution. The growth of Au on P(VDF-TrFE) is chosen as a model system of inert metal and reactive polymer. The analysis of the GISAXS data yields morphological information about the different stages of the growing metal film. These results will be compared to results of a parallel GISAXS-study on the growth of Au on PS and already published results on the growth of Au on Si [1].

[1] Schwarzkopf et al., Nanoscale 5, 5053-5062 (2013)

DS 43.16 Thu 16:00 P1

Investigation of the thermal stability and structure of 4,4'-dimercaptostilbene on Au(111) — •Johannes Völkner, Andre Pick, and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, 35032 Marburg

Sensing devices for biological molecular species such as proteins or sugars in solution are receiving increasing interest because they enable monitoring of physiological parameters or can lead to bioelectronics. One approach is a photoelectrochemical biosensor which requires an efficient coupling of involved semiconductor nano-particles and the gold electrode to enable charge transfer from the NP towards the electrode without direct quenching the optical excitation with the NP. In a previous study it was shown that self-assembled monolayers of 4,4'-dimercaptostilbene provide a suitable linker that combines structural order and sufficient conductance [1]. However, the ordering and quality of this thiolate-bound interlayer critically depends on several preparation parameters, such as assembling temperature and the choice of solvent. Therefore we investigated the thermal stability and structural order of differently prepared 4,4'-dimercaptostilbene self-assembled monolayers on Au(111) surfaces by means of TDS, XPS and NEXAFS.

[1] W. Khalid et al. ACS Nano, 5, 9870 (2011).

DS 43.17 Thu 16:00 P1

A comparison of dielectric elastomers and electrostrictive polymers for vibration energy harvesting applications — •Kirstin Bornhorst, Christian Schirrmann, Andreas Weder, Andreas Heinig, and Florenta Costache — Fraunhofer Institute for Photonic Microsystems IPMS, Dresden, Germany

Harvesting energy from the surrounding environment and converting it into usable electrical energy has become an attractive approach to producing sustainable power sources for wireless sensors and low-power electronics.

In this paper, electroactive polymers (dielectric elastomers and electrostrictive polymers) are compared in terms of their potential for vibration energy harvesting applications. Stacks consisting of polymer thin films placed in between thin metallic electrodes were subjected to dynamic deformation by means of a pneumatic piston of variable frequency and pressure characteristics. A self-priming energy harvesting circuit was developed and used to harvest the generated energy. We investigated the polymer harvester performance, i.e. energy gained from the capacity change, when employing electroactive polymers of different elastic moduli, dielectric constants or electrostrictive constants. Furthermore, we studied the influence of the stack geometry. It is shown that for instance by using a polymer with high electromechanical coupling a harvested energy density of about 0.2 mJ/cm^3 at 15 Hz could be obtained. The harvested energy could be further increased by increasing the frequency of the induced deformation. Applications such as power generation for wireless sensors will be addressed.

DS 43.18 Thu 16:00 P1

Crystalline phase formation during the atomic layer deposition of TiO_2 — •Barbara Abendroth, Solveig Rentrop, Theresa Moebus, Hartmut Stöcker, and Dirk C. Meyer — Institut für Experimentelle Physik, TU Bergakademie Freiberg, Germany

Titanium dioxide is a wide gap semiconductor and is, based on its optical and electronic properties, widely used in various applications. For its use as thin dielectric layer in microelectronic data storage or in electrochemical energy storage devices, TiO_2 is commonly produced by atomic layer deposition (ALD). In this work we present the deposition of TiO_2 thin films by ALD from tetrakis(dimethylamino) titanium and water on silicon and polycrystalline TiN substrates for the use in metal - insulator - metal resistive switching random access memory cells. For this application, amorphous TiO_2 layers are desirable to minimize leakage currents, however, other applications of TiO_2 layers, such as a high k dielectric or photocatalysis require crystalline structures of either rutile or anatase polymorph. For our ALD process, we find a dependence of crystallisation of anatase and rutile on deposition temperature and layer thickness. A survey of literature data on TiO_2 ALD based on various precursors, shows that our results are representative for thermal ALD of TiO_2 on silicon substrates and can be summarized in a general thickness - temperature - phase diagram.

DS 43.19 Thu 16:00 P1

In-situ gold cluster growth kinetics on polystyrene thin films during sputter deposition - Influence of molecular weight — •Matthias Schwartzkopf[1], Gonzalo Santoro[1], Jan Perlich[1], Oleksandr Polonskyi[2], Alexander Hinz[2], Thomas Strunskus[2], Ezzeldin Metwalli[3], Yuan Yao[3], Franz Faupel[2], Peter Müller-Buschbaum[3], and Stephan V. Roth[1] — [1]Deutsches Elektronen-Synchrotron, Notkestr. 85, 22607 Hamburg — [2]CAU Kiel, Institut für Materialwissenschaft, LS Materialverbünde, Kaiserstr.2, 24143 Kiel. — [3]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching.

The adjustment of size-dependent catalytic, electrical and optical properties of gold cluster assemblies and to tailor their morphology with polymer templates is a very significant issue in modern applied nanotechnology. We investigate in situ the growth kinetics of gold nanostructures on polystyrene thin films with different molecular weights during RF-sputter deposition with high time resolution by means of GISAXS. The morphological parameters related to the metallic layer growth such as cluster size, correlation distance and surface coverage are deduced from a general model solely based on geometrical assumptions [1]. Our study opens up the opportunity to deduce the influence of polymer chain length on the wetting behaviour of gold films and provides a better understanding of the growth process kinetics at the polymer-metal interface during sputter deposition. [1] Schwartzkopf et al., Nanoscale 5, 5053-5062 (2013)

DS 43.20 Thu 16:00 P1

Characterization of diamond-like carbon (DLC) coatings on industrial polyethylene and polyoxymethylene by SEM, AFM and NEXAFS — •Liz M. Rösken[1], Magdalena Rohrbeck[1], Alberto Catena[1], Stefan Wehner[1], Christian B. Fischer[1], Matthias Richter[2], Matthias Städter[2], and Dieter Schmeisser[2] — [1]Department of Physics, University Koblenz-Landau, 56070 Koblenz, Germany — [2]Department of Applied Physics and Sensors, Brandenburg University of Technology, 03046 Cottbus, Germany

Diamond-like carbon (DLC) coatings are often utilized to change the base properties of raw materials, e. g. to gain robust or chemically inert surfaces. Here the deposition of hard DLC layers on soft polymers is tested. The common industrial polymers polyethylene (PE) and polyoxymethylene (POM) serve as model substrates in the present work. In order to examine the effect of the carbonaceous layers on PE and POM thin diamond-like carbon films were realized via PECVD. The topography of the different coatings was detected by AFM and SEM uncovering the different influence of the substrate material, e. g. interlayer formation for PE. The composition of the surface structures were analyzed in more detail by NEXAFS, showing the hybridization of carbon atoms in chemical different surroundings from the pure polymer to the carbon coating. The comparison of carbon coated PE- and POM-composites enables valuable insights into the interaction between soft substrates and hard coatings. For the chosen settings in PECVD, POM showed incomplete coating, while on PE a very stable and robust composite has formed.

DS 43.21 Thu 16:00 P1

Sputter yield amplification of carbon by serial magnetron co-sputtering — •Patrick Ries[1], Rüdiger Schmidt[1], Andreas Pflug[2], Tomas Kubart[3], and Matthias Wuttig[1,4] — [1]I. Physikalisches Institut (IA), RWTH Aachen, Germany — [2]Fraunhofer IST, Braunschweig, Germany — [3]Solid State Electronics, Uppsala University, Sweden — [4]JARA - Fundamentals of Future Information Technology

Carbon has been doped by serial co-sputtering with two different elements, namely Tungsten and Niobium. Both elements provide a significant rate increase for the doping concentrations analyzed. A dopant concentration of 3 at.% Nb increases the deposition rate of carbon by 130%, whereas W increases it by 280%. Due to its higher mass, W is significantly more effective than Nb. TRIDYN simulations have been performed which reproduce the experimental data and show that saturation occurs at higher dopant concentrations, which have not been reached in the experiments. Additionally our experiments indicate very long residual times of the dopant in the target as a result of recoil implantation.

DS 43.22 Thu 16:00 P1

Al-doped zinc stannate thin films as amorphous transparent conductive oxides prepared by reactive DC magnetron sputtering — •Roland Sittner, Rüdiger Matti Schmidt, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany

Transparent conductive oxides (TCOs) combine the contrary material properties of low electrical resistivity and high optical transparency. Indium tin oxide and aluminum doped zinc oxide are widely used in optoelectronic devices such as photovoltaic modules and flat panel displays. Amorphous TCOs, like indium gallium zinc oxide and zinc stannate, are utilized as channel material in transparent thin film transistors. The most common stoichiometries of the $Zn_xSn_yO_z$ system are $ZnSnO_3$ and Zn_2SnO_4, with the latter possessing a lower electrical conductivity in the amorphous state.

In this work, we deposited aluminum doped $Zn_xSn_yO_z$ thin films with a high Zn to Sn ratio via reactive DC magnetron sputtering. Doping occurred in a serial co-deposition process in order to obtain films with improved electrical properties compared to undoped zinc tin oxide films. The process parameters and dopant concentrations were varied to deposit films with optimized properties. The electrical, optical and structural properties were determined via van der Pauw method, UV/Vis spectroscopy and X-ray diffraction.

DS 43.23 Thu 16:00 P1

Influence of film thickness on structural properties of TiO_2 films coated with RF and DC magnetron sputtering — •Sebastian Schipporeit[1], Sanat Kumar Mukherjee[1], Abdelkader Nebatti[2], Farhad Mohtascham[1], Christian Notthoff[2], and Dieter Mergel[1] — [1]Faculty of Physics, University Duisburg-Essen — [2]Faculty of Engineering, University Duisburg-Essen

TiO_2 thin films were deposited by reactive sputtering of a Ti target on unheated substrates and post-heated at 300 °C and 500 °C. The dc-sputtered films are amorphous after deposition and crystallize to pure anatase only at 500 °C. The rf-deposited films are crystalline (purely anatase) already after deposition without post-heating. Above a thickness of 100 nm, the crystallite size is constant at 35 nm and decreases to zero when the thickness decreases to 25 nm. Below 25 nm the films are x-ray amorphous. Height and half-width of the XRD peaks of rf-sputtered films do not change upon post-heating at 300 or 500 °C, contrary to the intensitiy of Raman lines [1]. A larger lattice parameter ratio c/a is observed compared to the bulk value that decreases with increasing film thickness and is about 1 % larger for a film thickness larger than 100 nm.

[1] Sanat Kumar Mukherjee, Dieter Mergel, J. Appl. Phys. 114, 013501 (2013).

DS 43.24 Thu 16:00 P1

Pulsed Laser Deposition of thin Metal-Oxide Multilayers for thermal barrier coatings — •Anna Major[1], Florian Döring[1], Christian Eberl[1], Sarah Hoffmann[2], Felix Schlenkrich[1], and Hans-Ulrich Krebs[1] — [1]Institute for Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute for X-Ray Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Multilayers consisting of metals and oxides are highly interesting for modern high-quality coatings especially with regard to their unique thermal conducting properties which could be used for thermal barrier coatings in different applications like gas turbine coatings, cryogenic applications or modern power plants.

Therefore, we have studied pulsed laser deposited (PLD at 248 nm) multilayers consisting of various metals (e.g. W, Ti, Cu) and oxides (e.g. ZrO_2 or MgO) with different layer thicknesses. Their structure, interface roughness and thermal stability were characterized by X-Ray-Reflectivity, Scanning-Electron-Microscopy and cross-sectional Transmission-Electron-Microscopy. Especially we focus on the material combination of W and ZrO_2, which is highly useful for high temperature applications due to its high thermal stability. For effective multilayer insulation it is necessary to produce very thin individual layers with a high interface density and therefore many scattering and reflection centers for heat transporting phonons.

In this contribution, we show our results in producing these multilayers with high quality and thin individual layer thicknesses.

DS 43.25 Thu 16:00 P1

High quality TiN as bottom electrode for zinc ferrite based magnetic tunnel junctions grown by pulsed laser deposition — •Michael Bonholzer, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig

A highly conductive interlayer is required for a successful device implementation of spinel oxides in magnetic tunnel junctions (MTJs) [1]. We use zinc ferrite ($ZnFe_2O_4$) as ferromagnetic electrodes. To reduce the series resistance of these devices we add a highly conductive titanium nitride (TiN) layer between the magnesium oxide (MgO) substrate and the $ZnFe_2O_4$ layer. We have achieved to grow atomically smooth hetero-epitaxial TiN thin films on (001) MgO single crystals by pulsed laser deposition (PLD).

In order to generate perfect conditions for two-dimensional growth of TiN on MgO, the substrates are annealed at 950°C for 2h in vacuum using a CO_2 laser heater. The annealed substrates show smooth and uniformly stepped surfaces. The terrace height is half a unit cell of MgO; a value of 0.21 nm was measured by atomic force microscopy (AFM). On these substrates we grew TiN thin films by pulsed laser deposition (PLD). In situ RHEED oscillations indicate two dimensional growth mode up to a film thickness of about 50 nm. This is confirmed by AFM measurements; the TiN films show smooth, stepped surfaces with a uniform terrace height of about 0.21 nm. The existence of intensity fringes in the X-ray pattern indicates a high film quality, as well.

[1] M.Opel *et al.*, Phys. Status Solidi A **208**, 232 (2011)

DS 43.26 Thu 16:00 P1

Structural and magnetic properties of ultrathin epitaxial magnetite films grown on $SrTiO_3$(001) — •Olga Schuckmann[1], Nico Pathé[1], Tobias Schemme[1], Frederic Timmer[1], Timo Kuschel[2], Florian Bertram[3], Karsten Küpper[1], and Joachim Wollschläger[1] — [1]Osnabrück University, Germany — [2]Bielefeld University, Germany — [3]Lund University, Sweden

In this study, structural and magnetic properties of ultrathin magnetite (Fe_3O_4) films grown on $SrTiO_3$ (STO) have been investigated. The films of thicknesses between 10 - 120 nm, as determined by x-ray reflectivity (XRR), were deposited on single crystalline niobium doped STO(100) substrates by reactive molecular beam epitaxy (RMBE, Fe evaporation in O_2 atmosphere).

The stoichiometry of the oxide films was controlled by x-ray photoelectron spectroscopy (XPS). The film structure was characterized by high-energy surface x-ray diffraction (HESXRD) using 85 keV photons as well as lab based conventional XRD. The in-plane and out-of-plane lattice parameters show that compressive strain (-7.5 % lattice mismatch) is reduced with increasing film thickness. In addition, the magnetic properties were studied by magnetooptic Kerr effect (MOKE) showing that the thickness and epitaxial strain affect the magnetic anisotropy of the films.

DS 43.27 Thu 16:00 P1

Thickness dependency of the magnetic anisotropy of iron oxide on MgO(001) — •Tobias Schemme[1], Nico Pathé[1], Timo Kuschel[2], and Joachim Wollschläger[1] — [1]Barbarastr. 7, 49076 Osnabrück — [2]Universitätsstr. 25, 33615 Bielefeld

Iron oxide films with different thicknesses were prepared on MgO(001). The MgO substrates were cleaned by annealing at 400 °C in a 10^{-4} mbar oxygen atmosphere. Afterwards, the surface quality and cleanness was checked in-situ by low energy electron diffraction (LEED) and x-ray photoelectron spectroscopy (XPS), respectively. Iron oxide films with different thicknesses were grown using reactive molecular beam epitaxy (MBE) at 250 °C depositing Fe in a 10 $^{-4}$ mbar oxygen atmosphere. Film thickness and the lattice constants were analyzed by x-ray reflectometry (XRR) and x-ray diffraction (XRD), respectively. These experiments reveal the singlecrystalline and epitactic state of the films. XPS spectra and LEED patterns indicate the stoichiometry and the surface structure of magnetite. Ex-situ magneto optic Kerr measurements were performed to investigate the magnetic properties. While the thinnest film shows a magnetic isotropic behavior, the thicker films exhibit a fourfold magnetic in-plane anisotropy. However, the anisotropy gets weaker with increasing film thickness.

DS 43.28 Thu 16:00 P1

Pseudo-rotational Epitaxy of Octadecyltrichlorosilane Monolayers on Sapphire (001) — •Hans-Georg Steinrück[1], Andreas Magerl[1], Moshe Deutsch[2], and Ben Ocko[3] — [1]1Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen Nürnberg, Germany — [2]Bar-Ilan University, Ramat- Gan, Israel — [3]Brookhaven National Laboratory, Upton NY, USA

Octadecyltrichlorosilane (OTS) self-assembled monolayers (SAMs) on the (001) sapphire surface are vertically aligned, well-packed and have hexagonal ordering like the underlying sapphire as shown by X-ray grazing incidence diffraction. The SAM lattice planes are preferentially aligned along the sapphire in-plane structure albeit with an angular rotational distribution, which is well described by a Lorentzian profile with a FWHM of 10 degrees. The hexagonal SAM lattice constant is incommensurate with the sapphire by 1.2% at room temperature, and the degree of incommensuration increases at higher temperatures. The radial correlation length of 232 $\AA$ is three times larger than for the same monolayers on a native silicon oxide surface and scales with the orientation ϕ of domains via $\xi \sim 1/sin \cdot \phi$. Our results suggest that a commensurate epitaxial arrangement is distorted by steric hindrances caused by both the packing density of the alkyl chains and the dimension and the cross-linking of the head groups. This results in a size-dependent strain within the OTS domains. We call these novel structural properties of a SAM pseudo-rotational epitaxy.

DS 43.29 Thu 16:00 P1

High-resolution TEM investigation of an epitaxially strained LaNiO3/LaGaO3 superlattice — •Haoyuan Qi[1], Michael Kinyanjui[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-89069 Ulm, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70579 Stuttgart, Germany

An epitaxially strained LaNiO3/LaGaO3 (LNO/LGO) superlattice grown on (001) SrTiO3 (STO) has been investigated. Due to the lattice mismatch, the superlattice is subject to tensile strain. The strain-induced distortions and deformations of the octahedral network may drastically influence the magnetic, electrical and structural functionalities of the heterostructures. We have studied the structural change, particularly the tilt system, of the octahedral network by means of aberration-corrected high-resolution transmission electron microscopy (AC-HRTEM). Each atomic column can be resolved clearly by applying negative Cs conditions. The two different octahedral tilt angles viewed in [110] projection indicate non-identical tilt systems in LNO and LGO layers. The atomic structure of the superlattice has been resolved, including in-plane and out-of-plane lattice parameters, distortions and rotation of the oxygen octahedral.

DS 43.30 Thu 16:00 P1

Soft X-ray emission spectroscopy used for the characterization of a-C and CN$_x$ thin films — Sergej Nepijko[1], Alisa Chernenkaya[1], Katerina Medjanik[1], •Sergey Chernov[1], Michael Klimenkov[2], Oleksandr Vlasenko[3], Svetlana Petrovskaya[4], Larisa Odnodvorets[3], Yaroslav Zaulichnyy[5], and Gerd Schönhense[1] — [1]Institute of Physics, University of Mainz, Germany — [2]Institute for Applied Materials, Karlsruhe Institute of Technology, Germany — [3]Sumy State University, Sumy, Ukraine — [4]Frantsevich Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Kiev, Ukraine — [5]National Technical University of Ukraine (KPI), Kiev, Ukraine

We have studied a-C and CN$_x$ films characterized by an outstanding mechanical properties (hardness, elasticity, low friction coefficient) and chemical inertness thus being a good protection against corrosion and mechanical damage for underlying layers. We present the results of a soft X-ray emission spectroscopy study of a-C and CN$_x$ films on Si(100) and glass substrates. Also for the characterization of the homogeneity in depth electron energy loss spectroscopy measurements with localization better than 4 nm were carried out. In case of CN$_x$ films the highest diamond-like modification occurs in the region close to Si(100) substrate. Film density decreases with increasing distance from the substrate and becomes almost constant in range of thicknesses more than 2 nm. By means of X-ray absorption and photoelectron spectroscopies it was shown that a CN$_x$ film (a-C film also) as thin as 1.5 to 2 nm thickness effectively prevents oxidation of the underlying Co film.

DS 43.31 Thu 16:00 P1

Measurement of lattice parameters of ultrathin films with an improved Guinier diffractometer — •Markus Meyl and Arno Ehresmann — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Straße 40, D-34132 Kassel

Lattice parameters of ultrathin films are quantified with the X-ray Guinier thin film diffractometer *Huber* G 653. One advantage of this Guinier diffractometer includes the use of a focussing monochromator between the X-ray tube and the sample for achieving strictly monochromatic X-rays. Another benefit lies in the very small angle of incidence ($< 10°$) between the incident X-rays and the surface of the sample to attain a large distance in the ultrathin films and thereby higher diffraction intensities. Furthermore the sample surface is aligned with height accuracy by utilizing a home built adjustment stage. The measurement setup behind the monochromator is the one of a Seemann-Bohlin camera. In this camera the focal line of the monochromator, the surface of the sample and the detector entrance slit are situated on a constant focussing cylinder. Before a measurement the angle of incidence is appointed and reflected X-rays are measured when Bragg's law is fulfilled. As a consequence the Guinier thin film diffractometer is especially suitable for analysing thin polycrystalline films on a crystalline or amorphous substrate. From the diffraction spectrum e.g. lattice parameters can be calculated. Exemplary results of Si / Cu / Ir$_{17}$Mn$_{83}$ / Ti samples deposited by radio frequency sputtering will be presented.

DS 44: Poster III: Focus session: Resistive switching by redox and phase change phenomena

Time: Thursday 16:00–19:00 Location: P1

DS 44.1 Thu 16:00 P1

Memristive operation mode of floating gate transistors for neuromorphic applications — •Martin Ziegler[1], Dietmar Schroeder[2], Wolfgang Krautschneider[2], and Hermann Kohlstet[1] — [1]Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel, 24143 Kiel, Germany — [2]Technische Universität der Hamburg-Harburg, Institut für Nanoelektronik, Hamburg, Germany

A memristive operation mode of a single floating gate transistor (MemFlash-cell) is presented. To ensure the memristive operation mode, the three-terminal device is reduced to a two-terminal device in such a way that the device resistance varied accordingly to the charge flow through the device during source-drain voltage application. In particular, we provide evidence that the MemFlash-cell can be used to mimic synaptic functionality. Furthermore, based on Hebbian learning, a synaptic analytical expression for the learning rate of this device is derived. The experimental findings are theoretically supported by a capacitive based model. The presented two-terminal MemFlash-cell can be considered as a potential substitute for any memristive device in neuromorphic circuits, cross bar arrays, or reconfigurable logics, and is compatible with state-of-the-art Si-fabrication technology. — [1] Ziegler, M., Kohlstedt, H., JOURNAL OF APPLIED PHYSICS 114, 194506 (2013). [2] Ziegler, M.; Oberlaender, M.; Schroeder, D.; et al., APPLIED PHYSICS LETTERS 101, 263504 (2012).

DS 44.2 Thu 16:00 P1

High resolution electrocoloration study of Fe:STO single crystals — •Viktor Havel[1], Astrid Marchewka[1], Stephan Menzel[2], Susanne Hoffmann-Eifert[2], and Rainer Waser[1,2] — [1]Institut für Werkstoffe der Elektrotechnik II, RWTH Aachen University, Germany — [2]Forschungszentrum Jülich GmbH, PGI 7, Jülich, Germany

Strontium titanate (STO) single crystals and thin films are utilized as model materials for the understanding of the resistive switching (RS) mechanism of valence change oxides like TiOx, HfOx and TaOx. Prior to the bipolar RS an electroforming step is typically required, which impacts the device performance. A thorough understanding of the physical processes involved in the electroforming step is fundamental for future device optimization.

In this study, the electroforming process in Fe doped STO single crystals is made optically visible. Color changes in the transparent Fe:STO crystals are caused by a valence change of the Fe ions as a result of a local redox processes. Thus, the Fe redox reaction is utilized as an indirect proof of the oxygen vacancy drift-diffusion in the crystal. The custom designed electrocoloration set-up enables to put the samples under temperature and electrical stress, to measure the current and resistance change over time and in parallel to monitor the evolution of the color front by high resolution optical microscopy.

The results are discussed on the basis of 1D drift-diffusion simulations of the temporal evolution of the oxygen vacancy distribution, which represent the initial progress of the virtual cathode region.

This work was supported in part by the DFG (SFB917).

DS 44.3 Thu 16:00 P1

The importance of local temperture for the SET kinetics in valence change memories — •Karsten Fleck[1,2], Stephan Menzel[2,3], Ulrich Böttger[1,2], and Rainer Waser[1,2,3] — [1]Institut für Werkstoffe der Elektrotechnik II, RWTH Aachen — [2]JARA Fundamentals of Future Information Technology — [3]Forschungszentrum Jülich GmbH

Resistive switching random access memories (ReRAM) based on the valence change mechanism (VCM) have gained much attention due to their scalability, endurance and switching speed. By the application of bipolar voltage signals of appropriate amplitude the resistance can be switched between a high resistive (HRS) and a low resistive state (LRS).

Commonly this resistance change is attributed to the modulation of an oxygen vacancy enriched nano-sized filament in the oxide layer. The switching kinetics of VCM cells are highly nonlinear which can be attributed to a positive temperature feedback due to local Joule heating in the filament.

The resistive switching of Ti/SrTiOx/Pt cells is investigated at varying background temperature by pulse measurements and voltage sweeps, both covering several orders of magnitude on the timescale. We found evidence for the importance of local temperature for the switching kinetics.

DS 44.4 Thu 16:00 P1

Switching processes induced by partial joule heating in vanadium dioxide two-terminal devices — •Danilo Bürger[1], Varun John[1], Kerstin Bernert[2], György Kovacs[2], Ilona Skorupa[2], Oliver Schmidt[3], and Heidemarie Schmidt[1] — [1]Material Systems for Nanoelectronics, Chemnitz University of Technology — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — [3]Institute for Integrative Nanosciences, IFW Dresden

Vanadium dioxide thin films with the reversible semiconductor-metal phase transition at the thermochromic switching temperature of around 340 K have been prepared by pulsed laser deposition on (0001)-sapphire substrates. We fabricated different two-terminal devices and measured the switching properties by time domain reflectometry as well as switching with a pulse generator. We find repeatable switching behavior for billions of voltage pulses and switching times shorter than 50 ns by using a pulse generator. After measurements with time domain reflectometry at higher voltage amplitudes, we observe a local degredation of VO2 between the two metallic contacts. We think that the inhomogenous electrical fields in the VO_2-structure due to the used conventional contact geometry lead to the local degredation. The main consequence is a partial switching due to local joule heating. This is in contradiction with the often used assumption of the homogenous switching of the complete volume of VO_2 in two-terminal devices [1]. [1] Y. Zhou et al., Electron Device Letters, IEEE **34**, 220 (2013)

DS 44.5 Thu 16:00 P1

Thermal stability of VO_2 — •Marcel Hopfe[1], Jura Rensberg[1], Sebastian Vatterodt[1], You Zhou[2], Shriram Ramanathan[2], György J. Kovàcs[3], Ilona Skorupa[3], Heidemarie Schmidt[4], and Carsten Ronning[1] — [1]Institute for Solid State Physics, Friedrich Schiller University Jena — [2]School of Engineering and Applied Sciences, Harvard University — [3]Helmholtz-Zentrum Dresden-Rossendorf — [4]Material Systems for Nanoelectronics, Technical University Chemnitz

Pure vanadium dioxide (VO_2) has a totally reversible metal-insulator transition (MIT) at about 68°C, making it very interesting for photonic and electric applications. It is known that doping reduces the MIT-temperature. One possibility to dope VO_2 thin films is ion implantation. Lattice defects are introduced during ion irradiation, worsening the MIT properties and making annealing indispensable. Thus, our aim was to investigate the thermal stability of VO_2 at a base pressure of around 10^{-6} mbar. The low pressure is necessary for the ion beam doping process. VO_2 thin films were annealed at temperatures ranging from 100°C to 600°C. All samples were optically and electrically characterised in order to investigate possible changes of MIT properties. With increasing annealing temperature the MIT at 68°C vanishes. This is due to oxygen outdiffusion causing a reductoin of VO_2 towards V_2O_3. Same experiments at higher base pressures show, that oxygen outdiffusion can be prevented. Additionally, post-implantation annealing of irradiated VO_2 thin films will be discussed on the poster.

DS 44.6 Thu 16:00 P1

Growth and characterization of free-standing VO_2 nanowires — Matthias Ogrisek, •Tim Barth, Jura Rensberg, and Carsten Ronning — Institut für Festkörperphysik Friedrich Schiller Universität Jena

Recently, Vanadium dioxide has attracted much attention because of its "metal to insulator transition (MIT)" at ≈68°C. This transition causes a significant change of the electrical and optical properties, allowing applications like sensing or switching. The growth of high-quality VO_2 films is challenging due to stress caused by different thermal expansion coefficients and a lattice mismatch between the film and the substrate. For this reason the growth of VO_2 nanowires (NW's) is of particular interest, because stress can quickly relax laterally in NW's. The aim of our study was to grow free-standing VO_2 NW's. The wires have been grown in a 3-zone tube furnace utilizing Vapor-Solid (VS) growth. VO_2 powder was placed in an alumina boat and heated up to 1325 K to evaporate. The vapor was transported to the substrate by an argon gas flow and grew the wires by self alignment. In-plane grown wires had a length of 200 μm and a diameter of 1-2 μm. Out of plane growth of the nanowires has been achieved by using r-plane sapphire substrates but caused a decrease of the wirelength to 10 μm. EDX-spectrometry revealed only vanadium and oxygen signals and the Raman spectrum measured at RT confirmed the VO_2 nature of the nanowires.

DS 44.7 Thu 16:00 P1

Resistive switching characteristics of $Pr_{0.48}Ca_{0.52}MnO_3$ heterostructures — •Benedikt Arndt[1], Anja Herpers[1], Christian Lenser[1], Regina Dittmann[1], and Rainer Waser[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Jülich, 52425, Germany — [2]Institut für Werkstoffe der Elektrotechnik II, RWTH Aachen University, Aachen, 52074,Germany

Resistive random access memory (RRAM), which is based on hysteretic resistive switching in transition-metal oxides, is believed to be a promising candidate for high-density nonvolatile memory. It has been demonstrated for many oxides, that the resistive switching and its related redox processes take place in a spatially restricted filament region. In contrast, it has been demonstrated that the currents from high and low resistive states in praseodymium calcium manganate (PCMO) RRAM cells scale with the electrode area. The underlying mechanisms in these systems have not yet been fully understood.

We could experimentally prove that resistive switching in PMCO/Ti heterostructures is based on a redox-process, which mainly happens on the side Ti of the PCMO/Ti interface. In particular, the amount of fully oxidized Ti-ions determines the thickness of the insulating TiO_2 tunnel barrier, which forms at this interface.

Furthermore, we compare these devices to cells which comprise an yttria stabilized zirkonia (YSZ) layer at the interface of PCMO and platinum top electrodes. The YSZ is intended as an artificial tunnel barrier whose properties can be influenced by the deposition process. This extra layer allows further to tune the device properties.

DS 44.8 Thu 16:00 P1

Oxygen-vacancy behavior in strontium titanate — •Marcel Schie[1], Roger A. De Souza[2], and Rainer Waser[1] — [1]Institute of Materials in Electrical Engineering and Information Technology, RWTH Aachen University, 52074 Aachen — [2]Institute of Physical

Chemistry, RWTH Aachen University and JARA-FIT, 52056 Aachen

We investigate the effect of acceptor-type cation dopants on oxygen-vacancy migration in the perovskite oxide SrTiO3 by static lattice simulation techniques. We focus on two themes: cation dopants modifying the activation energies for vacancy migration, and cation dopants (Ni2+, Fe2+, Co2+, Mn2+ and Al3+) binding oxygen vacancies in binary associates. In both cases a variety of defect configurations exceeding the scope of nearest neighbor (NN) interaction is examined Our results predict that, regardless of the cation dopant, the binding energy of an oxygen vacancy to a dopant is negative at NN sites, but only converges to zero for NNNNN sites. In addition the simulations show that the migration energy of a vacancy is affected by an acceptor dopant cation over a length scale of several unit cells. The results are also used in an analytic three frequency model of ionic conductivity in SrTiO3 to show trends for different dopants and concentrations. For comparison, a simple defect-chemical model containing only dopant-vacancy association at nearest neighbor sites is employed to reconcile literature data. Within this model two major results that are apparently inconsistent with different migration enthalpies are combined.

DS 44.9 Thu 16:00 P1

Influence of Au-nanoparticles on the resistive switching properties of $SrTiO_3$ thin films — •Nicolas Raab[1], Oliver Schmidt[2], Ulrich Simon[2], and Regina Dittmann[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Jülich, 52425, Germany — [2]Institut für Anorganische Chemie, RWTH Aachen University, Aachen, 52074,Germany

The strong impact of defects on the resistive switching properties of $SrTiO_3$ is generally assumed. Therefore we investigated a method of tailoring defect positions and thereby locally modifying the resistive switching properties of $SrTiO_3$ thin films.

To induce locally defined defects we processed Au-nanoparticles (AuNPs) from solution onto 0.5%wt-Nb:$SrTiO_3$ substrates. We expect the AuNPs to act as defect nuclei for the subsequently PLD-grown $SrTiO_3$ thin films. We investigated the correlation between the topography and the local conductivity by performing *in-situ* LC-AFM measurements with area scanning as well es grid measurements. These measurements combine topography scans with single point spectroscopy, leading to I-V curves correlated with defined positions on the surface.

We measured differences in the resistive switching behavior between the AuNPs, their immediate vicinity and the more distant areas. In the immediate vicinity of the AuNPs the $SrTiO_3$ thin film can be switched, whereas the other areas show no change in the conductivity. We will discuss the influence of defects formed in the vicinity of the AuNPs on the local switching properties.

DS 44.10 Thu 16:00 P1

Chemical investigation of buried active layers in resistive switching materials by hard x-ray photoemission electron microscopy (HAXPEEM) — •Christoph Schmitz[1], Marten Patt[1], Carsten Wiemann[1], Alexandra von der Heiden[2], Manfred Martin[2], Andrei Gloskovskii[3], Wolgang Drube[3], and Claus M. Schneider[1,4] — [1]Peter Grünberg Institut PGI-6, FZ Jülich, Jülich, Germany — [2]Institute of Physical Chemistry, Aachen, Germany — [3]Deutsches Elektronen-Synchroton DESY, Hamburg, Germany — [4]Fakultät f. Physik and Center for Nanointegration Duisburg-Essen (CeNIDE), Duisburg, Germany

Energy filtered photoemission electron microscopy (EF-PEEM) offers a lot of valuable insights into chemically driven processes at surfaces. In our work we want to apply this method to resistive switching materials to understand the origin of the different resistive states of such materials by investigating changes of band structure, chemical bonding and composition. However, devices based on resistive switching materials are commonly designed in layered structures where the active material is buried beneath a metal top electrode and usually not accessible by conventional photoemission techniques due to their high surface sensitivity. Here we present a way to increase the probing depth of EF-PEEM up to several nm in a non-destructive manner by using hard x-ray photons (hν=6550eV). Advantages and limitations of this method will be discussed on the basis of recent data of GaOx-based resistive switching devices and a Cr/Au/Si wedge sample collected at PETRA III Beamline P09.

DS 44.11 Thu 16:00 P1

Spectroscopic investigations of resistively switching Ta_2O_{5-x} thin films — •Oliver Peters[1], Katharina Skaja[1], Christoph Bäumer[1], Regina Dittmann[1], and Rainer Waser[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Jülich, 52425, Germany — [2]Institut für Werkstoffe der Elektrotechnik II, RWTH Aachen University, Aachen, 52074,Germany

The subject of resistive switching in metal oxides and its utilisation in resistive random access memory (RRAM) has received abundant research interest during the last years.

Within the valence change memory (VCM) type of RRAM, Tantalum Oxide is one of the materials of choice, recently being introduced to the market. Thus, the proposed physical model of resistive switching in VCM, which is linked to the diffusion of oxygen vacancies and the formation of conducting filaments, has been analysed by different approaches. Although there are several publications dealing with the spectroscopic analysis of stacked structures, such as capacitors, the details of the chemical changes induced by electrical treatments at the electrode/Ta_2O_{5-x} interface are not completely understood so far.

Employing an in-situ electrode delamination technique, the electrode/Ta_2O_{5-x} interface was analysed by means of energy filtered photoelectron emission microscopy (PEEM). We will present characteristics of the low and high resistance state as well as non-switched areas of a Ta/Ta_2O_{5-x}/Pt stacked sample.

DS 44.12 Thu 16:00 P1

TaOx based memristive systems with variable oxygen concentration — •Stefan Niehörster[1], Savio Fabretti[1], Markus Schäfers[1], and Andy Thomas[1,2] — [1]Bielefeld University, Bielefeld, Germany — [2]Mainz University, Mainz, Germany

TaOx based devices show reversible and nonvolatile memristive switching effects for a large number of cycles. This property makes them very interesting for data storage applications or imitating synapses in a neural network. We prepared devices with Pd and Ta electrodes and a TaOx barrier. The electrodes were deposited by magnetron sputtering and the tunnel barrier was fabricated by in-situ oxidation of a thin sputtered Ta film. This approach gives us the possibility to manipulate the oxygen concentration of the barrier compared to sputter deposition of a TaOx target. We varied the bias voltage of the oxygen plasma to regulate the thickness of the barrier by the penetration depth, and we varied the oxidation time to regulate the oxygen concentration. We used optical lithography to define squares of 10x10, 15x15 or 25x25μm^2. The junctions were characterized by transport measurements in two point geometry. The measurements of our devices show memristive switching, where the amplitude and the noise of the switching show a dependence on the oxidation time. In addition, we were able to reach more than two states. The data is compared to our earlier results with MgO based memristive tunnel junctions. Here, the amplitude of the memristive switching was increased by a factor of 3.

DS 44.13 Thu 16:00 P1

Setup for optical switching of single antenna resonances in the mid-infrared using phase-change materials — •Thomas Kalix, Ann-Katrin Ursula Michel, Martin Salinga, and Thomas Taubner — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Metallic nanostructures become more important in the field of plasmonics and metamaterials, since they locally enhance electromagnetic fields. For example the resonance frequency of rod-like shaped nanoantennas depends on the geometry, the material they are fabricated of and the refractive index n of the surrounding media [1].

Phase-change materials (PCM) are characterized by a fast phase transition between the amorphous and crystalline state. The structural change is accompanied by a huge modulation of n, which allows us to tune the resonance frequency of nanoantennas which are embedded in a PCM thin film [2]. The switching between the amorphous and crystalline phase can be realized reversibly for example by an optical pulse [3]. We built a laser setup which allow us the local switching of single nanostructures which are fabricated on the PCM $Ge_3Sb_2Te_6$ with single nanosecond pulses.

[1] F. Neubrech *et al.*, J. Appl. Phys. 89, 253104 (2006).
[2] A. Michel *et al.*, Nano Lett., 13(8), pp 3470-3475 (2013).
[3] J. Siegel *et al.*, J. Appl. Phys. 103, 023516 (2008).

DS 44.14 Thu 16:00 P1

Sputter Deposited Chalcogenide Superlattices (CSL) for Energy Efficient Data Storage — •Felix R. L. Lange[1], Enrico Varesi[2], Andrea Redaelli[2], Luigi Avaro[2], Jamo Momand[3], Bart J. Kooi[3], Stefan Jakobs[1], and Matthias Wuttig[1,4] — [1]1.

Physikalisches Institut (IA), RWTH Aachen University, Germany — [2]Micron Semiconductor Italia, Process R&D, Agrate Brianza, Italy — [3]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — [4]JARA - FIT, RWTH Aachen, Germany

Phase change materials (PCM) are a unique sub-class of chalcogenides where both, an amorphous and a crystalline state are stable at ambient conditions. Since the phase transition can proceed on a nanosecond timescale PCM are already exploited in rewritable optical data storage solutions (CD-RW, Blu-ray-RW) and first solid state memories are commercially available. The phase transition in both cases is induced via melt quenching and crystallizing of the material, respectively. Only recently a very different mechanism was proposed for highly textured multilayers of GeTe and Sb_2Te_3. Here, a change of the coordination number of Ge atoms at the interface was argued to be responsible for the pronounced electrical contrast between these two states [1]. These superlattices furthermore exhibit rather low switching powers as compared to ordinary PCM which makes this novel stack design highly valuable for future 'green' data storage solution. Here we explore the feasibility to grow highly textured thin alternating layers of GeTe and Sb_2Te_3 using DC magnetron sputter deposition.
[1] R. E. Simpson *et al.*, Nat. Nanotechnol. **6**, 501-505 (2011)

DS 44.15 Thu 16:00 P1

Analysis of the switching behaviour of Phase Change Materials using s-SNOM — •Martin Lewin, Benedikt Hauer, Ann-Katrin U. Michel, and Thomas Taubner — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Phase Change Materials (PCM) show at least two stable states in the solid phase: One amorphous and one crystalline state. These two states have significantly different dielectric functions. The fact that the two states can be switched reversibly by optical or electrical means (laser-, voltage-pulses) makes PCM very interesting for storage applications (Re-Writable-Discs, Phase-Change-RAM) or even logical photonic devices [1]. PCM are often characterised by TEM, AFM or far-field reflection measurements (diffraction-limited).

Scattering-type scanning near-field optical microscopy (s-SNOM) is based on an illuminated metal coated tip being scanned over a sample. The backscattered light is measured in a detector yielding the near-field optical amplitude and phase signals which depend on the dielectric function of the sample. Due to the local detecting approach the lateral resolution is no longer wavelength-dependent (here: approx. 25 nm). S-SNOM does not rely on thin samples as TEM does and yields subsurface information in contrast to AFM.

Here we present our progress in resolving the state of switched PCM (both thermally and by laser-pulse sequences) on a nm-scale using s-SNOM.

[1] Simone Raoux and Matthias Wuttig. In Nanoelectronics and Information Technology. Rainer Waser (ed.). Wiley-VCH Verlag, 2012.

DS 44.16 Thu 16:00 P1

Textured growth of pulsed laser deposited Ge2Sb2Te5 thin films — •Erik Thelander, Ulrich Ross, Xinxing Sun, Andriy Lotnyk, and Bernd Rauschenbach — Leibniz Institute of surface modification, Leipzig, Germany

Phase change materials based on the material system Ge-Sb-Te have been widely used for optical storage for decades and are gaining more interest as a candidate for storage class memory. Pulsed laser deposition (PLD) is a deposition method with hyper-thermal species that could have a large influence on the film and crystal growth and hence also on the phase change properties. Although a number of groups have studied PLD-deposited phase change films, until now no investigations of the growth of the material has been presented. This investigation show that it possible to synthesize high quality thin films of Ge2Sb2Te5 using a stoichiometric compound target and a pulsed laser deposition process. X-ray diffraction (T-2T, RC and pole figure measurements) was employed to determine the crystalline quality of the samples and selected samples was investigated with HRSTEM using a probe corrected FEI Titan* G2 60-300kV transmission electron microscope. As substrates, HF-dipped Si (100) and freshly cleaved KCl (100) have been used. Thermally annealed as-deposited films show a polycrystalline nature whereas films that are deposited at elevated temperature show a preferred 111-growth direction independent of substrate. This could have implications for the switching behavior of the material and for further studies on epitaxial growth.

DS 44.17 Thu 16:00 P1

Laser-induced phase transitions of PLD-deposited GeTe films — •Xinxing Sun[1], Erik Thelander[1], Hongbing Lu[2], Jürgen W. Gerlach[1], and Bernd Rauschenbach[1] — [1]Leibniz Institute of Surface Modification, Permoserstr. 15, D-04318, Leipzig, Germany, — [2]Hubei University, Wuhan 430062, China

Phase change memory materials based on chalcogenides can rapidly and reversibly be switched between an amorphous and a crystalline phase. Since both phases are characterized by very different optical and electrical properties, there materials can be employed for rewritable optical and electrical data storage. In this letter, phase transformations in Ge-Te thin films (grown using pulsed laser deposition system) are induced by irradiation with nanosecond laser pulse at 248 nm has been investigated. The influence of laser fluence between 20- 300 mJ/cm2 on the structure and properties of Ge-Te phase-change films were studied by X-ray diffraction and reflectivity measurements. The results show that switching is possible under irradiation with nanosecond pulses using single pulses for amorphization and multiples pulses for crystallization. For comparison, the large structural differences between the laser irradiated and thermally annealed films are also revealed, in between those of the crystalline and amorphous.

DS 44.18 Thu 16:00 P1

An alternative route for crossing the metal-insulator transition in GeTe-Sb_2Te_3-alloys — •Annika Poitz, Hanno Volker, Peter Jost, Peter Zalden, Tobias Schäfer, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen, 52056 Aachen

Phase-change materials (PCMs) are outstanding materials: Besides a fast transition between the amorphous and the crystalline state, these materials show a high contrast in their optical and electrical properties. Due to these properties PCMs can be employed in optical and electrical memory technologies.
Recently it has been demonstrated[1] that the resistivity in the crystalline phase in some PCMs such as $Ge_1Sb_2Te_4$ depends on the annealing temperature. Higher annealing temperatures lead to smaller resistivities and even a change from non-metallic to metallic behavior. This is explained by a reduction of disorder upon annealing, which leads to a disorder-driven metal-insulator transition (MIT). This MIT has been proven to be independent of structural transitions[1]. However $Ge_1Sb_2Te_4$ shows a cubic to trigonal transition near the MIT, which hampers a clear distinction between the influences of disorder and crystalline structure.
In this study we report an MIT in PCMs without such a structural change. Instead of annealing, we control disorder by varying the stoichiometry of $(Sb_2Te_3)_{1\text{-}x}(GeTe)_x$-alloys with $0.75 \leq x \leq 1$. In this study we employ low- and high-temperature resistivity, Hall-effect and XRD measurements for a characterization of the samples.
[1] T. Siegrist et al., Nat. Mat. 10, 202 (2011)

DS 44.19 Thu 16:00 P1

Nanodiffraction and fluctuation electron microscopy of phase-change material — Manuel Bornhöfft[1,2], Paul Voyles[3], Tobias Saltzmann[4], •Ulrich Simon[4], and Joachim Mayer[1,2] — [1]Gemeinschaftslabor für Elektronenmikroskopie, RWTH Aachen University, Ahornstraße 55, 52074 Aachen, Germany — [2]Ernst Ruska-Centre, FZ Jülich and RWTH Aachen, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [3]Department of Materials Science and Engineering, University of Wisconsin, Madison, Madison, Wisconsin 53706, USA — [4]Institute of Inorganic Chemistry and JARA - Fundamentals of Future Information Technology, RWTH Aachen University, Landoltweg 1, 52074, Aachen, Germany

We studied phase-change materials in a scanning transmission electron microscopy (STEM) dedicated Titan transmission electron microscope (TEM) by nanodiffraction and fluctuation electron microscopy. In both techniques the samples are investigated by a coherent and parallel electron probe in the nanometer scale by STEM. This is in contrast to the normal STEM, which is executed with a convergent beam. The coherent and parallel illumination enables us to image the diffraction patterns of probe size (1-11nm) limited regions. Nanodiffraction is used to get nanometer scale information of the phase of phase-change materials and its structures. Fluctuation electron microscopy is sensitive to the medium-range order of materials. The grade of order can influence the crystallization kinetics of the materials, which are important for the application as memories.

DS 44.20 Thu 16:00 P1

Resistive Switching Properties of Chemically Synthesized Metal Oxide and Higher Chalcogenide Nanoparticles — •Tobias Saltzmann[1], Oliver Schmidt[1], Michael Noyong[1], and

Ulrich Simon[1,2] — [1]Institut für Anorganische Chemie, RWTH Aachen University, 52074 Aachen, NRW, Germany — [2]JARA - Fundamentals of Future Information Technologies

We apply chemical approaches for the fabrication of metal oxide and higher chalcogenide nanoparticles (NPs) as resistively switching nanostructures. By varying size, crystallinity, morphology as well as composition, we aim to explore structure-composition-property relations.

As a model phase change material we studied the narrow band gap semiconductor Sb2Te3. Its highly anisotropic crystal structure consists of quintuple Te Sb Te Sb Te layer stacks, with covalent bonding in ab-, but v. d. Waals bonding in c-direction. Synthesized via a solvothermal route, Sb2Te3 is formed as single crystalline hexagonal platelets (HPs) with sizes of 1 to 10 *m in ab-direction and with a few tens up to 250 nm in c-direction. We electrically addressed single HPs in situ in a SEM in ab- and c-direction, respectively, and monitored switching between two differently conducting states in both directions.

As model valence change material we synthesized TiO2. Via a sol-gel process amorphous TiOx NPs are formed and subsequently calcined to form crystalline TiO2. To study the influence of defect concentration and crystallinity on the resistive switching behavior, amorphous as well as NPs calcined in oxidizing or reducing environments are electrically characterized in situ in a SEM.

DS 44.21 Thu 16:00 P1

Simulation of nucleation and growth in crystallization of phase change metrials — •Fatemeh Tabatabaei[1], Markus Apel[2], and Efim Brener[1] — [1]Peter Grünberg Institut (PGI-2), Forschungszentrum Jülich, 52428, Jülich — [2]Access e.V., RWTH Aachen, 52072 Aachen

Chalcogenide materials like GeSeTe and AgInSbTe showing phase change properties suitable for the use in non-volatile rewritable memory devices. Their crystallization mechanism in the course of switching is known to be nucleation dominated or growth dominated, respectively [1]. The phase field simulation technique is applied in order to study crystallization of the amorphous state to the crystalline state. We extended our work by adding a nucleation model to the simulation of crystallization. The impact of different model parameter like critical radius for nucleation or maximum nucleation frequency has been investigated as a function of process parameter, e.g. the substrate temperature, for non-isothermal and transient conditions. Results of the simulations are grain size, temperature evolution and the crystallization rate.

[1] Raoux S. and Wuttig M., (2010) *Phase Change Materials, Science and Application*, New York, NY: Springer

DS 45: Poster IV: One-Dimensional Metals: Reality or Fiction

Time: Thursday 16:00–19:00 Location: P1

DS 45.1 Thu 16:00 P1

Structural investigations of Au quantum wires on Ge(100) — •Heiko Teiken, Timo Lichtenstein, Christoph Tegenkamp, and Herbert Pfnür — Leibniz Universität Hannover, Institut für Festkörperphysik, AbteilungATMOS, 30167 Hannover

Ge(100) is known as a substrate for self-organized growth of one dimensional quantum wires by adsorption of Au. As shown recently (C. Blumenstein et.al. Nature 7, 776) the signatures of a Luttinger liquid behavior depends crucially on the quality of the ensemble and, consequently, on the quality of the Ge(100) sample prior to adsorption. Furthermore, there is a debate regarding details of the atomic structure of the atomic wires induced upon Au adsorption. In this study we have measured systematically roughness parameters on variously prepared surfaces by means of spot profile analysis of low energy electron diffraction patterns (SPA-LEED). From G(S)- and H(S)-analyses Ge-monoatomic step heights of $1.42\AA$ with average terrace lengths around 20 nm are found. Ex-situ chemically treated Ge-samples followed by in-situ thermal annealing reveal slightly lower rms-values (1.3 Å) as samples which have undergone multiple in-situ sputter/annealing cycles. The G(S)-curves reveal additional structurs after growth of the Au-wires corresponding to step heights of 1.8 Å which we suggest to be due to interference between gold covered islands and clean terraces. The overall roughness of the Ge-template does not increase due to growth of the Au-induced wires. Details of the G(S)-curves will be discussed in terms of different structural models (Au-dimer chains vs. Au-induced Ge-facet structures) currently proposed in literature.

DS 45.2 Thu 16:00 P1

Structural and electronic properties of Si(111)-(5×2)-Au surface from first-principles calculations — •Kaori Seino and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Jena, Germany

Self-assembled atomic wires fabricated on semiconductor surfaces are promising candidates for future nanoelectronics. The Si(111)-(5×2)-Au surface is one of the examples where atomic nanowires appear. For a long time it has been the subject of experimental and theoretical studies. The experimental determination of the Au coverage has been recently revised to be 0.6 ML instead of 0.4 ML. Correspondingly, a structural model was proposed from first-principles calculations [1]. However, recently an alternative model is proposed from structural studies [2]. Still the surface reconstruction of the Si(111)-(5×2)-Au surface is under debate.

Here we present *ab-initio* calculations of structural and electronic properties of Si(111)-(5×2)-Au. To assess the accuracy of our first-principles total energy methods, we also used different exchange correlation functionals including the Perdew-Becke-Ernzerhof functional for solids and surfaces (PBEsol) and the van der Waals density functional (vdW-DF). We clearly favor the model proposed by Erwin *et al.* [1] versus that proposed by Abukawa and Nishigaya [2].

[1] S. C. Erwin *et al.*, Phys. Rev. B **80**, 155409 (2009).

[2] T. Abukawa und Y. Nishigaya, Phys. Rev. Lett. **110**, 036102 (2013).

DS 45.3 Thu 16:00 P1

Rare Earth Silicides from Density Functional Theory — •Kris Holtgrewe, Simone Sanna, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn, Paderborn, Germany

Rare earth silicide nanowires are of high interest both because of their fundamental physics properties and for applications such as nanoscale interconnects, optical waveguides and quantum devices. However, the exact knowledge of their atomic structure is still incomplete. The detailed knowledge of the bulk phase of the rare earth silicides is a prerequisite for a fundamental understanding of the ground and excited state properties of the nanowires. As a first step towards the nanowire modeling, we have investigated the hexagonal and tetragonal phases of several rare earth disilicides, including $\mathrm{ErSi_2}$, $\mathrm{DySi_2}$ and $\mathrm{HoSi_2}$ from *first-principles*. The $4f$ electrons of the rare earth are treated both as valence states, explicitly taking into account the on-site Coulomb interactions, or as frozen state in the atomic core. Structural and electronic properties of the investigated systems are discussed. While all the silicides are characterized by rather similar lattice parameters, these are found to strongly depend on the Si vacancy concentration.

DS 45.4 Thu 16:00 P1

Tb silicide nanowires on planar and vicinal Si(001): growth and characterisation — •Stephan Appelfeller, Stefan Kuls, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Deutschland

Metallic nanowires are interesting not only because of their possible future applications in nanoelectronics but also because of unique one-dimensional phenomena, e.g. the Peierls instability or Luttinger liquid behavior. A model system for metallic nanowires are silicide nanowires on Si(001). Here, the growth of Tb silicide structures by molecular beam epitaxy on planar and vicinal Si(001) surfaces was studied for the first time. Submonolayer amounts of Tb were deposited at room temperature and subsequently annealed at elevated temperatures. A wire-like 2×7 reconstruction and – for coverages surpassing a critical coverage – Tb silicide nanowires were observed and analysed by scanning tunnelling microscopy. The critical coverage reduces for more structured surfaces, e.g. vicinal surfaces. At moderate annealing temperatures, the 2×7 reconstruction, which shows a strongly voltage dependant appearance, remains intact upon nanowire formation. In contrast, the 2×7 reconstruction disappears during nanowire formation at higher temperatures. The structure of the nanowires could be identified as hexagonal TbSi$_2$. They are highly anisotropic with widths of few nanometers and lengths of several hundred nanometers and grow parallel to each other on well ordered vicinal surfaces. This work was supported by the DFG through FOR 1700 project E2.

DS 45.5 Thu 16:00 P1

Pb nanowires on Si(557) — •Frederic Timmer[1], Sebastian Gevers[1], Thomas Weisemöller[1], Christoph Tegenkamp[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover

The restructuring of the Si(557) surface during formation of Pb nanowires has been investigated in-situ by surface x-ray diffraction (SXRD) studies which were performed at the beamline ID03 of ESRF. For this purpose, Pb has been deposited on the bare Si(557) - (3×1) at room temperature until 3D Pb islands were grown on the initial Pb wetting layer. The formation of Pb islands was monitored by the appearance of 3D Pb Bragg peaks.

Thereafter, Pb was carefully desorbed by annealing to 600K. This process was controlled by recording corresponding 3D Pb Bragg peaks directly in-situ by SXRD. Desorption of Pb has been stopped when the Pb islands have vanished and the Pb wetting layer is transformed into a $\left(\sqrt{3} \times \sqrt{3}\right)$ superstructure on the nano-(111) terraces of the Si(557) surfaces. Reciprocal space mappings were recorded in the $[7, 7, \bar{1}0]$ direction, i.e. perpendicular to the atomic steps, clearly indicating a strong refacetting of the initial (557) orientation. It turns out that the restructured Si(557) surface is indeed stabilized by the $\left(\sqrt{3} \times \sqrt{3}\right)$ Pb overlayer on the Si(111) terraces.

DS 45.6 Thu 16:00 P1

Structural studies on self-assembled atomic gold nanowires of the Si(111)-(5x2)-Au reconstruction by Surface X-Ray Diffraction — •Patrick Bayersdorfer[1], Frederic Timmer[2], Julian Aulbach[1], Henrik Wilkens[2], Lenart Dudy[1], Joachim Wollschläger[2], Ralph Claessen[1], Friedrich Reinert[1], and Jörg Schäfer[1] — [1]Universität Würzburg, D-97074 Würzburg — [2]Universität Osnabrück, D-49076 Osnabrück

Self-assembled nanowires on semiconductors have recently attracted high attention in terms of one-dimensional (1D) physics. The structural confinement on the order of atomic width gives rise to an enhancement of electron correlation effects, leading to exotic many-body phenomena.

As a prototype of 1D metallic chain systems, the Si(111)-(5x2)-Au reconstruction has been widely studied by a variety of spectroscopic and structural techniques. Particularly, it remains unclear whether or not the superstructure relates to a frozen Peierls distortion or to a structural component. However, the definite structural model is still unknown, although it is of vital importance for a precise understanding of the unusual 1D properties in terms of lattice instabilities or correlation physics.

We present a structural investigation of the Si(111)-(5x2)-Au reconstruction by Surface X-Ray Diffraction (SXRD) yielding the two-dimensional Patterson function, as well as several crystal truncation rods. This will be compared with recent theoretical structural models. In addition, we applied spot-profile low-energy electron diffraction (SPA-LEED) to analyse the morphological aspects of this 1D system.

DS 45.7 Thu 16:00 P1

STM study of Dy-induced nanowires on Ge(001) — •Michael Lochner, Robert Bienert, Ulrike Kürpick, and René Matzdorf — Universität Kassel

Quasi one dimensional nanowire structures on semiconductor surfaces are of interest for more than ten years. The scope of this research is the understanding of exotic quantum phenomena like Luttinger-Liquids, Charge-Density-Waves or magnetic ordering in 1D or quasi-1D.

While the atomic structure of Rare Earth metal induced nanowires on silicon surfaces is investigated in many publications, there are less publications on Rare Earth metals on germanium. In this poster, we present our latest STM and LEED data of Dy-induced nanowires on Ge(001).

Similar to Dy-induced nanowires on Si(001), they have different widths, but there is no wetting layer on the Ge(001) surface. The thinnest wires have a width of four Ge lattice constants and their length can vary from just a few to more than 50 nm. We present STM data of the electronic structure in the wires.

DS 45.8 Thu 16:00 P1

Dimensionality and Metallicity of quasi-1D Ag:Si(557) Investigated by Angle-Resolved Photoemission — •Chris Nicholson[1], Claude Monney[1], Ulrich Krieg[2], Michele Puppin[1], Yunpei Deng[1], Christoph Tegenkamp[2], Herbert Pfnür[2], Karsten Horn[1], Ralph Ernstorpher[1], and Martin Wolf[1] — [1]Fritz-Haber-Institut of the Max Planck Society, Berlin, Germany — [2]Leibniz Universität, Hannover, Germany

Self-assembled quasi-one-dimensional (1D) atomic wires on semiconductor surfaces show a range of interesting physical phenomena, and are promising for nanoscale devices. However, the number of metallic systems available is relatively small. Angle-Resolved Photoemission Spectroscopy (ARPES) is a powerful tool that can directly address the metallicity of these systems, and can additionally connect macroscopic conductivity to specific parts of the electronic band structure. We apply ARPES to Ag:Si(557): around 1ML coverage, plasmonic losses with a 1D dispersion have been observed at room temperature in Electron Energy Loss Spectra (EELS), in contrast to insulating behaviour observed with EELS and ARPES at lower Ag coverage. Preparation has been optimised by LEED and ARPES measurements with He I, while high resolution ARPES near the Fermi level allows us to search for metallic surface states and measure their dispersion, in order to assess their relation to the low-dimensional plasmonic excitations. Furthermore, we have developed a new high-repetition rate VUV light source for ultrafast time-resolved ARPES measurements, which will provide complementary dynamic information on such quasi-1D systems.

DS 45.9 Thu 16:00 P1

Evidence of Spin-Orbit Density Waves in Atomic Pb-Wires on Si(557) — •Christian Brand[1], Daniel Lükermann[1], Herbert Pfnür[1], Gabriel Landolt[2], Hugo Dil[2,3], and Christoph Tegenkamp[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland — [3]Institute of Condensed Matter Physics, École Polytechnique Fédérale de Lausanne, Switzerland

Growth of 1.3 monolayers Pb on Si(557) results in a highly anisotropic wire ensemble structure which undergoes a 2D/1D transition when cooling below 78 K as seen by surface sensitive transport measurements. In particular, the system becomes insulating in the direction across the wires. We will show that the mutual interplay between superlattice structures, band filling factors, and spin-orbit coupling results in a highly correlated electronic spin and charge state. By means of spin- and angle-resolved photoemission spectroscopy (SR-ARPES), supplemented by LEED and STM, the spin texture close to the Fermi surface was found to be alternating and equidistant; thus, Fermi nesting occurs in between bands with the same spin texture, giving rise to spin spirals in the direction across the wires. An out-of-phase superposition of both Rashba channels is manifested by an extraordinary large Rashba splitting of $\Delta k_0 = 0.2\,\text{Å}^{-1} = g/2$, where g is a reciprocal lattice vector defined by the interwire distance and fits into the model of spin-orbit density waves in antiferromagnetically ordered chain structures. The implications towards spin-polarized transport along the wires will be discussed.

DS 45.10 Thu 16:00 P1

Spin-Polarization and Spin-Orbit Coupling in Au-Induced Atom Chains on High-Index Silicon Surfaces — •Julian Aulbach[1], Jörg Schäfer[1], Steven C. Erwin[2], Sebastian Meyer[1], Lenart Dudy[1], Bartosz Slomsik[3], Gabriel Landolt[3], Hugo Dil[3], and Ralph Claessen[3] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg, Germany — [2]Naval Research Laboratory, Washington DC, USA — [3]Paul Scherrer Institut, Villigen, Switzerland

Atoms can form chain-like architectures by self-assembly on various semiconductor surfaces. Such may offer physical realizations of 1D electronic ground states like Peierls instabilities or Tomonaga-Luttinger liquids. Here we report on Au-stabilized nanowires on a high-index silicon substrate, namely Si(553). The two chain types present in that system, one built by Au and one by Si atoms, develop two- and threefold periodicities at low temperatures, which were previously assigned to Peierls instabilities. However, our results from scanning tunneling microscopy and spectroscopy are in astounding agreement with the Si(553)-Au ground state predicted by density-functional theory , where every third Si atom is spin polarized [1]. Moreover, the structural model [2] suggests strong spin-orbit coupling for the Au chains. Using spin- and angle-resolved photoemission we find direct evidence for such a spin-splitting in both Au-induced bands, rendering this system an intriguing 1D material with spin ordering in real and reciprocal space.

[1] J. Aulbach *et al.*, Phys. Rev. Lett. **111**, 137203 (2013).

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

DS 45.11 Thu 16:00 P1

Rashba splitting and relativistic energy shifts in In/Si(111) nanowires — •Nora Jenny Vollmers, Andreas Lücke, Uwe Gerstmann, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn, Germany

The electronic properties of quasi-1D systems are of both scientific interest and technological relevance, e.g., for atomic-scale interconnects. The ordered array of In "nanowires" formed upon room temperature (RT) In monolayer deposition on Si(111) substrates and sub-sequent annealing is one of the most intensively investigated model systems in this context. We investigate the influence of relativistic effects, notably the spin-orbit coupling, on the energetics and electronic properties of the In nanowires. Spin-orbit (SO) coupling is well-known to be the driving force behind ferromagnetism und can be used to control the functionality of electronic devices in spintronics. On the other hand, spin-split electron gases may form in asymmetric quantum wells or at surfaces and give rise to the so-called Rashba-(Bychkov) effect even in non-magnetic materials: The break of the spatial symmetry caused by the surface in conjunction with the SO related break of time reversal symmetry lifts the spin degeneracy. Here it is shown that in case of In/Si(111) nanowires – due to an enlarged out-of-plane potential gradient caused by structural anisotropies of the In nanowires – a pronounced splitting of the Rashba type is found at the X point, i.e., at the Brillouin zone boundary.

DS 45.12 Thu 16:00 P1

Raman Spectroscopy of gold-induced nanostructures on plain and high index Si(111) — •Jochen Räthel[1], Eugen Speiser[1], Sandhya Chandola[1], Arne Baumann[1], Norbert Esser[1], Julian Aulbach[2], Sebastian Meyer[2], Utz Bass[2], Martin Liebhaber[2], Lenart Dudy[2], Jean Geurts[2], Jörg Schäfer[2], and Ralph Claessen[2] — [1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Albert-Einstein-Str. 9, 12489 Berlin — [2]Physikalisches Institut and RCCM, Universität Würzburg, Physikalisches Institut, Am Hubland, 97074 Würzburg

Atomic chains formed by metal adsorption on semiconductor surfaces are used as model systems for determining exotic electronic ground states. Here we present the vibrational properties of Au-induced nanostructures on Si(111) (($\sqrt{3}\times\sqrt{3}$) and (5×2) phase) and on Si(553) (local (5×2) phase), probed by polarized Raman spectroscopy (RS). Plenty of new surface vibration modes were identified for all three Au related surfaces. By comparing the results from RS of these three Au phases under consideration of different substrates, common structural elements were identified. These results could have a high impact on the verification of theoretical structures models of these systems, e.g., the lowest-energy reconstruction models of Krawiec [1] and the structural model of Erwin and Himpsel [2]. [1] M. Krawiec, Phys. Rev. B 81, 115436 (2010); [2] S. C. Erwin, Nat Commun 1, 58 (2010)

DS 45.13 Thu 16:00 P1

Optical and electronic properties of gold nanowires on Si(553) — •Sandhya Chandola[1], Eugen Speiser[1], Jochen Räthel[1], Arne Baumann[1], Nobert Esser[1], Conor Hogan[2], Julian Aulbach[3], Sebastian Meyer[3], Jörg Schäfer[3], and Ralph Claessen[3] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Albert Einstein Strasse 9, 12489 Berlin — [2]Institute for Structure of Matter, National Research Council (CNR-ISM), Rome — [3]Universität Würzburg, Physikalisches Institut, Am Hubland 97074, Würzburg

Reflectance Anisotropy Spectroscopy (RAS) of the clean Si(553), Si(553)-Au and hydrogenated Si(553)-Au surfaces are measured and compared with density functional theory simulations. The lowest energy reconstruction models of Krawiec [1] are used for the calculations of the structure and optical response. Good agreement between experiment and theory is obtained. Local structural elements such as the Si honeycomb chains and the gold atomic wires, which are usually found on gold reconstructed vicinal Si surfaces, yield distinctive features in the optical spectra. By comparing the optical response of the freshly prepared and hydrogenated Si(553)-Au surfaces, the spectral features can be directly attributed to particular structural elements on the surface. Hydrogen adsorption attenuates the anisotropic response at spectral regions associated with the honeycomb chains at the Si step edges and the gold atomic wires. This combination of experiment and theory is very useful in helping to identify specific structural sites on the surface, which generate distinctive features in the optical response. [1] M. Krawiec, Phys. Rev. B **81**, 115436 (2010)

DS 45.14 Thu 16:00 P1

Optical and vibrational characterization of gold-induced atomic wires on germanium (001) — •Jochen Räthel[1], Eugen Speiser[1], Sandhya Chandola[1], Arne Baumann[1], Norbert Esser[1], Utz Bass[2], Jean Geurts[2], Sebastian Meyer[2], Julian Aulbach[2], Lenart Dudy[2], Jörg Schäfer[2], and Ralph Claessen[2] — [1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Albert-Einstein-Str. 9, 12489 Berlin — [2]Physikalisches Institut and RCCM, Universität Würzburg, Physikalisches Institut, Am Hubland, 97074 Würzburg

Atomic chains formed by metal adsorption on semiconductor surfaces are known as model systems for determining exotic electronic ground states, such as the Tomonaga-Luttinger liquid (TTL). A system of Au-induced atomic wires on the Ge(001) surface has been reported to host such TTL behaviour [1]. Here we present the results of temperature dependent reflection anisotropy spectroscopy (RAS) and Raman spectroscopy (RS) on clean Ge(001) and Au/Ge(001). RAS probes optically surface and surface to bulk electronic transitions between 0.5 and 5 eV with linear polarized light at normal incidence. From polarized RS measurements the vibrational properties of clean Ge(001) and Au/Ge(001) were characterized and in particular surface phonon modes identified. In combination with calculated ab-initio optical and vibrational spectra , the experimental data from RS and RAS provide a basis for structural modeling of these complex surface reconstructions. [1] C. Blumenstein, Nat. Phys. 7, 776 (2011)

DS 45.15 Thu 16:00 P1

Optical properties of gold and indium atom chains on Si(111) — •Fabian Hötzel[1], Olaf Skibbe[1], Eugen Speiser[2], and Annemarie Pucci[1] — [1]Kirchhoff Institute of Physics, Heidelberg University, Heidelberg, Germany — [2]ISAS-Institute for Analytical Sciences, Department Berlin, Berlin, Germany

Optical properties of self-assembled gold atom chains on Si(111) are investigated by Fourier transform infrared spectroscopy in transmittance geometry. Reflection high energy electron diffraction patterns reveal two different domains of 5x2 reconstruction showing metallic behavior between 20 and 423K. Therefore a metal-to-insulator transition of this system can be excluded in this temperature range. The infrared absorption is proportional to the fraction of gold-reconstructed surface and higher at low temperatures. Transmittance spectra can be depicted by a Drude type dielectric function. The resulting sheet conductance is inversely proportional to temperature which emphasizes the metallic character of this system. By means of polarization dependent measurements the orientations of the two domains of gold chains can be identified. Reflectance anisotropy spectra of indium atom chains on the stepped Si(111) surface show an anisotropic interband transition at 1.9eV. The splitting of this feature at 40K along with structural changes of the LEED pattern confirms the metal-to-insulator transition at low temperatures caused by Peierls instability. This contribution is related to DFG-FOR1700.

DS 45.16 Thu 16:00 P1

Optical and electronic properties of rare-earth silicide nanowires on vicinal Si(001) — •Sandhya Chandola[1], Eugen Speiser[1], Stephan Appelfeller[2], Martin Franz[2], Norbert Esser[1], and Mario Dähne[2] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Berlin — [2]Institut für Festkörperphysik, TU Berlin

Dy and Tb silicide nanowire structures on vicinal Si(001) surfaces are studied using *in-situ* Reflectance Anisotropy Spectroscopy (RAS) and Scanning Tunneling Microscopy (STM). Two different types of structures, metallic nanowires or a wire-like reconstruction, are formed by molecular beam epitaxy depending on the coverage and the annealing temperature. RAS of clean surfaces shows the typical features due to dangling bonds at the steps and Si dimers on the terraces. The silicide growth has a significant effect on the optical anisotropy, e.g. a feature develops at 3.8 eV for both structure types. This peak disappears after the surface is contaminated, confirming that it is unambiguously related to surface state transitions. Furthermore, RAS can identify how well-ordered the metallic nanowires are by the relative magnitude of this peak. The feature of the dangling bonds at the steps is significantly more affected for the wire-like reconstruction than for the metallic nanowires, as supported by the STM data showing that the reconstruction decorates many steps, thereby saturating the dangling bonds. Thus, RAS can be used as an optical fingerprint to distinguish different silicide nanowire structures. This work was supported by the DFG through FOR 1700 projects E2 and E3.

DS 45.17 Thu 16:00 P1

Transport in spatially restricted ensemble wire systems — Frederik Edler, •Stephanie Demuth, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany

Low dimensional electron gas systems can be grown by self-organized growth of metals on appropriate semiconducting surfaces. In the recent past various atomic wire structures are found with special properties like Luttinger liquid behavior or Peierls-driven metal insulator phase transitions. Instabilities are directly accessible by surface transport measurements. In order to reveal a deeper insight into the role of coupling of the systems to their environment, transport in spatially restricted areas is highly desirable to correlate imperfections and/or finite size effects directly with transport findings. We have developed a fully in-situ process for Si(111) surfaces to perform such measurements by means of a 4-tip STM/SEM system. For this, oxidation of Si samples is necessary. The SEM e-beam is used to reduce locally the SiO$_2$ to SiO which is volatile at around 760 °C resulting in Si-windows of arbitrary shape. The subsequent adsorption of 1 ML Ag at 550 °C leads to Ag $\sqrt{3}$-reconstructions only within these windows. Feedback controlled Au-coated W-STM tips are navigated under SEM control for contacting the Ag reconstructions. Transport measurements reveal 2D conductivity of 1.4 kΩ in reasonable agreement with former studies and no contribution of remaining not percolated Ag clusters on SiO$_2$. We are extending this technique to the In/Si(111) system for a systematically study of finite size effects.

DS 45.18 Thu 16:00 P1

Oxygen Adsorption on the In/Si(111) Nanowire Array: Structure and influence on metal insulator transition — •Stefan Wippermann[1], Duck Mahn Oh[2], Han Woong Yeom[2], and Wolf Gero Schmidt[3] — [1]Max-Planck-Institute for Iron Research, Düsseldorf — [2]Pohang University of Science and Technology — [3]University of Paderborn

The ordered array of In nanowires that self-assembles at the Si(111) surface is an extremely popular model system for one-dimensional (1D) electronic systems. It exhibits an intriguing metal-insulator (MI) transition, that was recently shown to occur as a first order transition starting from condensation nuclei. While the nature of these condensation nuclei remains controversial, Oxygen has recently been observed experimentally to facilitate the metal-insulator transition.

Here we present density functional theory calculations to study the influence of O adsorption on the structural properties and the MI transition of the In/Si(111)-(4x1)/(8x2) nanowire array. We find three different low energy adsorption sites. However, a single oxygen adsorbed at any of these sites does not facilitate the phase transition. Instead, two oxygen atoms acting in concert catalyze the MI transition by lowering the energy barrier for the formation of 4x2 In hexagons. These in turn act as condensation nuclei for the MI transition.

S. Wall, B. Krenzer, S. Wippermann, S. Sanna, F. Klasing, A. Hanisch-Blicharski, M. Kammler, W. G. Schmidt, M. Horn-von-Hoegen, Phys. Rev. Lett. 109, 186101 (2012)

DS 45.19 Thu 16:00 P1

An Atomistic Picture of Charge Density Wave Formation at Surfaces: Indium Atomic Wires on Si(111) — S. Wall[1], T. Frigge[1], B. Hafke[1], V. Tinnemann[1], B. Krenzer[1], S. Wippermann[2], S. Sanna[2], F. Klasing[1], A. Hanisch-Blicharski[1], W.G. Schmidt[2], and •M. Horn-von Hoegen[1] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Fachbereich Physik, Universität Paderborn

Ultrafast time-resolved reflection high energy electron diffraction was employed to investigate the dynamics of the Peierls-instability-driven phase transition on the (8x2) In/Si(111) surface. At 20 K, far below the critical temperature of 90 K, the (8x2)-(4x1) phase transition is electronically driven through weak excitation with a fs-laser pulse and results in a long-lasting super-cooled excited (4x1) phase. The immediate recovery of the low temperature groundstate is hindered by an activation barrier for the collective motion of the atoms. The recovery of the (8x2) ground state on a timescale of 500 ps is then only triggered by adsorbates that act as nucleation seeds. With increasing density of pre-existing adsorbates the recovery to the groundstate proceeds much faster. The surface unit cells fall back into their ground state one at a time, one-dimensionally like a row of falling dominoes. The phase front propagates at about 100 m/s, comparable to the speed of sound.

DS 45.20 Thu 16:00 P1

Proof of First Order: The (4x2)<>(8x2) Phase Transition in the Indium on Si(111) Atomic Wire system — F. Klasing, T. Frigge, B. Hafke, V. Tinnemann, B. Krenzer, A. Hanisch-Blicharski, and •M. Horn-von Hoegen — Fakultät für Physik, Universität Duisburg-Essen

The In induced (4x1) reconstruction on Si(111) is a prototype for an atomic wire type arrangement of metal atoms on a surface. It has attracted much attention because the In wires undergo a reversible Peierls like phase transition at Tc = 130 K to a (8x2) reconstructed groundstate. In a high resolution LEED study we observed the existence of a robust hysteresis loop upon slow increase and decrease of the sample temperature at Tc. The critical temperatures of the transition are T+c = 135 K and T-c = 125 K for increasing and decreasing temperatures, respectively. The width of the hysteresis loop of 8.6 K is almost independent on the heating and cooling rate and is thus direct evidence for the existence of an energy barrier between the (8x2) ground state and the (4x1) excited state. It unambiguously answers the question about the nature of the phase transition: it is first order.

DS 45.21 Thu 16:00 P1

The conductance phase transition of Si(5 5 7)-Pb probed by Raman and reflectance anisotropy spectroscopy — •Arne Baumann[1], Sandhya Chandola[1], Jochen Räthel[1], Eugen Speiser[1], Daniel Lükermann[2], Christoph Tegenkamp[2], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e. V., Albert-Einstein-Straße 9, 12489 Berlin, Germany — [2]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover, Germany

Si(5 5 7)-Pb is a model system for a quasi-1D conductor below a phase transition at 78 K, resulting in an anisotropic 2D-phase. The adsorption of 1.31 ML of Pb on the vicinal Si(5 5 7) surface induces a refacetting of the surface into evenly stepped (2 2 3) facets, decorated by wire-like Pb nanostructures. Reflectance anisotropy spectroscopy (RAS) is applied to probe surface band structure transitions and polarized Raman spectroscopy (RS) to characterize vibrational properties.

In RAS measurements the low and high temperature phases exhibit an anisotropic optical conductance behavior and optical transitions in the region between 0.7 and 1.7 eV. This can be assigned to the Pb induced reformation of the surface.

Temperature-dependent RS measurements show new Pb-induced surface phonon modes, while Si-adatom surface vibrational modes persist. A reformation of the terrace structure at 78 K can be excluded. A structural phase transition can only occur on the step edges or between the individual (2 2 3) facets.

DS 45.22 Thu 16:00 P1

Experimental and theoretical evidence for a Peierls insulating state in the low-temperature phase of In/Si(111) — •Eric Jeckelmann[1], Wolf Gero Schmidt[2], Simone Sanna[2], Norbert Esser[3], and Eugen Speiser[3] — [1]Leibniz Universität Hannover — [2]Universität Paderborn — [3]ISAS, Berlin

We reinvestigate the phase transition in indium atomic wires on a Si(111) substrate experimentally with Raman spectroscopy and theoretically using first-principles simulations and model calculations. We construct an effective one-dimensional model for the electronic properties of In wires including a coupling to shear and rotary lattice deformations. Thereby the input parameters for the model calculations are obtained from first-principles frozen-phonon and deformation-potential calculations based on density-functional theory within the local density approximation (DFT-LDA). The present investigation demonstrates that both shear and rotary modes in the low-temperature phase can be interpreted as Peierls lattice deformations which are significantly softened as the temperature increases. This agrees remarkably well with the measured temperature dependence of the surface phonon frequencies in the In/Si(111) atomic wire structure.

DS 45.23 Thu 16:00 P1

HREELS on the In/Si(111)-(4x1) to (8x2) phase transition — •Raphael Müller, Olaf Skibbe, Jan Pischel, and Annemarie Pucci — Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany

Interest in 1D-metallic systems on the nanoscale has increased lately due to interesting properties such as transport anisotropy, charge density waves, Luttinger liquid behavior et cetera.
One example for such systems are self-assembled Indium nanochains on vicinal Si(111) surfaces showing anisotropic collective excitations [1] and a characteristic phase transition whose nature is still under debate [2]. Whilst the In/Si(111)-system was investigated intensively by STM, ARPES and other techniques [3,4], electron energy loss spectroscopy (EELS) with an energy resolution appropriate for surface phonon investigation in the various temperature ranges had not been performed in a comprehensive manner. In order to gain more insight into the reported excitations and the connected phase transition, we used an ELS-22 spectrometer with high energy resolution to probe plasmonic and phononic excitations in the In/Si(111)-nanochains. Here, we report on measurements conducted above and below the phase transition temperature of 120K with excitation parallel and perpendicular to the 1D-metallic chains.

[1] Liu et al., Phys. Rev. B **77**, 205415, 2008.
[2] Wippermann and Schmidt, Phys. Rev. Lett. **105**, 126102, 2010.
[3] Yeom et al., Phys. Rev. Lett. **82**, 4898-4901, 1999.
[4] S. Hasegawa, J. Phys.: Condens. Matter **22**, 084026, 2010.

DS 45.24 Thu 16:00 P1

Tuning of 1d plasmons via selective doping at the edges — •Ulrich Krieg, Timo Lichtenstein, Heiko Teiken, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany

We prepared Ag-$\sqrt{3}$ nanowires on the regularly stepped Si(557) surface via self assembly. These wires are of monoatomic height and have an average width of 3.6 nm. Using the intrinsic semiconducting nature of the Ag-$\sqrt{3}$ phase we recently showed that it is possible to tune the 1d plasmon dispersion in a wide range by adsorption of additional silver atoms [1]. This leads to a 1d metallic surface. Using an electron loss spectrometer (EELS) with simultaneous high energy and momentum ($k_{||}$) resolution and SPA-LEED we found strong evidence that the silver doping process is indeed not due to a silver adatom gas, as seen on Ag-$\sqrt{3}$ on Si(111), but due to chemical adsorption of silver atoms at the step edges. This is compatible with the saturation coverage of 0.12ML and the temperature independence of the plasmon energy.

[1] Krieg U, Zhang Y, Tegenkamp C and Pfnür H 2013 *arXiv:1308.5591*

DS 45.25 Thu 16:00 P1

Plasmonic excitations in Au quantum wires on Ge(001) — •Timo Lichtenstein, Heiko Teiken, Christoph Tegenkamp, and Herbert Pfnür — Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung ATMOS, 30167 Hannover

One dimensional electronic systems show exceptional transport properties such as Peierl's transitions or Tomonaga-Luttinger liquid behavior. The latter has been found in Au quantum wires on Ge(001). Their plasmonic excitations should feature a dispersion relation different from the well-known characteristics in two or three dimensions.

Ge substrate preparation was done ex-situ via chemical etching and in-situ by heating to 900 K in a UHV chamber with a base pressure of 7×10^{-11} mbar. The wires were then formed by evaporation of different amounts of Au at 720 K via self-assembly. The sample quality was controlled with SPA-LEED. Finally, the plasmon dispersion was investigated via EELS combined with a SPA-LEED setup providing both high energy and momentum resolution.

For Au coverages higher than 0.7 ML low-dimensional plasmon modes appear in the loss spectra. Their dispersion relation increases linearly for parallel momentum $k_{||} > 0.1\,\text{Å}^{-1}$, but significantly deviates from the known dispersion of a quasi one-dimensional plasmon for $k_{||} < 0.1\,\text{Å}^{-1}$. A contribution coming from Au clusters seen in SEM can be excluded as the FWHM in the loss spectrum decreases steadily with decreasing $k_{||}$. A dipole excitation can also be ruled out since it would be observable down to zero momentum.

DS 45.26 Thu 16:00 P1

Vibrational properties of Au/Si(553) nanowires — •Sergej Neufeld, Simone Sanna, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany

Metallic nanowires on semiconducting substrates such as silicon and germanium have been attracting considerable interest in the last decade. Besides various potential applications as non ohmic conductors, they are candidate systems for the demonstration of the basic concepts of one-dimensional physics such as electron correlation and Luttinger liquid behavior. Furthermore the phase transitions observed on these systems have been controversially discussed and are still poorly understood. Self organizing gold chains at vicinal surfaces such as the Si(553) and Si(557) are of particular interest, as the use of stepped templates allows to vary the geometric parameters and, thus, tune the inter-chain coupling. While well-established microscopic structural models of the Au/Si(553) and Au/Si(557) systems based on density functional theory are available in the literature, few is known about their vibrational properties. In this work, the phonon eigenmodes and eigenfrequencies of the Au/Si(553) wires are calculated from *first-principles* at the center of the Brillouin zone. Several surface localized phonon modes are found, whose phonon frequencies can be directly compared with the spectra obtained by Raman measurements.

DS 45.27 Thu 16:00 P1

Time- and angle-resolved 2PPE studies of Pb nanowires on Si(557) — •Abdul Samad Syed[1], Vesna Mikšić Trontl[1], Manuel Ligges[1], Mathias Sandhofer[1], Ishita Agarwal[1], Isabella Avigo[1], Daniel Lückermann[2], Christoph Tegenkamp[2], Herbert Pfnür[2], and Uwe Bovensiepen[1] — [1]Fakultät für Physik, Univ. Duisburg-Essen — [2]Institut für Festkörperphysik, Leibniz Univ. Hannover

Strongly anisotropic systems, like, e.g., metallic nanowire arrays grown on semiconducting surfaces, are expected to exhibit significantly different electronic dispersion - along and perpendicular to the wire structure. Angle-resolved photoemission is an excellent tool to study electronic band dispersion, but is often limited to (i) one momentum direction in a single measurement and (ii) the occupied electronic structure. Here, we report on femtosecond-laser based two-photon photoemission experiments on Pb/Si(557) nanowires that map the unoccupied electronic structure. Using a position-sensitive time-of flight spectrometer [1], the dispersion along and perpendicular to the wires can be analyzed simultaneously in a single measurement. Furthermore, by delaying two light pulses with respect to each other, the lifetimes of these unoccupied electronic states can be measured in a pump-probe experiment. We present first time- and momentum-resolved studies on the unoccupied states in this system. We gratefully acknowledge funding by the DFG through FOR1700.

[1] Kirchmann et al., Appl. Phys. A 91,211 (2008)

DS 46: Organic Electronics and Photovoltaics VI (jointly with CPP, HL, O)

Time: Thursday 17:45–19:45 Location: CHE 91

DS 46.1 Thu 17:45 CHE 91

The role of residual additives on the stability of polymer blend materials for organic photovoltaic applications. — •Aurélien Tournebize[1,2], Agnès Rivaton[2], Heiko Peisert[1], and Thomas Chassé[1] — [1]Institute of Physical and Theoretical Chemistry, Tübingen, Germany — [2]Institut de Chimie de Clermont-Ferrand, France

Processing additives for improved the morphology of the bulk heterojunction (BHJ) materials used in organic solar cells (OSCs) is now very popular. Thus, by optimizing the donor and acceptor nano domains, the efficiency of OSCs devices could be significantly increased. [1] The impact of those additives on the performances has been widely explored recently but nothing in terms of stability. And yet, a part of the additives stays trapped in the thin film [2] and could participate in the complex photodegradation of the polymer blend materials.

In the present work, we have investigated the impact of residual additives on the polymer blend photostability. By using essentially spectroscopic technics, we have observed an acceleration of the polymer blend photodegradation in presence of additives. In this context, the use of new additives providing a better morphology and by the way a better stability was also explored.

[1] J.K. Lee, W.L. Ma, C.J. Brabec, J. Yuen, J.S. Moon, J.Y. Kim, K. Lee, G.C. Bazan, and A.J. Heeger JACS. 2008, 130, 3619-3623 [2] L. Ye, Y. Jing, X. Guo, H. Sun, S. Zhang, M. Zhang, L. Huo, and J. Hou J. Phys. Chem. C 2013, 117, 14920-14928

DS 46.2 Thu 18:00 CHE 91

Electronic States and Electrochemical Properties of Polymeric Phthalocyanine Sheets — •Clemens Geis and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Phthalocyanines are forming organic semiconducting thin films applicable in field-effect transistors, organic solar cells and as heterogeneous chemical catalysts. They consist of a planar organic aromatic ligand around a central metal atom like *Cu*, *Fe* or *Co*. In a chemical vapour deposition reaction (CVD) phthalocyanines with polymerized ligands were synthesized by reactions of bifunctional 1,2,4,5-tetracyanobenzene with thin metal films. By these means a high concentration of the catalytically active metal-sites on the substrate is established, they are electronically coupled and a molecular network is formed by such sheet polymers. Photoelectron spectroscopy was used to characterize the electronic states of the metals and ligands. Metal ions in the complexes as well as neutral metal clusters were detected in the films. Optical transmission spectroscopy was used to discuss the uniformity of the electronic excitation energy and its dependence on preparation conditions. The films were electrochemically reduced and oxidized to further study their accessible electronic states, study consequences for their optical absorbance and to test the polymeric phthalocyanines as electrocatalysts for water oxidation to oxygen and reduction to hydrogen, reactions of highest interest for the chemical storage of electrical energy from fluctuating renewable sources.

DS 46.3 Thu 18:15 CHE 91

Asymmetry of mixing length scales and kinetics of phase-separation in co-evaporated donor-acceptor organic thin film blends — •Rupak Banerjee, Christopher Lorch, Alexander Gerlach, Jiří Novák, Christian Frank, Johannes Dieterle, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Small molecular organic semiconductors have found widespread usage in organic photovoltaics (OPV) due to their attractive optical, structural and electronic properties [1]. One of the many ways to tune the efficiency of an OPV is by mixing donor (D) and acceptor (A) materials [1] since the efficiency depends on the interplay of the diffusion lengths of the excitons generated by the absorption of light and the structural length scales of the D:A mixture. Controlling the structural length scales in D:A mixtures is thus of paramount importance [2]. We discuss *in situ* and real-time x-ray scattering studies on the structure of mixed D:A films as a function of mixing ratio which reveal the kinetics and thickness dependence of phase separation and in particular the asymmetry between top and bottom interfaces [3]. We further discuss the influence of interrupted growth on the phase-separation kinetics of such systems.

[1] W. Brütting and C. Adachi, Physics of Organic Semiconductors, Wiley-VCH, Weinheim (2012).

[2] A. Opitz *et al.*, IEEE J. Sel. Top. Quant. **16**, 1707 (2010).

[3] R. Banerjee, J. Novák, C. Frank, C. Lorch, A. Hinderhofer, A. Gerlach, and F. Schreiber, Phys. Rev. Lett. **110**, 185506 (2013).

DS 46.4 Thu 18:30 CHE 91

UPS studies on different air-stable molecular n-dopants — •Martin Schwarze[1], Max L. Tietze[1], Paul Pahner[1], Ben Naab[2], Zhenan Bao[2], Björn Lüssen[1], Daniel Kasemann[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Chemical Engineering, Stanford University, Stanford, California 94305, United States

Understanding the working mechanism of electrical doping in organic semiconductors is essential for the optimization of organic semiconductor devices. A defined doping level allows for the control of the Fermi level position and the conductivity of transport layers. In comparison to molecular p-doping of organic semiconductors, n-doping has the additional problem of air instability. To successfully transfer an electron to the lowest unoccupied molecular orbital (LUMO) of the matrix material, dopants exhibiting shallow highest molecular orbitals (HOMO) are necessary, rendering them prone to reactions with e.g. oxygen. In this study, three different types of n-dopants are compared, an air stable cationic DMBI and DMBI dimer with the air sensitive W2(hpp)4. Doping efficiency, Fermi-level shift, air stability, and conductivity at different doping concentrations are investigated by ultraviolet photoelectron spectroscopy (UPS) and electrical measurements.

DS 46.5 Thu 18:45 CHE 91

Fracture and corrosion protection for thin-film encapsulation - Fine-tuning the electrical calcium corrosion test for water vapor permeation measurements — •Frederik Nehm, Hannes Klumbies, Lars Müller-Meskamp, and Karl Leo — Institut für Angewandte Photophysik, TU Dresden, Dresden, Deutschland

In recent years, the demand for ultra-high moisture barriers has strongly increased due to the ongoing development of organic electronics. Thus, the ability to measure water vapor transmission rates (WVTRs) below $10^{-5}\,\frac{g(H_2O)}{m^2d}$ - less than a monolayer in 10 days - is crucial for barrier development. The electrical calcium corrosion test - monitoring the decreasing conductivity of a thin calcium film turning into calcium hydroxide - is a sensitive, cost-efficient method to measure such low WVTRs. However, poor design can cause a high background rate or test breakdown. We show that calcium corrosion causes barrier breaking by both expansion and hydrogen emission. As a countermeasure, we introduce organic (C_{60}) buffer layers for decoupling on both sides of the calcium film. Further investigations show elevated calcium corrosion at the calcium-electrode-interface which can be prevented by a proper choice of the electrode material. Finally, the massive corrosion of barrier thin films is shown to be prevented by glueing a polymer foil onto the barrier under testing. With these precautions, we show atomic layer deposited alumina barriers measured in thin film encapsulation structure close to an actual device architecture. At 30°C, 90% rh, WVTRs of below $5 \cdot 10^{-5}\,\frac{g(H_2O)}{m^2d}$ were obtained.

DS 46.6 Thu 19:00 CHE 91

Commensurability as the determining factor for molecular tilt and multilayer growth: In-situ and real-time growth study of the nanographene HBC on SiO_2 and HOPG — •Paul Beyer[1], Tobias Breuer[2], Saliou Ndiaye[2], Anton Zykov[1], Andreas Viertel[1], Manuel Gensler[1], Jürgen P. Rabe[1], Stefan Hecht[1], Gregor Witte[2], and Stefan Kowarik[1] — [1]HU Berlin, 12489 Berlin — [2]Philipps-Universität Marburg, 35032 Marburg

We investigate the influence of symmetries and the substrate-molecule commensurability on the structure and growth kinetics of the nanographene hexa-*peri*-hexabenzocoronene (HBC). We study organic molecular beam deposited ultrathin HBC films on SiO_2, pristine and sputtered HOPG because of the similar surface energies, singling out the influence of the lattice-matching between HBC and graphite. Using real-time and *in situ* x-ray growth oscillations we find the first ad-layer to grow lying down on both substrates. On pristine HOPG we find a superstructure of hexagonally arranged, recumbent molecules in a new polymorph using GIXD, XRR and NEXAFS. The loss of commensurability in the sputtered HOPG leads to mainly upright molecules. Equally, we find a transition to upright molecules on amorphous SiO_2 surfaces. On SiO_2 micro-crystallites in the bulk structure that completely cover the substrate are found, while the strong ordering on HOPG leads to island growth of the new polymorph as observed by AFM. Our results demonstrate that the (lack of) symmetry- and lattice-matching critically determines the molecular orientation and occurrence of surface induced polymorphs.

DS 46.7 Thu 19:15 CHE 91

Spray coating process for highly conductive silver nanowire networks as transparent top electrode for small molecule organic photovoltaics — •Franz Selzer[1], Nelli Weiss[2], David Kneppe[1], Ludwig Bormann[1], Christoph Sachse[1], Nikolai Gaponik[2], Lars Müller-Meskamp[1], Alexander Eychmüller[2], and Karl Leo[1] — [1]IAPP, TU Dresden — [2]Phy. Chem., TU Dresden

Organic photovoltaics are a promising technology for fabrication in high throughput R2R-coating machines. Therefore, flexible and highly conducting transparent electrodes on temperature sensible polymer films are required. Percolative networks made of silver nanowires (AgNWs) are a flexible alternative, showing an opto-electrical performance comparable to ITO. Usually, they are deposited from solution, followed by post-annealing (200°C). The solvents involved in the deposition limit the versatility of this type of electrode and do not allow the direct deposition as top contact onto evaporated small molecule devices. Here, we present a novel spray-coated AgNW mesh, showing excellent opto-electrical performance although processed below 80°C. We investigate different types of wire functionalization and the consequences on typical network parameters of AgNWs. By comparing all investigated materials for different parameters like varying concentration and by scanning electron microscopy, the basics of the sheet resistance reduction mechanism are extracted and AgNW electrodes (<50Ohm/sq@>80%) are processed at 30°C. Finally, the successful implementation as transparent top electrode for high-performance organic p-i-n type solar cells is demonstrated.

DS 46.8 Thu 19:30 CHE 91

Tuning the energy levels of carbon nanotubes by functionalization — •Gerhard Lackner[1], Wei Xia[2], Vladimir Shvartsman[1], Martin Muhler[2], and Doru C. Lupascu[1] — [1]Institute for Materials Science, University of Duisburg-Essen, 45141 Essen, Germany — [2]Laboratory of Industrial Chemistry, Ruhr-University Bochum, 44801 Bochum, Germany

Carbon nanotubes (CNT) are a promising material for electrical applications due to their extraordinary properties. Nevertheless, a defined tuning of the energy levels of this material has not been reported so far. We show a possible route to set the energy levels of CNT by functionalization. The energy levels before and after the functionalization are analysed by Kelvin Probe measurements. Additionally, the functionalized and non-functionalized CNT are applied in organic solar cells and a comparative study about the solar cell performances is given.

DS 47: Micro- and Nanopatterning (jointly with O)

Time: Friday 9:30–11:15 Location: CHE 89

DS 47.1 Fri 9:30 CHE 89

Effect of periodic pre-patterned structures on ripple wavelength and propagation velocity on ion-irradiated surfaces — •Detlef Kramczynski[1], Bernhard Reuscher[2], and Hubert Gnaser[1,2] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institute for Surface and Thin-Film Analysis (IFOS), 67663 Kaiserslautern, Germany

Glass surfaces were patterned by milling periodic trench structures with wavelengths from 150 to 750 nm in a focused ion beam (FIB) system. Upon exposure to 30 keV Ga^+ ion irradiation under an incidence angle of 52° with respect to the surface normal, these patterns were found to transform into "ripple"-like nanostructures. Their evolution was monitored in situ for ion fluences up to 2.5×10^{18} Ga^+ ions/cm^2 using the scanning electron microscope incorporated in the FIB. With increasing fluence, the wavelengths of the ripples were found to stay constant (and equal to their original feature size) while they propagate across the surface, in a direction which coincides with the projection of the ion beam's incident direction onto the surface. The propagation velocity was determined to scale inversely proportional to the wavelength, being in the range (60-100) nm/(10^{17} ions/cm^2). On pristine surface areas (which had not been pre-patterned) ripples were also formed by ion bombardment. However, their wavelength was found to increase with ion fluence from initially ∼250 nm to ∼420 nm.

DS 47.2 Fri 9:45 CHE 89

structural evolution upon thermal annealing for Fe ion irradiated Si(100) — •behnam khanbabaee[1], jörg grenzer[2], stefan facsko facsko[2], and ullrich pietsch[1] — [1]Universität Siegen, Festkörperphysik,Siegen, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

Off-normal irradiation of Si(100) by Fe ions leads to the surface patterning. In order to understand the mechanism of pattern formation, chemical reactions between Fe and Si atoms have to be considered to influence the surface instability required for pattern formation. Since the as-irradiated surface area is amorphous, we examined the recrystallization process of the Fe-Si layer formed by off-normal 20 keV irradiation using a Si(100) substrate comparing the effect of low (1*10ˆ16 ions/cmˆ2) and high (5*10ˆ17 ions/cmˆ2) fluencies, where only the higher fluence leads to patterned surface. The samples were annealed up to a temperature of 800°C and characterized by in-situ grazing incidence X-ray diffraction (GI-XRD). Depth profiling by GI-XRD confirmed that ϵ-FeSi was formed close to the surface changing to a β-FeSi2 phase with lower Fe content at larger depths. While the polycrystalline β-FeSi2 phase dominates for higher ion fluencies, a nearly equal ratio between ϵ-FeSi and β-FeSi2 is found for lower ones. Our results suggest that phase distribution is related to the Fe concentration profile and can be considered as the relevant factor in the process of pattern formation.

DS 47.3 Fri 10:00 CHE 89

Nano-structured surfaces produced by low energy ion beam sputtering of amorphous Fe_xSi_{1-x} films — •Kun Zhang, Christoph Brüsewitz, and Hans Hofsäss — II. Physikalisches Institut, Universität Göttingen, Göttingen, Germany

It is well known that metallic surfactants induce pronounced dot and ripple patterns on Si substrate surfaces during normal ion incidence sputter erosion. These surfactant atoms are co-deposited on the substrate surface either from intentional co-deposition or inadvertently contaminations from sputtering of the vacuum chamber walls. In the present contribution we investigate the pattern formation on amorphous Fe_xSi_{1-x} thin films with different Fe atomic fraction x, irradiated with Xe ions of 5 keV and 10 keV energies and normal incidence. In this situation the Fe atoms work as surfactants, but are supplied from the bulk of the substrate. The resulting surface morphologies were examined ex-situ by AFM, while the Fe concentration and its depth profile were determined with RBS and high resolution RBS. Nanopattern forms on the substrates with $x = 0.02$ - 0.08. In this case Fe atoms accumulate in the surface near region (13 nm in depth) after ion irradiation, revealing a phase separation towards a FeSi2 phase. For the samples with $x > 0.09$, the average Fe concentration near the surface exceeds $x=0.33$ and the surface remains flat. For $x < 0.02$ no pattern formation occurs. The results give further evidence of phase separation as a major drive force for surfactant induced the pattern formation.

DS 47.4 Fri 10:15 CHE 89

Redeposition during ion-beam erosion can stabilize well-ordered nanostructures — •Christian Diddens and Stefan J. Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster

We investigate the redeposition effect, i.e. the reattachment of eroded particles on the surface, in the context of self-organized pattern formation on semiconductor targets during ion-beam erosion. Within the framework of a continuum model for this non-local, inherently complicated process, we present (i) the distribution of redepositing particles on the surface, (ii) an approximation of the redeposition effect in terms of the surface height and (iii) the spatio-temporal evolution of one- [1] two-dimensional [2,3] surface morphologies subject to combined erosion and redeposition. We are able to conclude that an interplay of erosion, diffusion and redeposition can reproduce the hexagonally arranged nanodots found in experiments in extended regions of the parameter space.

[1] C. Diddens and S. J. Linz, Eur. Phys. J. B, 86 (2013) 397
[2] C. Diddens and S. J. Linz, EPL, 104 (2013) 17010
[3] C. Diddens and S. J. Linz, (in preparation)

DS 47.5 Fri 10:30 CHE 89

Nanoscale low energy electron induced graphitization in tetrahedral amorphous carbon thin films — •Frederik Klein and Thomas Mühl — Leibniz Institute for Solid State and Materials Research Dresden, PF 270116, D-01171 Dresden, Germany

Under ambient or vacuum conditions diamond and related materials like tetrahedral amorphous carbon (ta-C) are in a metastable state. By application of energy the material is able to undergo a phase change to a graphitic or sp^2-hybridised state. We induce local phase changes in ta-C thin films by eV and low keV electron beams in ultrahigh vacuum provided by a scanning tunneling microscope (STM) and a scanning electron microscope (SEM), respectively. These are accompanied by huge changes in many physical properties such as electrical conductivity.

The graphitization is analyzed by STM-based current-distance spectroscopy and conductive atomic force microscopy (c-AFM). The total tip-sample circuit contains the tunneling gap resistance in series with the resistance of the carbon thin film R_{carbon}. An analysis of the STM spectra provides the tunneling barrier height Φ and R_{carbon}.

We observe a decrease of R_{carbon} as well as an increase of Φ in the graphitized areas. However, an expected surface elevation due to a reduction of the material's mass density cannot be seen.

DS 47.6 Fri 10:45 CHE 89

Surface nanostructuring of fused silica assisted by laser-induced self-assembling of thin metal layers: Theory and experiment — •Pierre Lorenz[1], Michael Klöppel[2,3], Tomi Smausz[4], Tamas Csizmadia[4], Frank Frost[1], Martin Ehrhardt[1], Klaus Zimmer[1], Bela Hopp[1], and Pu Li[2] — [1]Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany — [2]Simulation and Optimal Processes Group, Institute of Automation & Systems Engineering, Ilmenau University of Technology, POB 10 05 65, 98684 Ilmenau, Germany — [3]Institute of Scientific Computation, Department of Mathematics, TU Dresden, 01062 Dresden — [4]Department of Optics and Quantum Electronics, University of Szeged, H-6720 Szeged, Dóm tér 9, Hungary

The introduced laser method demonstrates a novel concept of complex nanostructuring of dielectric surfaces assisted by a laser-induced molten metal layer deformation process. This method allows the fast, large-scale, and cost-effective production of randomly distributed surface nanostructures with a lateral dimension down to 10 nm. However, for an optimizing of this process a profound physical understanding is necessary. For this, the process was simulated under the assumption of the heat equation and the Navier-Stokes equations. Furthermore, the resultant structures were investigated dependent on the metal layer thickness and the laser parameter by AFM and SEM. Additionally, the dynamics of the deformation process were analysed by time-dependent reflection and transmission as well as time-dependent optical microscopic measurement.

DS 47.7 Fri 11:00 CHE 89

Interference Lithography Combined with Hard Anodization Leading to Highly Ordered Nanoporous Alumina — Josep M. Montero Moreno[1], •Robert Zierold[1], Martin Waleczek[1], Stephan Martens[1], Victor Vega Martinez[2], Victor M. Prida[2], and Kornelius Nielsch[1] — [1]Institut für Angewandte Physik, Universität Hamburg — [2]Department of Physics, University of Oviedo

A perfect order of the pores in nanoporous alumina is desired for application in the fields magneto-optical and opto-electronic devices, photonic crystals, solar cells, fuel cells, and chemical and biochemical sensing systems, to name a few.

We present the fabrication of thick nanoporous Al_2O_3 membranes with mono-oriented, perfect hexagonal packing of pores, and precise control of all structural parameters over large areas by matching the conditions of three-beam laser interference lithography and subsequent hard anodization. The periodic concavities after the patterning step in the aluminum surface guide the pore nucleation during the anodization, and the self-ordering phenomenon guarantees the maintenance of the predefined arrangement throughout the entire layer.

The cylindrical pores—diameters adjustable between 20 and 450 nm with advanced post-processing techniques such as atomic layer deposition or selective-chemical etching—are uniform in shape and widely tunable in their dimensions with aspect ratios as high as 500. With that technique, the interpore distance can be easily and accurately tuned in the range of 200 to 500 nm without time-consuming prefabrication of hard-masking stamps.

DS 48: Topological Insulators (jointly with MA,HL,O,TT)

Time: Friday 9:30–12:00 Location: HSZ 04

DS 48.1 Fri 9:30 HSZ 04

Experimental characterization and simulation of quasi-particle-interference in the Bi-bilayer topological insulator — •Matteo Michiardi[1], Andreas Eich[2], Gustav Bihlmayer[3], Alex A. Khajetoorians[2], Jens Wiebe[2], Jianli Mi[4], Bo B. Iversen[4], Philip Hofmann[1], and Roland Wiesendanger[2] — [1]Department of physics and astronomy, Aarhus University, Denmark — [2]Institute of Applied Physics, University of Hamburg, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [4]Center for Materials Crystallography, Aarhus University, Denmark

Topological insulators (TI) are a new class of materials that host gapless surface states with spin helicity. While several 3D TIs have been discovered, the interest in 2D TI systems that can host topological edge state is rising. A single bilayer of bismuth is predicted to be such a 2D TI. Here we present an experimental and theoretical study of a Bi-bilayer grown on 3D TI Bi_2Se_3. The use of Bi_2Se_3 as substrate allows the epitaxial growth of the bilayer in the rhombohedral structure, as shown by Scanning Tunnelling Microscopy. We calculate the band structure of the Bi-bilayer/Bi_2Se_3 system by Density Function Theory (DFT) and experimentally study the quasi particle interference (QPI) on the bilayer. In order to clarify the scattering channels responsible for the QPI, we perform simulations based on the Joint Density of States method starting from our DFT calculations. The comparison with the experimental results reveals a good match for a wide range of binding energies for both occupied and unoccupied states.

DS 48.2 Fri 9:45 HSZ 04

Quasiparticle self-consistent *GW* study of bismuth under strain — •Irene Aguilera, Christoph Friedrich, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

It has been recently claimed on the basis of ARPES measurements that bulk bismuth is a topological semimetal. The discrepancies between this result and previous *ab-initio* calculations were attributed to the failure of density functional theory (DFT) in the prediction of band gaps, because the topological or trivial character of Bi depends only on the "sign" of the very small direct band gap at the L point. We show that bulk Bi is indeed predicted by DFT in the local-density approximation (LDA) to be a trivial semimetal, with a surprisingly overestimated gap at L. We have performed quasiparticle self-consistent *GW* (QS*GW*) calculations for bulk bismuth that support its trivial character. The QS*GW* gap at L as well as the energy overlap between the electron and hole pockets are in much better agreement with experiments than the LDA ones. Thus, the QS*GW* approach appears as the right tool to study the trivial-to-topological transition that Bi experiences under stress, as a result of a change of sign of the gap at L. We have analyzed the effect of strain on the topological properties of bulk Bi. Whereas LDA predicts that an impractical stress is needed for such a transition, QS*GW* shows that bulk Bi becomes a topological semimetal already under very small stress. This work is supported by the Helmholtz Virtual Institute for Topological Insulators (VITI).

DS 48.3 Fri 10:00 HSZ 04

Combined STM/STS- and ARPES-investigation of the quaternary Topological Insulator $\mathrm{Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}}$ — •Thomas Bathon[1], Felix Reis[1], Christoph Seibel[2], Hendrik Bentmann[2], Paolo Sessi[1], Friedrich Reinert[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We present a combined scanning tunneling microscopy/spectroscopy (STM/STS) and angular-resolved photoemission spectroscopy (ARPES) characterization of the electronic properties of the quaternary compound $\mathrm{Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}}$. ARPES-data evidence that this compound is still a Topological Insulator (TI) with a single Dirac cone, which is characteristic for the $\mathrm{Bi_2X_3}$-class. The topological properties of the surface state, i.e. forbidden backscattering, have been confirmed by Fourier-transformed differential conductance (dI/dU) maps. Measurements performed both above and below the Fermi level allow us to determine the energy dispersion relation, the carrier velocity, and—by extrapolation to zero momentum—the position of the Dirac point. The observed scattering vectors are not as well-defined as those observed in binary compounds, probably due to substitutional disorder which results in a spatial fluctuation of the chemical potential. Our investigations illustrate how the properties of the well-known TI $\mathrm{Bi_2Te_3}$ can be changed by chemical substitution.

DS 48.4 Fri 10:15 HSZ 04

Surface and bulk contributions to the electronic structure of the topological insulator $\mathrm{Sb_2Te_3}$(0001) — •Christoph Seibel[1,2], Hendrik Bentmann[1,2], Henriette Maass[1,2], Jürgen Braun[3], Jan Minár[3], Kenya Shimada[4], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe — [3]Department Chemie, Physikalische Chemie, Universität München, Butenandtstraße 5-13, D-81377 München — [4]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

Photon energy dependent angle-resolved photoemission measurements were performed to disentangle surface and bulk contributions to the electronic structure of the 3D topological insulator (TI) $\mathrm{Sb_2Te_3}$. We discover a penetration of the topological surface state (TSS) into the bulk valence band regime where it coexists with bulk states without considerable hybridization. Our results indicate an emerging $k_\perp$-dispersion of the TSS at higher binding energies, which we attribute to an increasing bulk character. These observations deviate from previous findings for the isostructural TIs $\mathrm{Bi_2Se_3}$ and $\mathrm{Bi_2Te_3}$. Our results are supported by fully relativistic one-step photoemission calculations. [1] Seibel *et al.* PRB 86, 161105(R) (2012)

15 min. break

DS 48.5 Fri 10:45 HSZ 04

Spin-dependent unoccupied electronic structure of the topological insulator $\mathrm{Sb_2Te_3}$ — •Anna Zumbülte[1], Anke B. Schmidt[1], Markus Donath[1], Peter Krüger[2], Gregor Mussler[3], and Detlev Grützmacher[3] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

Studies on three-dimensional topological insulators focus mainly on the well-known systems of $\mathrm{Bi_2Se_3}$ and $\mathrm{Bi_2Te_3}$ and the related ternary compounds. Theoretical predictions of chalcogenides as topological insulators with a single Dirac cone [1] include an additional compound, $\mathrm{Sb_2Te_3}$. There, due to p-type doping of the available samples, the Dirac point lies above the Fermi level, making it inaccessible to photoemission experiments unless the surface is modified with an adsorbate [2]. Consequently, the electronic structure of this system has been left almost unstudied.

We present spin- and angle-resolved inverse-photoemission measurements of the unoccupied electronic states of $\mathrm{Sb_2Te_3}$. In addition to the Dirac state, further spin-dependent features have been obtained which show a distinct Rashba splitting. The experimental data will be discussed along with bandstructure calculations.

[1] H. Zhang *et al.*, Nat. Phys. **5**, 438 (2009)

[2] C. Seibel *et al.*, Phys. Rev. B **86**, 161105 (2012)

DS 48.6 Fri 11:00 HSZ 04

Comparitive study of the ternary topological insulators $\mathrm{Bi_2Se_2Te}$ and $\mathrm{Bi_2Te_2Se}$ — •Felix Reis[1], Thomas Bathon[1], Christoph Seibel[2], Hendrik Bentmann[2], Paolo Sessi[1], Friedrich Reinert[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The 3D topological insulators $\mathrm{Bi_2Se_2Te}$ and $\mathrm{Bi_2Te_2Se}$ have been investigated by combining the complementary experimental techniques scanning tunneling microscopy (STM/STS) and angular-resolved photoemission spectroscopy (ARPES). With low temperature STM/STS technique we investigate the structural and electronic properties of both systems. Fourier-transformed quasi-particle interference (QPI) maps give access to the scattering events within the topological surface state. Taking QPI maps for several energies allows us to obtain information on the position of the Dirac point and the carrier velocity by fitting the linear energy dispersion relation of the Dirac fermions. These results will be compared with the band structure as obtained by ARPES measurements.

DS 48.7 Fri 11:15 HSZ 04

A large-energy-gap oxide topological insulator based on the superconductor BaBiO3 — •Binghai Yan[1,2,3], Martin Jansen[1], and Claudia Felser[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden — [3]Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg University of Mainz, 55099 Mainz

Topological insulators are a new class of quantum materials that are characterized by robust topological surface states (TSSs) inside the bulk-insulating gap, which hold great potential for applications in quantum information and spintronics as well as thermoelectrics. One major obstacle is the relatively small size of the bulk bandgap, which is typically around 0.3eV for the known topological insulator materials. Here we demonstrate through ab initio calculations that a known superconductor BaBiO3 (BBO) with a Tc of nearly 30 K emerges as a topological insulator in the electron-doped region. BBO exhibits a large topological energy gap of 0.7 eV, inside which a Dirac type of TSSs exists. As the first oxide topological insulator, BBO is naturally stable against surface oxidization and degradation, distinct from chalcogenide topological insulators. An extra advantage of BBO lies in its ability to serve as an interface between TSSs and superconductors to realize Majorana fermions for future applications in quantum computation.

Reference: B. Yan, M. Jansen, C. Feler, Nature Physics 9, 709*711 (2013) (arXiv:1308.2303).

DS 48.8 Fri 11:30 HSZ 04

Topological surface states of HgTe and Heulser compounds — •Shu-Chun Wu[1], Binghai Yan[1,2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany. — [2]Max Planck Institute for Physics of Complex Systems, Dresden, Germany.

We studied the topological electronic structures of HgTe and half Heusler compounds (e.g.: XYZ, X = rare earth elements, Y = trasition metal and Z = main group elements) by both *ab initio* calculations. The topological surface structures were investigated by the Wannier function based tight-binding method. The effects of external strains induced from the substrate and surface terminations are taken into account by the atomic positions. Our results agree well with recent photoemission experiments.

DS 48.9 Fri 11:45 HSZ 04

Sputter Deposition of Half-Heusler Topological Insulators — •Benedikt Ernst, Daniel Ebke, Stanislav Chadov, Gerhard Fecher, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

Heusler compounds have exhibited manifold physical properties in the recent years and attracted a lot of interest in the field of spintronic applications due to their half-metallic properties. Recently, a topological insulating state has been predicted by theory for some of these compounds.

In this work, we have prepared Heusler materials such as LaPdBi and LaPtBi for which a topological insulating behavior was predicted.

Co-deposition by DC- and RF magnetron sputtering was used to prepare corresponding thin films. To realize an epitaxial film growth in the crystallographic C1_b structure on MgO-substrates, a buffer layer was applied and optimized. Initial transport properties will be discussed with regard to the film composition and the crystallographic properties.

DS 49: Atomic Layer Deposition

Time: Friday 9:30–12:30 Location: CHE 91

Invited Talk DS 49.1 Fri 9:30 CHE 91

Synthesis, Characterization, and Application of Tunable Resistance Coatings — •Jeffrey W. Elam — Argonne National Laboratory, Argonne, IL, USA

We used atomic layer deposition (ALD) to synthesize nanocomposite coatings comprised of M:Al2O3 where M= W or Mo using alternating exposures to trimethyl aluminum (TMA) and H2O for the Al2O3 ALD and alternating MF6/Si2H6 exposures for the metal ALD. By varying the ratio of metal and the Al2O3 ALD cycles, we can tune precisely the resistance of these coatings over a very broad range from 1012-105 Ohm-cm. These films exhibit Ohmic behavior and resist breakdown even at high electric fields of 107 V/m. Moreover, the self-limiting nature of ALD allows us to grow these films inside of porous substrates and on complex, 3D surfaces. To investigate the growth mechanism we employed in situ QCM and FTIR absorption spectroscopy studies. For the Mo:Al2O3 films, QCM showed that the Mo ALD inhibits the Al2O3 ALD and vice versa. Surprisingly, FTIR revealed that the reducing agent for the Mo is not the Si2H6, but rather the TMA exposure from the subsequent Al2O3 ALD cycle. Cross sectional TEM revealed the film structure to be metallic nanoparticles (~1 nm) embedded in an amorphous matrix. We utilized these coatings to fabricate large-area microchannel plates for large-area photodetectors, and as charge drain coatings in MEMS devices for a prototype electron beam lithography tool.

DS 49.2 Fri 10:00 CHE 91

ALD on Multi-Stacked Polystyrene Opals for Thermal Barrier Coatings — •Robert Zierold[1], Martin Waleczek[1], Josep M. Montero Moreno[1], Roman Kubrin[2], Hooi Sing Lee[3], Alexander Petrov[3], Manfred Eich[3], Gerold A. Schneider[2], and Kornelius Nielsch[1] — [1]Institut für Angewandte Physik, Universität Hamburg — [2]Institut für Keramische Hochleistungswerkstoffe, Technische Universität Hamburg-Harburg — [3]Institut für Optische und Elektronische Materialien, Technische Universität Hamburg-Harburg

Thermal Barrier Coatings (TBC) are used to protect thermally highly loaded metallic components, such as turbine blades in gas engines, from excessive heat and thus prolong the life time of the component.

Herein, we present a novel synthesis route for multi- stacked, photonic crystals made of titania and zirconia revealing a multi-bandgap structure in the infrared, a prerequisite for a TBC. Sequential self-assembly of monodisperse polystyrene particles with different diameters between 315 and 756 nm results in multi-stacked direct opals. The polymer template is then conformally molded by low temperature ALD—with its capabilty to coat complex nanostructures without shadowing effects due to its self-limited nature—processes with TiO_2 and ZrO_2 from the precursors titanium isopropoxide (TTIP) or tetrakis(ethylmethylamino) zirconium (TEMAZ), respectively, and H_2O. Subsequently, calcination of the polystyrene leads to high quality photonic crystals. Optical characterization of the tailor-made samples reveals reflectance peaks in the near infrared corresponding to the different stop-gaps of the individual layers with different periodicities.

DS 49.3 Fri 10:15 CHE 91

New opportunities with Plasma enhanced atomic layer deposition (PE-ALD) of oxides — •Massimo Tallarida[1], Karsten Henkel[1], Hassan Gargouri[2], Jörg Häberle[1], Bernd Gruska[2], Matthias Arens[2], and Dieter Schmeisser[1] — [1]Brandenburg University of Technology, Konrad Wachsmann Allee, 17, 03046, Cottbus Germany — [2]Sentech Instruments GmbH, Schwarzschildstrasse 2, 12489 Berlin, Germany

Thermal Atomic layer deposition (T-ALD) of oxides is obtained by the pulsed alternation of a metal precursor and an oxygen source, typically H_2O or O_3, and the reactions leading to ALD are thermally activated. With plasma enhanced ALD (PE-ALD), instead, the oxygen source is represented by an oxygen-containing plasma. The higher reactivity of the plasma-generated species extend the capabilities of ALD: improved film quality and increased flexibility in process conditions, such as growth at low temperature, are typical advantages of PE-ALD over T-ALD. We report on results on the preparation of thin (<100 nm) aluminum oxide (Al_2O_3) films on silicon substrates using T-ALD and PE-ALD in the SENTECH SI ALD LL system. Films were deposited in the temperature range between room temperature (RT) and 200°C. We characterized the films with spectroscopic ellipsometry (thickness, refractive index, growth rate) over 4" wafers and with X-ray photoelectron spectroscopy. All films resulted in a high degree of homogeneity, independent of the deposition temperature. Investigations with capacitance-voltage and conductance-voltage measurements showed a very low interface states density for the PE-ALD films.

DS 49.4 Fri 10:30 CHE 91

X-ray linear dichroism in atomic layer deposited Titanium dioxide layers — •Chittaranjan Das, Massimo Tallarida, and Dieter Schmeisser — Applied physics and sensors,BTU Cottbus, Germany

Among the various metal oxides TiO2 has been investigated because of its wide range of applications in various fields such as self-cleaning, photocatalysis, solar cell, water splitting, bio-implants. In order to increase its efficiency in water splitting and solar cell energy conversion, it is necessary to understand the crystal structure and electronic properties of thin films. Generally the process of synthesis may modify the electronic properties of TiO2. In the present work we show X-ray linear dichroism (XLD) measurements of TiO2 thin films of different polymorphs. Titania thin films were produced by atomic layer deposition (ALD) and were characterized in-situ with X-ray photoelectron and absorption spectroscopy at synchrotron radiation center BESSY-II. We found that that all titania phases show XLD at Ti-L and O-K edges, but the intensity of XLD is different for different phases. We discuss our data in terms of the partial density of states.

DS 49.5 Fri 10:45 CHE 91

Control of thickness of SiO2 interfacial layer for photocatalytic water splitting on Si photocathodes — •Chittaranjan Das, Massimo Tallarida, and Dieter Schmeisser — Applied physics and sensors,BTU Cottbus, Germany

Silicon with a band gap of 1.1eV is an excellent candidate for visible photocatalytic water splitting. But p-type Si has a low quantum yield and are less efficient for water splitting [1]. It has been shown that preventing oxidation of Si surface can shift the onset potential for water reduction by about 300mV towards more positive [2]. We investigated in detail the influence of the SiO2 layer thickness on the onset potential for water splitting on Si photocathodes: we used p-type Si substrates covered with SiO2 layers of varying thickness. Then, we deposited a thin TiO2 film on using atomic layer deposition (ALD) to inhibit Si oxidation during the electrochemical experiment. In this way we could shift the onset potential up to 200mV, depending on the SiO2 thickness.

[1]E. L. Warren, S. W. Boettcher, M. G. Walter, H. A. Atwater, and N. S. Lewis: J. Phys. Chem. C 115 (2011) 594. [2]B. Seger, Anders B. Laursen, P. C. K. Vesborg, T. Pedersen, O. Hansen, S. Dahl, I. Chorkendorff, Angew. Chem. Int. Ed. 2012, 51, 9128 *9131

Coffee break (15 min)

DS 49.6 Fri 11:15 CHE 91

Atomic layer deposition of $Sr_xTi_{1-x}O_y$: Stoichiometry variation and layer characterization — •Solveig Rentrop[1], Barbara Abendroth[1], Hartmut Stöcker[1], Ralph Strohmeyer[1], Jura Rensberg[2], Juliane Walter[1], and Dirk C. Meyer[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg — [2]Institut für Festkörperphysik, Universität Jena

Resistance switching of metal-insulator-metal (MIM) capacitor structures is one of the possible routes for future non-volatile random access memories. A promising ternary dielectric for MIM devices is $Sr_xTi_{1-x}O_y$. In this material, the layer composition is found to determine dielectric and optical properties as well as the band gap.

Here, we present studies on the atomic layer deposition of amorphous $SrTiO_3$ from $Sr(iPr_3Cp)_2$, $Ti[N(CH_3)_2]_4$ and H_2O at substrate temperatures of 300 °C and 320 °C, resp. By changing the Sr/Ti pulse ratio, we are able to tailor the stoichiometry from stoichiometric to Sr or Ti excess. The layer composition is obtained from X-ray fluorescence spectroscopy and Rutherford backscattering. The tuned band gap value is determined by using a Tauc plot of the ellipsometric absorption coefficient. Moreover, we investigated the dependencies of optical constants, layer density and surface morphology on the layer composition.

Carbon incorporated during deposition increases the leakage current. By X-ray photoelectron spectroscopy the carbon content was measured after Ar ion cluster sputtering. The results show that we are able to deposit carbon free $Sr_xTi_{1-x}O_y$ layers for different Sr/Ti ratios.

DS 49.7 Fri 11:30 CHE 91

Ta_2O_5 by thermal-activated ALD — •Marcel Junige[1], Ralf Tanner[1], Christian Wenger[2], Grzegorz Lupina[2], Matthias Albert[1], and Johann W. Bartha[1] — [1]Technische Universität Dresden — [2]IHP GmbH, Frankfurt (Oder), Germany

Ta_2O_5 is a dielectric material with a comparably high permittivity as well as refractive index and thus gains interest for several electronic or optical applications. Atomic Layer Deposition (ALD) is a vacuum technique, which enables the coating of complex-shaped surfaces by alternatively applying self-terminating physicochemical reactions.

We investigated the thermal-activated ALD using the halogen-free metal-organic precursor TBTEMT and ozone gas (O_3) as co-reactant at an actual deposition temperature of 215 °C. We pre-heated a Silicon sample for 30 min at the respective process conditions and pre-cleaned the initial surface for 180 s in O_3 in order to remove ambient carbon contaminations prior to the ALD.

In-situ real-time Spectroscopic Ellipsometry with a highest possible sampling rate of ca. 1 data point/s confirmed a timewise saturation of the TBTEMT adsorption and of the subsequent ligand removal. An ellipsometric multi-time analysis of a deposition run with 100 ALD cycles determined the homogeneous growth per cycle around 0.64 Å/cycle, the refractive index at 500 nm wavelength around 2.1 and the Tauc optical band gap around 4.3 eV, indicating an amorphous phase. Invacuo X-ray Photoelectron Spectroscopy revealed a Ta_2O_5 film of high purity with a tantalum-to-oxygen ratio of (29:71) at.% as well as carbon and nitrogen contaminants below the detection limit.

DS 49.8 Fri 11:45 CHE 91

Simulation of the deposition and growth of nano-crystalline MgF2 films via the low-temperature atom beam deposition method — Sridhar Neelamraju, •Johann Christian Schön, and Martin Jansen — MPI for Solid State Research, D-70569 Stuttgart

We model the deposition of magnesium difluoride (MgF2) clusters on a sapphire substrate and the subsequent growth of ordered MgF2-phases via the low-temperature atom beam deposition method. For the modeling procedure we use empirical potentials to describe the interactions within the substrate and the MgF2 deposit, and between the deposited atoms and the substrate. First, we established that primarily MgF2- and Mg2F4-clusters form in the gas phase, and thus the deposition could be described by the adsorption of such molecules on the substrate at low temperatures [1]. Next, the deposited MgF2-layers are annealed, and the structure of the resulting amorphous and nano-crystalline compounds is analyzed and compared with the results (pair distribution functions) of the experimental deposition [2]. We show that the appearance of an (at standard conditions) kinetically unstable CaCl2-type phase in the experiment [3] is due to the concurrent existence of a nano-crystalline CdI2-type modification of MgF2 predicted in earlier theoretical studies [4].

[1] S. Neelamraju et al., J. Chem. Phys. 137:194319 (2012); S. Neelamraju et al., Phys. Chem. Chem. Phys. 14:1223 (2012) [2] X. Mu et al., J. Appl. Cryst. 46:1105 (2013) [3] A. Bach et al., Inorg. Chem. 50:1563 (2011) [4] M.A.C. Wevers et al., J. Solid State Chem. 136:223 (1998)

DS 49.9 Fri 12:00 CHE 91

Structural changes in HfO_2 thin films: thickness and doping dependence — •Simone Brizzi[1], Massimo Tallarida[1], Christoph Adelmann[2], Lars-Ake Ragnasson[2], Sven Van Elshocht[2], and Dieter Schmeisser[1] — [1]Brandenburg University of Technology, Konrad-Wachsmann Allee 17, 03046 Cottbus, Germany — [2]Imec, Kapeldreef 75, B-3001 Leuven, Belgium

In this work we show results regarding MOCVD and ALD HfO_2 as well as Al-doped HfO_2. We use Synchrotron Radiation Photoemission Spectroscopy (SRPES) to determine Hf/O atomic ratios and X-ray Absorption Spectroscopy (XAS) to investigate the electronic properties related to their crystallization. MOCVD films are synthesized at temperatures ranging from ambient to 400°C and show structures from completely amorphous to monoclinic. ALD films are amorphous as deposited, and can crystallize after post-deposition anneal depending on the percentage of Al-doping. We discuss PES results in order to determine how close to stoichiometry the Hf/O atomic ratios of the films are, as well as the doping level. From XAS data, instead, we can point out how orbital hybridizations are related to structural and physical properties.

DS 49.10 Fri 12:15 CHE 91

Charging effect in HfO2 films deposited on SiO2/Si by atomic layer deposition — •Silma Alberton Correa, Simone Brizzi, Massimo Tallarida, and Dieter Schmeisser — Department of Applied Physics and Sensors, Brandenburg University of Technology, 03046 Cottbus, Germany

Thin films of hafnium oxide (HfO2) deposited by atomic layer deposition (ALD) have been studied extensively as a high-k replacement for the SiO2 gate in field effect transistors. The use of ALD process allows one to grow homogeneous thin films at low temperatures with a precise control of thickness [1]. Some important electrical considerations for the application of a high-k dielectric include the presence of fixed charge (Qf) and charge trapping in the dielectric. For instance, in the case of Al2O3 thin films deposited on Si, the thickness of the interfacial SiO2 layer was identified as a key fundamental parameter determining Qf [2]. A similar trend can be also expected in HfO2/Si structures. Therefore, in this work, we proposed an in situ evaluation of photon induced charge trapping in HfO2 films deposited on SiO2/Si structures. For that, tetrakis-di-methyl-amino-hafnium (TDMAHf) and H2O were employed as precursors to deposit HfO2 films on SiO2/Si samples with variable thickness of the SiO2 interlayer. Measurements were performed by Synchrotron Radiation Photoemission Spectroscopy (SR-PES). Results indicated that the charging process is dependent on the thickness of the SiO2 interlayer and on the quality of the HfO2 film. [1] M. Leskelä and M. Ritala, Thin Solid Films 409, 138 (2002). [2] G. Dingemans et al., J. Appl. Phys. 110, 093715 (2011).

DS 50: Organic semiconductors: Material properties (jointly with HL, CPP)

Time: Friday 10:15–12:30 Location: POT 051

DS 50.1 Fri 10:15 POT 051

Pressure dependent Electronic Structure from First Principles — •Franz Knuth[1], Christian Carbogno[1], Volker Blum[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]MEMS Department, Duke University, Durham, NC, USA

The electronic properties of organic semiconductors typically exhibit a significant dependence on the strain, stress and pressure [1]. To clarify the role of these effects electronic-structure theory is uniquely suited. However, standard density-functional theory approaches that neglect van-der-Waals interactions and that treat exchange and correlation in a semi-local approximation often fail to describe organic materials properly. To overcome this limitation, we have extended our implementation of the analytical strain derivatives (stress tensor) to include the contributions that stem from (a) the van-der-Waals interaction [2] and (b) the Fock-exchange in hybrid functionals. We discuss the details of our implementation that is based on a local resolution of identity (LVL) of the Coulomb matrix [3]. We validate our approach by investigating the geometric and electronic changes that occur in polyacetylene, polyaniline, and anthracene under pressure. We show that the fraction of exact exchange included in the calculations is critical – and non-trivial to choose – for a correct description of these systems.

[1] J. H. Kim, S. Seo, and H. H. Lee, Appl. Phys. Lett. **90**, 143521 (2007).

[2] A. Tkatchenko, and M. Scheffler, PRL **102**, 073005 (2009)

[3] A. Sodt, and M. Head-Gordon, J. Chem. Phys. **128**, 104106 (2008)

DS 50.2 Fri 10:30 POT 051

DFT study of vibronic properties of partially fluorinated nickel phthalocyanine — •Davoud Pouladsaz — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Since fluorinated phthalocyanines are shown to be sensitive to reducing gases due to the withdrawing effect of fluorine atoms, by means of density functional theory, we have investigated the effect of fluorination on the vibronic couplings and ionization potential in nickel phthalocyanine.

DS 50.3 Fri 10:45 POT 051

Ab-initio investigation of Charge and Spin transport properties of Organic Semiconductors. — •Sandip Bhattacharya and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, Ireland

In this talk I will describe in detail our procedure to explore the spin and charge transport properties of organic single-crystal semiconductors from first principles. Our technique involves representing the organic semiconductor with a tight-binding model, including coupling of the charge carrier to phonons and spin relaxation due to hyperfine and spin-orbit coupling interaction. The ab-initio Hamiltonian parameters are extracted from DFT and the maximally localized Wannier functions scheme. We evolve the classical fields in the Hamiltonian via Monte Carlo simulations, and then compute the mobility from Kubo formula and the spin-diffusion length from a Landauer-Buettiker approach. We shall demonstrate calculated charge carrier mobilities very close to those measured in single-crystal rubrene-based organic field effect transistors and spin-diffusion length quite close to that estimated in experiments on rubrene-based spin valves. In the second part of my talk, I shall discuss the use of a similar procedure to predict the ab-initio spin and charge transport characteristics of Triarylamine-based organic nanowires, recently synthesized. We obtain quite superior estimates for hole mobilities as well as spin-diffusion lengths in such organic nanowires, corroborating the experimental find of exceptional conductance through nanodevices made out of such nanowires.

DS 50.4 Fri 11:00 POT 051

Growth control of AgTCNQ nanowire arrays by using template-assisted electro-deposition method — •Chengliang Wang[1], Liaoyong Wen[1], Thomas Kups[2], Ranjith Vellacheri[1], Yaoguo Fang[1], Peter Schaaf[2], Huaping Zhao[1], and Yong Lei[1] — [1]Institute for Physics and IMN MacroNano(ZIK), Ilmenau University of Technology, Ilmenau 98693, Germany — [2]Institute of Materials Engineering and IMN MacroNano(ZIK), Ilmenau University of Technology, Ilmenau 98693, Germany

One dimensional (1D) organic semiconductor nanostructures, especially their aligned arrays, have attracted extensive attention due to their potential application in organic optoelectronics, and template-assisted methods have been proved to be one of the most powerful methods to achieve this kind of arrays. Due to the small size of the AAO nanopores, diffusion of the objects into the nanopores is one of the crucial issues to achieve nanowire arrays. Here, the growth control of AgTCNQ (TCNQ: 7,7,8,8-tetracyanoquinodimethane) nanowire arrays is achieved by using template-assisted electro-deposition methods. We find that the diffusion of the electrolyte into the nanopores takes an important role in the electro-deposition process and the equilibrium between the reduction and the diffusion is necessary to achieve continuous AgTCNQ nanowire arrays. We believed that the analysis of the equilibrium between the deposition and the diffusion and the controllable synthesis of organic semiconductor arrays will benefit the preparation of other semiconductor arrays.

DS 50.5 Fri 11:15 POT 051

Energy-transfer in ZnO/ladder-type oligophenylenes hybrid structures — •Francesco Bianchi[1], Sylke Blumstengel[1], Fritz Henneberger[1], Björn Kobin[2], Stefan Hecht[2], Raffael Schlesinger[1], and Norbert Koch[1] — [1]Institut für Physik Humboldt-Universität, Berlin, Germany — [2]Department of Chemistry Humboldt-Universität, Berlin, Germany

Inorganic/organic hybrid systems designed to inherit the advantageous properties of each of their constituents are of great interest both to basic science as well as for optoelectronic applications. In this regard it is required to find an organic material that exhibits specific properties like narrow transitions, large dipole moment, small emission-absorption Stokes shift and an optical gap that corresponds to the inorganic material. The design we use consists in a three spiro-bridged ladder-type quarter-phenyl (SP3-L4P) grown on ZnO-based single quantum wells (SQW) to obtain incoherent coupling. In such a setting, it should be possible to convert Wannier excitons of the SQW into Frenkel excitons of the organic layer via a Förster type energy transfer (FRET).

We investigate the FRET between SQW with different cap thickness and a 3Sp-L4P thin layer evaporated on top of them. With photoluminescence excitation and time-resolved spectroscopy we demonstrate that these hybrid structures exhibit energy transfer with an efficiency up to 65%. Despite the high efficiency, UPS measurements show a type II interface between ZnO and the molecules layer, leading to a charge separation process that limits the light emitted. Finally we investigate on the use of high gap material spacer to reduce this effect.

DS 50.6 Fri 11:30 POT 051

Temperature dependent PL measurements of rubrene single crystals with μm-resolution — •T. Schmeiler[1], J. Gabel[1], R. Claessen[1], and J. Pflaum[1,2] — [1]Inst. Exp. Phys. VI/IV, University of Würzburg, 97074 Würzburg — [2]ZAE Bayern e.V., 97074 Würzburg

Our previous demonstration of spatial confinement effects on exciton dynamics in rubrene (rub) single crystals, microcrystals and amorphous films [1] has raised fundamental questions on excitonic processes occurring at surfaces and interfaces of molecular stacks. We address this topic by analyzing the temperature dependent PL characteristics of rub single crystals on μm-length scales and under various boundary condition by e.g. capping them with thin films of different polarizability such as Au or LaVO. At first, a pronounced enhancement of the total PL intensity of up to two orders of magnitudes was observed in case of the Au top layer which can be attributed to a resonant coupling of the excited rub states to the surface plasmon modes of the metal. This coupling phenomenon is further corroborated by relative intensity changes within the PL spectra of the Au covered rub upon cooling below 100K. In case of a LaVO capping layer, providing high polarizability without significant contributions by exciton quenching, a strong temperature dependent influence in the rub PL peaks at short wavelengths is observed. This behavior will be discussed in the context of temperature dependent changes of the LaVO layer itself as well as different coupling mechanism for the interfacial excitonic species. Financial support by the DFG research unit FOR 1809 (project PF385/6) is gratefully acknowledged. [1] B. Gieseking et al., arXiv:1309.1107

DS 50.7 Fri 11:45 POT 051

Optical absorption and photoluminescence properties of perylene single-crystals — •Andre Rinn, Niklas Kraus, André Pick, Gregor Witte, and Sangam Chatterjee — Phillips Universität Marburg, Marburg, Germany

Organic semiconductors are considered promising candidates for next-generation optical devices. However, a detailed systematic understanding of the electro-optical response is in a much less holistic state than for inorganic materials such as Si or GaAs. Therefore, we investigated the two crystalline phases of perylene as model organic semiconductors and gain further insight in their optical response. This system crystallizes in two different phases: the beta-phase has a monomeric herringbone structure with two molecules per primitive unit cell, whereas the alpha phase grows in a dimeric herringbone configuration with four molecules per unit cell. The single -crystalline samples have been grown in silicon oil, which results in microcrystals of excellent quality. Hence, we can investigate the consequences of the respective crystal orientation on the Davydov splitting of the excitons as well as excimer formation. Both configurations have been investigated with polarization resolved absorption spectroscopy and time resolved luminescence experiments. Absorption spectroscopy reveals results with significant deviations from the widespread Davydov picture. The data obtained by time resolved luminescence shows characteristic excimer behavior. Additionally, the optical spectra are compared to the response of perylene in solution and the vapour phase.

DS 50.8 Fri 12:00 POT 051

Direct measurement of the charge carrier mobility in organic donor-acceptor blend in device geometry – including extreme stoichiometry — •Johannes Widmer[1], Janine Fischer[1], Christian Koerner[1], Karl Leo[1], and Moritz Riede[1,2] — [1]Institut für Angewandte Photophysik (IAPP), TU Dresden, Germany — [2]Current address: Clarendon Laboratory, UK

Blend layers of an organic donor (D) and a fullerene acceptor (A) are a key component of highly efficient organic solar cells. The charge carrier mobility in the blend sensibly affects the device efficiency concerning transport and recombination of charge carriers.

The applied method "POEM" – potential mapping by thickness variation – is a direct measurement giving model-free experimental access to the effective mobility $\mu(F, n)$ as a function of the electric field F and the charge carrier density n. It is based on a novel evaluation strategy for space-charge limited current (SCLC) in single carrier devices in a vertical device geometry.[Widmer et al., Org. El. (2013)]

Here, we apply POEM to characterize the hole transport in D:A blends of small molecules with different blend ratios. The measurements cover common ratios as well as strongly diluted blends with only $\approx 1\,\%$ donor content, which are known to yield efficient solar cells. Beyond characterizing disorder and trap states, which influence μ, the POEM measurements reveal that also in the diluted blend effective hole transport is possible, but takes place not only on the donor.

The obtained $\mu(F, n)$ functions allow for an advanced understanding of charge transport in D:A blends – also in moderate blend ratios.

DS 50.9 Fri 12:15 POT 051

Polymer aggregation control in polymer: PCBM bulk heterojunctions adapted from solution — •Christian Kästner[1], Daniel Egbe[2], and Harald Hoppe[1] — [1]Ilmenau University of Technology, Ilmenau, Germany — [2]Linz Institute for Organic Solar Cells, Linz, Austria

It is common knowledge that the polymer conformation and its phase separation with fullerene derivatives are delicate issues crucially impacting on the photovoltaic parameters of polymer based solar cells. Whereas strongly intermixed polymer:fullerene phases provide large interfacial area and consequently a high quantum efficiency of exciton dissociation, pristine and primarily ordered polymer and fullerene domains support efficient charge transport and percolation. To study the aggregation and phase separation in polymer solar cells we investigated counterbalancing influences of polymer solution concentration and PCBM ([6,6]-phenyl-C61-butyric acid methyl ester) blending ratio on the basis of a semi-crystalline anthracene-containing poly(p-phenylene-ethynylene)-alt-poly(p-phenylene-vinylene) (PPE-PPV) copolymer statistically bearing either branched 2-ethylhexyloxy or linear octyloxy side-chains (AnE-PVstat). The polymer aggregation varied with both, solution and PCBM concentrations, yielding a specific maximum within the parameter range. We explicitly demonstrate the counterbalancing effect on charge generation and transport for increasing polymer aggregation. Furthermore the influence of polymer aggregation on fundamental optoelectronic properties is discussed, providing detailed understanding of resulting photovoltaic parameters.

DS 51: Graphene (joint session with TT, MA, HL, DY, O)

Time: Friday 11:30–13:15 Location: CHE 89

DS 51.1 Fri 11:30 CHE 89

Plasma-enhanced chemical vapor deposition of graphene on copper substrates — •Nicolas Wöhrl, Oliver Ochedowski, Steven Gottlieb, and Volker Buck — Universität Duisburg-Essen und CENIDE, 47057 Duisburg, Germany

In this work we present the synthesis of graphene on copper by microwave Plasma-enhanced Chemical Vapor Deposition (PE-CVD) process. The special construction of the plasma source allows the deposition at a wide range of different process parameters giving a fast and inexpensive method to synthesize graphene. Additional advantages of the plasma deposition of graphene are lower substrate temperatures compared with thermal CVD processes. The PE-CVD process uses hydrogen and methane as reaction gases exactly like thermal CVD process does. The gaseous precursors are decomposed in the plasma and the catalytic influence of copper and the minor solubility of carbon in copper lead to the growth of one monolayer of graphene. Plasma parameters are varied to investigate the influence on the graphene properties. Raman spectroscopy and AFM measurements are used as non-destructive tools for the characterization of the synthesized graphene films. Especially Raman spectroscopy is used as an efficient tool to determine the number of graphene layers, the disorder and the defect density. We present a possible way to produce large area of monolayer graphene on a copper based substrate. This technology can help to make graphene available for industrial applications.

DS 51.2 Fri 11:45 CHE 89

Continuous wafer-scale graphene on cubic-SiC(001) — •Victor Aristov[1,2], Olga Molodtsova[2], Alexei Zakharov[3], Dmitry Marchenko[4], Jaime Sánchez-Barriga[4], Andrei Varykhalov[4], Marc Portail[5], Marcin Zielinski[6], Igor Shvets[7], and Alexander Chaika[1,7] — [1]ISSP RAS, Chernogolovka, Moscow dist. 142432, Russia — [2]HASYLAB at DESY, D-22607 Hamburg, Germany — [3]MAX-lab, Lund University, Box 118, 22100 Lund, Sweden — [4]HZB für Materialien und Energie, D-12489 Berlin, Germany — [5]CNRS-CRHEA, 06560 Valbonne, France — [6]NOVASiC, BP267-F73375 Le Bourget du Lac Cedex, France — [7]CRANN, School of Physics, Trinity College, Dublin 2, Ireland

The atomic and electronic structure of graphene synthesized on commercially available cubic SiC(001)/Si(001) wafers have been studied. LEED, LEEM, PEEM, STM and ARPES data prove the wafer-scale continuity and uniform thickness of the graphene overlayer and reveal that the graphene overlayer consists of only a few monolayers with physical properties of quasi-freestanding graphene: atomic-scale rippling, asymmetric distributions of carbon-carbon bond lengths etc. In addition, graphene overlayer consists of rotated nanometer-sized ribbons with four different lattice orientations connected through the grain boundaries. Thus, this graphene could be adapted for graphene-based electronic technologies and directly patterned using Si-electronic lithographic process. Supported by RFBR grant 14-02-00949, by Marie Curie IIF grant (7th ECFP) and by SPP 1459 of DPG.

DS 51.3 Fri 12:00 CHE 89

Characterization of single and few layer of molybdenum disulfide with spectroscopic imaging ellipsometry — •P. H. Thiesen[1], B. Miller[2], C. Röling[1], E. Parzinger[2], A. W. Holleitner[2], and U. Wurstbauer[2] — [1]Accurion GmbH, Göttingen, Germany — [2]Technische Universität München, Walter Schottky Institut, 85748 Garching, Germany

Molybdenum disulfide is a layered transition metal dichalcogenide. From the point of current research, 2D-materials based on MoS2 are very promising because of the special semiconducting properties. The bulk material has an indirect 1.2 eV electronic bandgap, but single layer MoS2 has a direct 1.8 eV bandgap. The monolayer can be used in prospective electronic devices like transistors or photo detectors. Like in the initial period of graphene research, the issue is to identify and characterize MoS2 crystallites of microscopic scale. Imaging ellipsometry is a nondestructive optical method in thin film metrology with a lateral resolution down to 1 micro meter. Imaging ellipsometry has been applied to characterize graphene flakes of few micrometer size [1],[2] and also to identify single layer steps in multilayer graphene/graphite stacks [3]. Delta and Psi Spectra of MoS2 monolayers as well as maps of the ellipsometric angles will be presented. The practical aspect of single layer identification will be addressed and the capability of ellipsometric contrast micrographs as a fast tool for single layer identification will be demonstrated. [1] Wurstbauer et al., Appl. Phys. Lett. 97, 231901 (2010) [2] Matkovic et al. J. Appl. Phys. 112, 123523 (2012) [3] Albrektsen et al. J. Appl. Phys. 111, 064305 (2012)

DS 51.4 Fri 12:15 CHE 89

Charge and Spin Transport in Turbostratic Graphene and Graphene Nanoribbons — •Nils Richter[1], Sebastian Schweizer[2], Ajit Kumar Patra[2], Yenny Hernandez[3], Akimitsu Narita[3], Xinliang Feng[3], Petr Ostrizek[1], Klaus Müllen[3], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]FB Physik, Universität Konstanz, 78457 Konstanz, Germany — [3]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

We present two specially selected allotropes of graphene: Turbostratic graphene (TG) and graphene nanoribbons (GNRs).

TG discs are graphitic microstructures where the twisting of adjacent layers leads to an electronic decoupling. Electrical transport measurements reveal quantum effects such as weak localization and huge charge carrier mobilities (100,000 cm^2/Vs) in protected bulk layers [1]. In non-local spin valves we find efficient spin injection over micrometer distances showing large spin diffusion lengths.

Using electromigrated nanojunctions we are able to investigate electrical and spin transport in chemically synthesized GNRs. As they are dispersed in a solvent [2] they can be drop cast on such junctions. With GNRs of different widths and edge geometries we will probe the exciting unconventional properties that have been predicted for these nanostructures [3].

[1] Y. Hernandez et al., arXiv:1301.6087 (under review 2013). [2] A. Narita et al., Nature Chem., in press, DOI: 10.1038/NCHEM.1819. [3] O. Yazyev, Rep. Prog. Phys. 73, 056501 (2010).

DS 51.5 Fri 12:30 CHE 89

Graphene functionalisation with N and O: reversible or permanent modification of the electronic properties? — •Peter Brommer[1,2], Alex Marsden[1], Neil Wilson[1], Gavin Bell[1], and David Quigley[1,2] — [1]Department of Physics, University of Warwick, Coventry, UK — [2]Centre for Scientific Computing, University of Warwick, Coventry, UK

For many applications it is essential to modify the electronic properties of graphene in a controlled fashion. This can be achieved via oxygen and nitrogen functionalisation in ultra-high vacuum, leading to a system in which electronic and structural properties can be systematically studied. Low dose oxygen functionalisation (< 5 atomic percent) can be reversed completely by annealing at 200 °C, while nitrogen permanently integrates itself into the material. Here we present insights from DFT calculations on this system, such as the low-energy configurations and simulated transmission electron microscopy (TEM) images, binding energies and effective band structures of the N and O decorated graphene sheets. We directly compare our results with experiments on CVD grown graphene. Angle-resolved photoemission spectroscopy (ARPES) resolves the band structure changes on functionalization, whilst X-ray photoelectron spectroscopy (XPS) provides information about the chemical environment of the defect atoms. Combined, the computational and experimental data can offer insights into the structural changes induced by the functionalisation process and their consequences on the electronic properties of the material.

DS 51.6 Fri 12:45 CHE 89

Revealing the ultrafast process behind the photoreduction of graphene oxide — •Daniel S. Badali[1], Regis Y.N. Gengler[1], Dongfang Zhang[1], Kostantinos Dimos[2], Kostantinos Spyrou[2], Dimitrios Gournis[2], and R.J. Dwayne Miller[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg Center for Ultrafast Imaging, University of Hamburg, Hamburg, Germany — [2]Department of Material Science and Engineering, University of Ioannina, Ioannina, Greece

Because of its unique electronic and structural properties, graphene has brought two-dimensional materials to the foreground of material science and nanoelectronic research. As such, reliable methods for producing graphene are in demand and have significant impact on the field of thin films. In recent years it has been found that irradiating dispersions of graphene oxide in water with ultraviolet light has led to the production of graphene. Although this has been observed in a variety of experimental conditionals, the exact mechanism of the reduction has remained elusive until now. To this end, we have performed careful optical pump-probe measurements which have revealed the chemistry of this process: rather than direct photoreduction, the reduction is mediated by solvated electrons which have been liberated from water molecules by the ultraviolet light. We show that this occurs on an ultrafast timescale in the tens of picoseconds range. Characterization of the final product confirms the removal of oxygen containing groups and the restoration of the honeycomb carbon network of graphene.

DS 51.7 Fri 13:00 CHE 89

Tuning of structural, electronic and optical properties in twisted bilayer MoS_2 — •Jens Kunstmann[1], Arend M. van der Zande[1], Alexey Chernikov[1], Daniel A. Chenet[1], YuMeng You[1], XiaoXiao Zhang[1], Timothy C. Berkelbach[1], Pinshane Y. Huang[2], Lei Wang[1], Fan Zhang[1], Mark Hybertsen[1,3], David A. Muller[2], David R. Reichman[1], Tony F. Heinz[1], and James C. Hone[1] — [1]Columbia University, New York, New York, 10027, USA — [2]Cornell University, Ithaca, New York, 14853, USA — [3]Brookhaven National Laboratory, Upton, New York 11973, USA

With the rise of graphene, atomically thin 2D materials have become the focus of many researchers worldwide. Among them, group 6 transition metal dichalcogenides, such as MoS_2 are new 2D direct gap semiconductors, have been used as field effect transistors and are promising for applications in valleytronics. However, little is understood about the interlayer interactions between 2D materials. We measured dozens of MoS_2 bilayers with well-defined twist angle by stacking single crystal monolayers using ultraclean transfer techniques. We observe that continuous changes in the interlayer twist angle lead to strong, continuous tuning in the indirect optical transitions, the Raman modes, the second harmonic generation, and the reflection spectra. We use electronic structure calculations to show that the tuning in the indirect band transitions arise from an increase of the bilayer separation caused by the van der Waals repulsion of sulfur atoms. These results indicate the possibility of producing new 2D materials with desired properties by tailoring the interlayer alignment in 2D heterostructures.