

## Thin Films Division Fachverband Dünne Schichten (DS)

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### Overview of Invited Talks and Sessions

(Lecture halls H32 and H39; Poster E)

#### Invited Talks

DS 1.1	Mon	9:30–10:00	H32	<b>Charge and ion exchange at electrochemical interfaces: atomistic insights by means of in-situ ellipsometry</b> — ●CHRISTOPH COBET
DS 11.1	Tue	9:30–10:00	H32	<b>Photoluminescence Analysis of Thin Films: What can it tell us about (Perovskite) Solar Cells?</b> — ●THOMAS UNOLD
DS 11.3	Tue	10:15–10:45	H32	<b>Defect activity in lead halide perovskite semiconductors</b> — ●SILVIA MOTTI
DS 11.5	Tue	11:15–11:45	H32	<b>Beyond traditional use of photoluminescence: Assessing halide perovskites quantitatively and qualitatively</b> — ●CAROLIN SUTTER-FELLA
DS 11.7	Tue	12:00–12:30	H32	<b>Photophysics of Sn-based hybrid perovskites</b> — ●MARIA ANTONIETTA LOI
DS 15.1	Wed	9:30–10:00	H32	<b>3D-Nanoprinting with Focused Electron Beams. Advances and Applications</b> — ●ROBERT WINKLER, JASON D FOWLKES, JÜRGEN SATTELKOW, PHILIP D RACK, HARALD PLANK
DS 15.7	Wed	11:30–12:00	H32	<b>Resist-free fabrication of graphene devices using focused ion beam patterning and direct-write ALD</b> — ●AGEETH BOL
DS 19.1	Wed	15:00–15:30	H32	<b>Fabrication of functional nanostructures by electron and ion beams</b> — ●MILOS TOTH
DS 19.6	Wed	16:45–17:15	H32	<b>Fundamentals of low-energy electron induced dissociation of focused electron beam induced deposition precursors</b> — ●ODDUR INGÓLFSSON
DS 21.1	Thu	9:30–10:00	H32	<b>Epitaxial graphene on SiC(0001) studied by electron spectroscopy and microscopy</b> — ●FLORIAN SPECK
DS 21.6	Thu	11:15–11:45	H32	<b>Patternable non-polar epigraphene for nanoelectronics and Dirac point physics</b> — VLADIMIR PRUDKOVSKIY, YIRAN HU, HUE HU, LEI MA, CLAIRE BERGER, ●WALT DE HEER
DS 21.9	Thu	12:15–12:45	H32	<b>Intrinsic stacking domains in graphene on silicon carbide: A pathway for intercalation</b> — TOBIAS A DE JONG, EUGENE E KRASOVSKII, CHRISTIAN OTT, RUDOLF M TROMP, SENSE JAN VAN DER MOLEN, ●JOHANNES JOBST
DS 23.1	Thu	15:00–15:30	H32	<b>Artificial nano-granular heterostructures: fundamentals and applications</b> — ●OLEG UDALOV, IGOR BELOBORODOV
DS 23.5	Thu	16:30–17:00	H32	<b>3D nanomagnetism and superconductivity: Current status and potential for future work</b> — ●OLEKSANDR DOBROVOLSKIY, MICHAEL HUTH

#### Invited talks of the joint Symposium SKM Dissertation-Prize 2019

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:50	H2	<b>Synchronization and Waves in Confined Complex Active Media</b> — ●JAN FREDERIK TOTZ
SYSD 1.2	Mon	9:50–10:10	H2	<b>Spin scattering of topologically protected electrons at defects</b> — ●PHILIPP RÜSSMANN
SYSD 1.3	Mon	10:10–10:30	H2	<b>Beyond the molecular movie: Revealing the microscopic processes behind photo-induced phase transitions</b> — ●CHRIS W. NICHOLSON
SYSD 1.4	Mon	10:30–10:50	H2	<b>Thermodynamic bounds on current fluctuations</b> — ●PATRICK PIETZONKA
SYSD 1.5	Mon	10:50–11:10	H2	<b>Lightwave-driven quasiparticle acceleration</b> — ●FABIAN LANGER

SYSD 1.6	Mon	11:10–11:30	H2	<b>Ultrafast plasmon-driven point-projection electron microscopy</b> — ●JAN VOGELSANG
SYSD 1.7	Mon	11:30–11:50	H2	<b>Helimagnets, sand patterns and fingerprints linked by topology</b> — ●PEGGY SCHÖNHERR

### Invited talks of the joint Symposium Mechanically Controlled Electrical Conductivity of Oxides

See SYCO for the full program of the symposium.

SYCO 1.1	Mon	9:30–10:00	H1	<b>Dislocation Dynamics and Their Conductivities in Oxides</b> — ●YUICHI IKUHARA
SYCO 1.2	Mon	10:00–10:30	H1	<b>Strain effects in ionic conductivity and electrode processes</b> — ●JÜRGEN JANEK
SYCO 1.3	Mon	10:30–11:00	H1	<b>Elastic dipoles of point defects in materials</b> — ●CELINE VARVENNE
SYCO 1.4	Mon	11:30–12:00	H1	<b>Mapping strain/pressure with ZnO nanowire arrays by piezo-phototronic effect</b> — ●CAOFENG PAN
SYCO 1.5	Mon	12:00–12:30	H1	<b>Bulk and Flexo-photovoltaic effect</b> — ●MARIN ALEXE

### Invited talks of the joint Symposium Patterns in Nature: Origins, Universality, Functions

See SYPN for the full program of the symposium.

SYPN 1.1	Mon	15:00–15:30	H1	<b>Engineering spatial-temporal organization of bacterial suspensions</b> — ●IGOR ARONSON
SYPN 1.2	Mon	15:30–16:00	H1	<b>Collective behaviour and pattern formation in phoretic active matter</b> — ●RAMIN GOLESTANIAN
SYPN 1.3	Mon	16:00–16:30	H1	<b>Control and selection of spatio-temporal patterns in complex systems</b> — ●SVETLANA GUREVICH
SYPN 1.4	Mon	16:45–17:15	H1	<b>Self-organization of Active Surfaces</b> — ●FRANK JÜLICHER
SYPN 1.5	Mon	17:15–17:45	H1	<b>Front instabilities can reverse desertification</b> — ●EHUD MERON

### Invited talks of the joint Symposium Geometry, Topology, and Condensed Matter

See SYGT for the full program of the symposium.

SYGT 1.1	Tue	9:30–10:00	H1	<b>Thermal Properties of Vortices on Curved Surfaces</b> — ●JOSÉ LORENZANA
SYGT 1.2	Tue	10:00–10:30	H1	<b>Curvature-induced effects in manomagnets</b> — ●DENIS SHEKA
SYGT 1.3	Tue	10:30–11:00	H1	<b>Magnetization configurations and reversal of individual ferromagnetic nanotubes</b> — ●MARTINO POGGIO
SYGT 1.4	Tue	11:15–11:45	H1	<b>An experimental perspective on topology and nanoelectronics in graphene and related 2D materials.</b> — ●IVAN J. VERA-MARUN
SYGT 1.5	Tue	11:45–12:15	H1	<b>Roles of the curvature in two-dimensional nematic films</b> — ●GAETANO NAPOLI

### Invited talks of the joint Symposium Interaction Effects and Correlations in twodimensional Systems - New Challenges for Theory

See SYTS for the full program of the symposium.

SYTS 1.1	Wed	15:00–15:30	H1	<b>Spectra of layered semiconductors from many-body perturbation theory</b> — ●MICHAEL ROHLFING
SYTS 1.2	Wed	15:30–16:00	H1	<b>Dark exciton dynamics in 2D materials</b> — ●ERMIN MALIC
SYTS 1.3	Wed	16:00–16:30	H1	<b>Excitons versus electron-hole plasma in monolayer transition metal dichalcogenide semiconductors</b> — ●ALEXANDER STEINHOFF
SYTS 1.4	Wed	16:45–17:15	H1	<b>Theory of near K-point optical properties of TMDC multilayers</b> — ●TINEKE STROUCKEN
SYTS 1.5	Wed	17:15–17:45	H1	<b>High-throughput modeling and discovery of novel 2D materials</b> — ●KRISTIAN THYGESEN

## Invited talks of the joint Symposium Czech Republic as Guest of Honor

See SYCZ for the full program of the symposium.

SYCZ 1.1	Thu	9:30–10:00	H4	<b>Crystal symmetries and transport phenomena in antiferromagnets —</b> •TOMAS JUNGWIRTH
SYCZ 1.2	Thu	10:00–10:30	H4	<b>Terahertz subcycle charge and spin control —</b> •RUPERT HUBER
SYCZ 1.3	Thu	10:30–11:00	H4	<b>1D molecular system on surfaces —</b> •PAVEL JELINEK
SYCZ 1.4	Thu	11:15–11:45	H4	<b>Tunneling microscopy on insulators provides access to out-of-equilibrium charge states —</b> •JASCHA REPP
SYCZ 1.5	Thu	11:45–12:15	H4	<b>Occam’s razor and complex networks from brain to climate —</b> •JAROSLAV HLINKA
SYCZ 1.6	Thu	12:15–12:45	H4	<b>Long range temporal correlations in complex systems —</b> •HOLGER KANTZ

## Invited talks of the joint Symposium Identifying Optimal Physical Implementations for beyond von Neumann Computing Concepts

See SYCC for the full program of the symposium.

SYCC 1.1	Fri	9:30–10:00	H1	<b>On the Link Between Energy and Information for the Design of Neuro-morphic Systems —</b> •NARAYAN SRINIVASA
SYCC 1.2	Fri	10:00–10:30	H1	<b>Encoding neural and synaptic functionalities in electron spin: A pathway to efficient neuromorphic computing —</b> •KAUSHIK ROY
SYCC 1.3	Fri	10:30–11:00	H1	<b>Neuromorphic computing with spintronic nano-oscillators —</b> •PHILIPPE TALATCHIAN
SYCC 1.4	Fri	11:15–11:45	H1	<b>Artificial Intelligence and beyond von Neumann architectures, a mutual opportunity —</b> •MIRKO PREZIOSO
SYCC 1.5	Fri	11:45–12:15	H1	<b>Brain-inspired approaches in ultrafast magnetism —</b> •JOHAN H. MENTINK

## Sessions

DS 1.1–1.7	Mon	9:30–11:45	H32	<b>Optical Analysis of Thin Films I (Reflection, Ellipsometry, Raman, IR-DUV Spectroscopy, ...</b>
DS 2.1–2.6	Mon	9:30–12:45	H34	<b>Focus Session: Oxide Semiconductors for Novel Devices (joint session HL/DS)</b>
DS 3.1–3.12	Mon	9:30–12:45	H39	<b>Layer Properties: Electronic, Optical and Mechanical Properties</b>
DS 4.1–4.9	Mon	10:30–13:00	H9	<b>Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge I (joint session O/TT/CPP/DS)</b>
DS 5.1–5.1	Mon	12:30–13:00	H32	<b>Prize talk Selina Olthof (joint session PRV/DS/VA)</b>
DS 6.1–6.10	Mon	15:00–17:30	H9	<b>Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge II (joint session O/TT/DS/CPP)</b>
DS 7.1–7.5	Mon	15:00–16:15	H32	<b>Optical Analysis of Thin Films II (Reflection, Ellipsometry, Raman, IR-DUV Spectroscopy, ...</b>
DS 8.1–8.4	Mon	15:00–16:30	PHY 5.0.21	<b>Instrumentation Micro-/Nano-Analysis and Lithography/Structuring (joint session KFM/DS/O)</b>
DS 9.1–9.6	Mon	15:00–16:30	H39	<b>Layer Deposition (ALD, MBE, Sputtering, ...)</b>
DS 10.1–10.5	Mon	16:45–18:00	H39	<b>Thermoelectric and Phase Change Materials</b>
DS 11.1–11.9	Tue	9:30–13:15	H32	<b>PhD-Symposium: Photoluminescence of halide perovskites: What does it tell us and what not? (joint session DS/AKjDPG/HL)</b>
DS 12.1–12.9	Tue	10:30–13:00	H9	<b>Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge III (joint session O/CPP/DS/TT)</b>
DS 13.1–13.10	Tue	14:00–16:45	H9	<b>Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge IV (joint session O/CPP/DS/TT)</b>
DS 14.1–14.60	Tue	17:00–20:00	Poster E	<b>Poster</b>
DS 15.1–15.9	Wed	9:30–12:30	H32	<b>Focus Session: Direct-Write Nanofabrication and Applications I (Electron Beam Induced Processing) (joint session DS/TT)</b>
DS 16.1–16.11	Wed	9:30–12:30	H39	<b>Organic Thin Films, Organic-Inorganic Interfaces</b>

DS 17.1–17.9	Wed	10:30–13:15	H9	<b>Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge V (joint session O/CPP/DS/TT)</b>
DS 18.1–18.11	Wed	15:00–17:45	H9	
DS 19.1–19.9	Wed	15:00–18:00	H32	<b>Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge VI (joint session O/DS/CPP/TT)</b>
DS 20	Wed	18:30–19:30	H39	<b>Focus Session: Direct-Write Nanofabrication and Applications II (Electron Beam Induced Processing) (joint session DS/TT)</b>
DS 21.1–21.9	Thu	9:30–12:45	H32	<b>Annual General Meeting of the Thin Films Division</b>
DS 22.1–22.10	Thu	9:30–12:15	H39	<b>Focus Session: Growth, Properties and Application of Epitaxial Graphene (joint session DS/O/HL)</b>
DS 23.1–23.8	Thu	15:00–17:45	H32	<b>Thin Film Applications</b>
DS 24.1–24.12	Thu	15:00–18:15	H39	<b>Direct-Write Nanofabrication and Applications III (Electron Beam Induced Processing) (joint session DS/TT)</b>
DS 25.1–25.12	Fri	9:30–12:45	H32	<b>Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...) Part I</b>
				<b>Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...) Part II</b>

### Annual General Meeting of the Thin Films Division

Wednesday 18:30–19:30 H39

## DS 1: Optical Analysis of Thin Films I (Reflection, Ellipsometry, Raman, IR-DUV Spectroscopy, ...)

Time: Monday 9:30–11:45

Location: H32

**Invited Talk**

DS 1.1 Mon 9:30 H32

**Charge and ion exchange at electrochemical interfaces: atomistic insights by means of in-situ ellipsometry** — ●CHRISTOPH COBET — Johannes Kepler University, Altenbergerstr 69, 4040, Linz, Austria

Recently, solid-liquid interfaces and electrochemical surface reactions received more and more attention. The motivation may arise by applications e.g. to solve energy harvesting problems or to develop novel (bio-)sensing techniques. The functionality, however, depends on the adjacent atomic layers near the interface and the development of respective surface sensitive methods allow nowadays a more detailed study. In general we have to deal with alternating charges and chemical compounds perpendicular to the interfaces. In the presented work we use polarization optical methods in the spectral range of transparency of the electrolytes. It is an advantage and at the same time a challenge that all boundaries in the light pass contribute to a polarization change. We show in comparison to conventional cyclic voltammetry, impedance spectroscopy, and electrochemical STM that spectroscopic ellipsometry and reflection anisotropy spectroscopy (RAS) can nevertheless provide quantitative information. At metal single crystal surface it was e.g. possible to determine the amount of surface adsorbates and the amount of interface charges. Thus, we could determine also the so called potential of zero total charge (PZTC). Furthermore, we got evidences for an increased density of the water film near the interface. Time resolved measurements gave supplementary insights in the dynamics of electrochemical absorption processes.

**15 min. break**

DS 1.2 Mon 10:15 H32

**Sensing and structure analysis by in situ IR spectroscopy: From ml flow cells to microfluidic applications** — ●KARSTEN HINRICH, LUCJAN GRZEGORZEWSKI, ANDREAS FURCHNER, and CHRISTOPH KRATZ — ISAS - e.V., Schwarzschildstr. 8, 12489 Berlin, Germany

The low penetration depths of IR radiation in aqueous solutions poses a challenge for utilizing IR spectroscopy in investigations with macro- and microfluidic flow cells. Probing the solid liquid interface through an IR transparent substrate can be advantageous in such experiments. In situ IR ellipsometry in combination with optical modeling can be applied for detailed analysis of molecular interactions and hydration states of ultrathin functional polymer films. The development of an optofluidic platform incorporating metal-island film substrates for signal enhancement translates this technique to the world of microfluidics. Time-resolved measurements of monolayer formation of organic molecules show that the developed concept can be employed to monitor dynamic processes under in situ conditions in nL volumes.

DS 1.3 Mon 10:30 H32

**Reflectance Anisotropy Spectroscopy as an analytical tool for phase transformation studies: order reactions in Cu-Au Thin Films** — ●MARCO VOLPI, ALLA SOLOGUBENKO, PHILIPP OKLE, and RALPH SPOLENAK — ETHZ, Zürich, Switzerland

Increasing interest of materials science in thin films is driven by a vast range of applications in many fields like mechanics, electronics and optics. Outstanding physical and mechanical properties originate from their morphology and microstructure, which are processing conditions dependent. Therefore, monitoring of film phase stabilities during their production is fundamental. In this work, we study thermally induced phase transformations of Cu-x at.% Au (x=15, 25, 50, 75) thin films produced with Plasma Assisted Physical Vapor Deposition (PA-PVD) by combining transmission electron microscopy (TEM) and X-Ray diffraction (XRD). Information gained on the order reactions were used to validate the phase state sensitivity in Reflectance Anisotropy Spectroscopy (RAS) [1]. As-deposited Cu-Au thin films show a solid solution state that disagrees with the equilibrium phase configurations expected from the bulk phase diagram. However, thermal treatment triggers order reactions that lead to equilibrium. Both TEM and RAS revealed the formation of intermetallic phases in Cu-25 at.% Au and Cu-50 at.% Au upon annealing. Yet, only RAS could reveal a two-

phase state that coexisted in the annealed Cu-25 at.% Au and Cu-50 at.% Au films. To conclude, RAS proves to be a very sensitive alternative to TEM that allows prompt and non-destructive phase analyses in films. [1] Cole R.J.et al., J Phys. D Appl. Phys., (2003), 36.

DS 1.4 Mon 10:45 H32

**Direct band gap of alpha-tin investigated by infrared ellipsometry** — RIGO A. CARRASCO<sup>1</sup>, CESY M. ZAMARRIPA<sup>1</sup>, ●STEFAN ZOLLNER<sup>1</sup>, and JOSE MENENDEZ<sup>2</sup> — <sup>1</sup>New Mexico State University, Las Cruces, NM — <sup>2</sup>Arizona State University, Tempe, AZ

Interest in gray tin has been revived because it is the endpoint constituent of Ge<sub>1-x</sub>Sn<sub>x</sub> alloys, which have potential applications as mid-infrared detectors and lasers.  $\alpha$ -tin also becomes a topological insulator or Dirac semimetal under stress. The band structure for gray tin is similar to Ge, but the  $\Gamma_7^-$  s-antibonding band, which is the conduction band in Ge, moves downward in gray tin and appears between  $\Gamma_8^+$  and  $\Gamma_7^+$  with a negative energy  $\bar{E}_0$  if we conventionally choose  $\Gamma_8^+$  as the zero energy level.

Using Fourier-transform infrared ellipsometry, we provide spectroscopic evidence about the valence band structure of  $\alpha$ -tin. The mid-infrared dielectric function of  $\alpha$ -tin grown pseudomorphically on InSb or CdTe by molecular beam epitaxy shows a strong  $\bar{E}_0$  peak near 0.41 eV. The peak can be attributed to allowed intra-valence band transitions from the  $\Gamma_7^-$  (electron-like) to the  $\Gamma_8^{+v}$  heavy hole valence band and/or interband transitions from the  $\Gamma_7^-$  band to the  $\Gamma_8^{+c}$  light "hole" conduction band. Possible sources for the strength of the peak, and its temperature dependence will be discussed. We would like to thank Dr. Arnold M. Kiefer and Stephanie Chastang for providing us the strained  $\alpha$ -tin samples.

DS 1.5 Mon 11:00 H32

**Temperature induced changes in monolayers observed by sum frequency generation spectroscopy** — ●DAMIAN FIRLA, ROBERT RAMEKER, JOSHUA MULTHAUP, and ECKART HASSELBRINK — Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen, Germany

A major component in cell membranes are phospholipids which form bilayers. The amphiphilic character of phospholipids was exploited to spread a solution on water in a Langmuir trough. This monolayer was compressed, transferred on a substrate and studied by sum frequency generation spectroscopy. The main goal was to observe changes upon raising the temperature. Typically conformational changes of alkyl chains from *all-trans* to a conformation with *gauche* defects were observed as recognized by the change of the intensities of the CH<sub>3</sub> and CH<sub>2</sub> vibrational modes. Different types of phospholipids and mixtures of phospholipids with varying chain lengths were studied. Investigations of single phospholipid species showed that the intensity of CH<sub>3</sub> vibrational modes decreased with rising the temperature whereas the intensity of the CH<sub>2</sub> symmetrical stretching mode was not increasing. This was attributed to the high density of such monolayers, in which conformational changes were not possible because of strong van der Waals interactions. Further on mixtures of phospholipids with different chain lengths were used. In these studies the symmetrical stretching mode of CH<sub>2</sub> was observed as well, consistent with the larger space for conformational changes. The thermal stability of phospholipid monolayers was also probed. Results showed that monolayers of single phospholipid species were more stable than monolayers of phospholipid mixtures.

DS 1.6 Mon 11:15 H32

**Raman spectroscopy characterization of silicon nanoribbons on Ag(110)** — ●DMYTRO SOLONENKO, ALEXANDER EHM, DIETRICH R. T. ZAHN, and PATRICK VOGT — Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Silicon nanoribbons, which can be grown epitaxially on the Ag(110) surface [1], have an unexpected chain-like structure of Si pentagons, originating from the missing row arrangement of the Ag surface and the adlayer-substrate interaction [2]. Such interplay has consequences for the Si-Si bond lengths and force constants, which can be probed by Raman spectroscopy. Our Raman results reveal the mode symmetries, which are necessary to properly assign the modes of these highly anisotropic quasi-1D crystals. Furthermore, the results allow the differ-

entiation between the two structural phases of the ribbons, *i.e.*, single- and double-strand ribbons, and the identification of structures, which appear at the super-monolayer growth regime. The spectroscopic signatures of Si nanoribbons are compared to those of epitaxial silicene, formed on Ag(111) [3], in order to understand the fundamental principles of the Si-Ag interaction and the hybridization states of the Si atoms. The functionalization of the nanoribbons and their application are also discussed. [1] P. De Padova, *et al.*, *Nano Lett.* 8, 271 (2008). [2] J. I. Cerdá, *et al.*, *Nat. Comm.* 7, 13076 (2016). [3] D. Solonenko, *et al.*, *2D Mater.* 4, 015008 (2017).

DS 1.7 Mon 11:30 H32

**Revealing the distinct structural and plasmonic properties of gold nanosponges through FIB nanotomographical reconstruction** — •PETER SCHAAF, LARS HAUKE HONIG, and DONG WANG — TU Ilmenau, Institute of Materials Science and Engineering and Institute of Micro and Nanotechnologies MacroNano(R), Gustav-Kirchhoff-Str. 5, 98693 Ilmenau, Germany

Individual gold nanosponges (nanoporous gold nanoparticles) which were fabricated by solid state dewetting of Ag/Au bilayers and subsequent dealloying, are reconstructed from SEM images captured by FIB nanotomography. The investigated particles have diameters in the range of a few hundred nanometers and ligament diameters around 12 nm. The optical and plasmonic properties of the gold nanosponges are clearly different from that of the solid nanoparticles, and are more complex and fascinating due to unique structural features. In this work, the 3D reconstructed models of gold nanosponges, which correspond precisely to the real structures, have been used for the simulation. The results show that the plasmon peak shifts red and multiple resonance behavior appears with increasing porosity. [1] D. Wang et al., *J. Mater. Chem.*, 2012, 22, 5344. [2] Fujita, T. et al., *Applied Physics Letters*, 2008, 92, 251902. [3] Vidal C. et al., *ACS Photonics* 2015, 2, 1436. [4] Rao W. et al., *ACS Appl. Mater. Interfaces* 2017, 9, 6273. [5] Vidal, C. et al., *Nano Lett* 2018, 18, (2), 1269. [6] Hergert, G. et al., *Light Sci. Appl.* 2017, 6, e17075.

## DS 2: Focus Session: Oxide Semiconductors for Novel Devices (joint session HL/DS)

The class of semiconducting oxides materials is currently investigated in terms of promising applications in devices, including low temperature processed amorphous thin films for bendable electronics and display technology as well as highly crystalline materials such as the wide band group-III sesquioxides. Possible devices applications are UV and DUV photo sensors, power electronics and even memristors. This session sets a focus on physical properties of semiconductor oxide materials, their growth methods and heterostructures for demonstrator devices.

Organizers: Holger Eisele (TU Berlin) and Holger von Wenckstern (Uni Leipzig)

Time: Monday 9:30–12:45

Location: H34

### Invited Talk

DS 2.1 Mon 9:30 H34

**The role of suboxide kinetics and thermodynamics for the catalysis and facet formation during the molecular beam epitaxy of oxides** — •OLIVER BIERWAGEN — Paul-Drude-Institut für Festkörperelektronik, Leibniz Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5–7, 10117 Berlin, Germany.

Based on its wide band gap of  $E_g=4.7$  eV  $\text{Ga}_2\text{O}_3$  is a promising oxide semiconductor for novel applications such as power electronics and UV detection. Band-gap engineering by alloying with  $\text{In}_2\text{O}_3$  ( $E_g=2.7$  eV) allows tuning the detection wavelength and enable heterostructure devices. Thin film growth of these oxides by molecular beam epitaxy (MBE) enables the high material quality (purity and crystallinity) required for novel applications. This contribution shows how the intermediate formation and desorption kinetics of  $\text{Ga}_2\text{O}$  and  $\text{In}_2\text{O}$  limits the MBE growth rate of  $\text{Ga}_2\text{O}_3$  (and of  $\text{In}_2\text{O}_3$  to a less extent). [1] Nevertheless, the stronger Ga-O than In-O bonds thermodynamically leads to a favorable incorporation of Ga into the alloy  $(\text{In}_x\text{Ga}_{1-x})_2\text{O}_3$ . [2] The collaborative effect of these kinetics and thermodynamics is shown to lift the growth rate limitation of  $\text{Ga}_2\text{O}_3$  in the presence of an additional In-flux by metal-exchange catalysis. [3,4] Finally, the impact of the metal-to-oxygen flux ratio on the anisotropy of surface free energy is shown to control the formation of surface facets on both oxides. [4,5] [1] Vogt et al., *Phys. Rev. Mater.* 2, 120401(R) (2018). [2] Vogt et al., *APL Mater.* 4, 086112 (2016). [3] Vogt et al., *Phys. Rev. Lett.* 119, 196001 (2017). [4] Mazzolini et al., *APL Mater.* 7, 022511 (2019). [5] Bierwagen et al., *J. Phys.: Condens. Matter* 28, 224006 (2016).

### Invited Talk

DS 2.2 Mon 10:00 H34

**Is There a Perspective of p-type Doping in Gallium Oxide?** — •DAVID ROGERS<sup>1</sup>, FERECHEH TEHERANI<sup>1</sup>, PHILIPPE BOVE<sup>1</sup>, ERIC SANDANA<sup>1</sup>, RYAN McCLINTOCK<sup>2</sup>, and MANIJEH RAZEGHI<sup>2</sup> — <sup>1</sup>Nanovation, 8 Route de Chevreuse, 78117 Chateaufort, France — <sup>2</sup>Center for Quantum Devices, Department of Electrical Engineering and Computer Science, Northwestern University, Evanston, IL60208, US

Recently, there has been a surge in interest for the ultra wide bandgap semiconductor  $\text{Ga}_2\text{O}_3$ . Key drivers for this are that bulk  $\beta\text{-Ga}_2\text{O}_3$  wafers have become commercially available and that a variety of film growth methods have been shown to give n-type doping control. A major drawback associated with  $\text{Ga}_2\text{O}_3$ , however, has been lack of a method for fabricating p-type material. Indeed, it is generally proposed that p-type doping is unlikely to be obtained because of a combi-

nation of factors including the relatively low energy level of the valence band, the lack of an identified shallow acceptor, the relatively high effective masses of holes at the top of the valence band, the propensity for self-trapping of holes and the comparatively low formation energy of the oxygen vacancy donor (which favors compensation of acceptors). Recently, however, Chikoidze et al. [1] and Razeghi et al. [2] independently presented direct evidence of majority p-type conduction  $\text{Ga}_2\text{O}_3$ . The former concerned nominally undoped layers grown by PLD and the latter concerned Si doped layers grown by MOCVD. In this talk we will give an overview of these results. [1] Chikoidze et al. *Materials Today Physics* 3 (2017) [2] Razeghi et al., *Photonics West*, Feb (2018)

### Invited Talk

DS 2.3 Mon 10:30 H34

**Highly rectifying contacts on  $\text{Ga}_2\text{O}_3$ ,  $\text{In}_2\text{O}_3$  and  $(\text{In,Ga})_2\text{O}_3$  thin films** — •DANIEL SPLITH — Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, Germany

Oxide semiconductors like gallium oxide or indium oxide are promising materials for a new generation of transparent electronic devices. Additionally, alloying both materials allows band-gap engineering, enabling e.g. the fabrication of wave-length selective photodetectors. In order to realize devices like diodes, field-effect transistors and photodetectors, the fabrication of rectifying contacts is essential. Further, such contacts also enable the investigation of the materials by means of space charge region based methods like thermal admittance spectroscopy.

In this contribution the properties of Schottky contacts and pn-heterojunctions on heteroepitaxial  $\text{Ga}_2\text{O}_3$  and  $\text{In}_2\text{O}_3$  thin films grown by pulsed laser deposition are discussed. Additionally, the properties of such rectifying contacts on  $(\text{In,Ga})_2\text{O}_3$  thin films having a lateral composition gradient are presented. In order to improve the rectification of the contacts, different vertical layouts were investigated. Further, a comprehensive model, taking into account thermionic emission, thermionic field emission and charging currents as well as non-idealities like barrier height inhomogeneities, current spreading and variations of the net-doping density in growth direction, was employed in order to understand the measured characteristics.

### 15 min. break

### Invited Talk

DS 2.4 Mon 11:15 H34

**Understanding the impact of vibrations and defects on the optical properties of phosphors** — •P. ERHART<sup>1</sup>, C. LINDERÄLV<sup>1</sup>, D. ÅBERG<sup>2</sup>, Y.-C. LIN<sup>1</sup>, M. BETTINELLI<sup>3</sup>, N. C. GEORGE<sup>4</sup>, S. F.

PARKER<sup>5</sup>, and M. KARLSSON<sup>1</sup> — <sup>1</sup>Chalmers University of Technology, Sweden — <sup>2</sup>LLNL, USA — <sup>3</sup>University of Verona, Italy — <sup>4</sup>UCSB, USA — <sup>5</sup>ISIS Facility, UK

Activator ions such as Ce are used to control the luminescent properties of phosphors, which are core components in white-light-emitting diodes. Their optical signatures are temperature dependent as they are sensitive to changes in the local environment due to atomic vibrations. Using a combination of experiment and first-principles calculations, we have recently provided a complete phonon assignment for the oxide garnet  $Y_3Al_5O_{12}$  (YAG). An increase in temperature causes larger tetragonal distortion of the  $CeO_8$  moieties and an increase of the crystal-field splitting, which gives rise to a redshift of the emitted light. The lattice thermal expansion on the other hand reduces the tetragonality and induces a blue-shift. The non-linear shift of the color of the emitted light with increasing temperature can then be explained as a competition between these two processes. Thermal quenching of the emission due to non-radiative processes limits the efficiency of these devices. In this context, we have investigated the potential contribution of oxygen vacancies. It is found that these defects exhibit very strong and localized electron-phonon coupling, providing an efficient non-radiative recombination channel.

**Invited Talk** DS 2.5 Mon 11:45 H34  
**atomically resolved termination engineering of electronic states at oxide semiconductors** — ●YA-PING CHIU — Department of Physics, National Taiwan University, Taipei, Taiwan

Termination engineering at oxide semiconductors has become highly attractive for next-generation electronic and spintronic devices due to a delicate interplay of different correlated processes including orbital, charge, and magnetic ordering as well as lattice degrees of freedom at the interfaces. Therefore, to achieve a detailed physical understanding of such exotic phenomena at oxide interfaces becomes important. Only with such detailed high resolution experimental data, will it be possible to explore the relevance of the different physical models. In our studies, cross-sectional scanning tunneling microscopy and spectroscopy is employed to provide direct experimental insight into the origin and

the natural evolution of the electronic properties with atomic precision across the heterointerfaces. In this talk, topics to be discussed include ferromagnetic/superconducting and multiferroic/ferromagnetic heterointerfaces. This study highlights the importance of a direct atomically resolved access to electronic interface states, which is useful in understanding the intriguing interface properties in oxide semiconductors and providing a lot of insights for these communities. [1-3] Selected references: 1.\*ACS nano, 12 (2), 1089 (2018). 2. Phys. Rev. Lett., 109, 246807 (2012). 3. Adv. Mater., 23, 1530 (2011).

**Invited Talk** DS 2.6 Mon 12:15 H34  
**Nanoscale Control of Native Point Defects and Doping in Oxide Semiconductors** — ●LEONARD BRILLSON — The Ohio State University, Columbus, OH, USA

Nanoscale optical and electrostatic techniques can directly measure the movement of native point defects inside oxide semiconductors and how they control space charge regions, tunneling, and contact rectification. Depth-resolved cathodoluminescence spectroscopy (DRCLS) with hyperspectral imaging measures 3-dimensional defect redistribution on a nanoscale for ZnO, Ga<sub>2</sub>O<sub>3</sub>, SrTiO<sub>3</sub>, and BaSrTiO<sub>3</sub>, revealing how intrinsic and applied electric fields drive defect movement. Defects at metal-ZnO diodes change carrier densities, tunneling, and trap-assisted hopping, altering Zn- vs. O-polar Schottky barriers. Nanoscale 3D measurement and imaging reveal electrically-active defects that extend deep inside wires, altering depletion widths, conducting channel volumes, and metal-ZnO nano-contact rectification. Electron and ion beams alter defect distributions to create rectifying, ohmic, or blocking contacts with the same metal on the same nanowire, demonstrating the interplay between the nature of native point defects, the intrinsic doping, and the physical dimensions of the nanostructure itself in determining the electronic properties of the oxide interface. DRCLS also enabled us to correlate the dominant luminescence features of Ga<sub>2</sub>O<sub>3</sub> with the most thermodynamically stable O vacancy, Ga vacancy, and Ga vacancy-hydrogen defect states in the band gap predicted theoretically. As with ZnO, the combined depth-resolved detection and processing of Ga<sub>2</sub>O<sub>3</sub> suggests new avenues for defect and doping control.

## DS 3: Layer Properties: Electronic, Optical and Mechanical Properties

Time: Monday 9:30–12:45

Location: H39

DS 3.1 Mon 9:30 H39  
**Ab initio description of layered excitonic insulators** — ●MALTE RÖSNER<sup>1</sup>, GIACOMO MAZZA<sup>2</sup>, HANNES HÜBENER<sup>3</sup>, SIMONE LATINI<sup>3</sup>, UMBERTO DE GIOVANNI<sup>3</sup>, ANGEL RUBIO<sup>3</sup>, and ANTOINE GEORGES<sup>1</sup> — <sup>1</sup>Center for Computational Quantum Physics, Flatiron Institute - Simons Foundation, New York, USA — <sup>2</sup>Ecole polytechnique, CNRS, Université Paris Saclay, Paris, France — <sup>3</sup>Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Although proposed more than half a century ago hints for excitonic ground states have been found in just a few materials so far. Among them, the layered van der Waals material Ta<sub>2</sub>NiSe<sub>5</sub> is a prominent candidate for realizing such a ground state defined by spontaneous electron-hole pair condensation. Here, we show how the excitonic ground state can be described by means of ab initio calculations. From this we learn how this exotic condensate can be manipulated by its environment.

DS 3.2 Mon 9:45 H39  
**Effects of screening on the optoelectronic properties of 2D materials** — ●ABDERREZAK TORCHE, JENS HÜHNERT, and GABRIEL BESTER — University of Hamburg, Germany

2D materials represent nowadays a promising route for new technologies due to their exceptional optical and electronic properties. These properties are highly dependent on the surrounding environment, consequently, one can modify a desired property such as the band gap or the doping simply by changing the environment. Despite the fact that 2D materials have been studied since the discovery of graphene in 2004, both at the experimental and the theoretical levels, the understanding of the effects of screening (e.g. substrate effects) is still not complete although some general rules are well established.

From a theoretical point of view, the study of screening in 2D materials is computationally heavy. Standard approaches to study the

optical properties of materials, such as the BSE formalism, have several limitations because the inclusion of the environment hinders the calculation of quasi-particle energies in 2D.

The goal of our research is to go beyond these limitations and treat larger systems (i.e. thousands of atoms) which are more relevant from an experimental (and/or industrial) point of view. For that goal, we propose a hybrid approach combining density functional theory and configuration interaction methods to predict the binding energies of excitations in 2D materials (excitons, trions, ...) taking the effect of the environment into account via screening.

DS 3.3 Mon 10:00 H39  
**Interlayer excitons in stacked TMDC heterostructures** — ●ROLAND GILLEN and JANINA MAULTZSC — Department Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, 91054 Erlangen

We computed the theoretical bandstructures and absorption spectra of bilayer MoSe<sub>2</sub>-WSe<sub>2</sub> and MoS<sub>2</sub>-WSe<sub>2</sub> heterostructures with different stacking orders by solution of the excitonic Bethe-Salpeter equation with GW quasiparticle corrections [1] and inclusion of spin-orbit-coupling. We find two spin-orbit split Rydberg series of low oscillation strength below the absorption onset of the monolayer materials, which arise from spatially indirect excitations between the K points of the hexagonal Brillouin zones of the constituent materials with a binding energy on the order of 250-300 meV. Additionally, our calculations firmly establish that the fundamental band gap of MoSe<sub>2</sub>-WSe<sub>2</sub> heterostructures is indirect and has a distinct interlayer nature, possibly giving rise to a momentum- and spatially indirect contribution [2]. These results confirm the recent experimental observation of a doublet nature of the interlayer photoluminescence. We further show that the local stacking order leads to small variations in the hybridization between the MoSe<sub>2</sub> and WSe<sub>2</sub> bands and has a decisive effect on the polarization dependence of the interlayer excitonic absorption [2]. Our results motivate detailed studies of electron-phonon coupling effects

and exciton dynamics in TMDC heterostructures by time-resolved optical experiments and ab initio methods.

- [1] Gillen et al., IEEE JSTQE 23, 1 (2017); arXiv:1605.01972 (2016)  
 [2] Gillen et al., Phys. Rev. B 97, 165306 (2018)

DS 3.4 Mon 10:15 H39

**Flexible anode materials - 2D transition metal carbides** — ●DOMINIK LEGUT<sup>1</sup>, HANG ZHANG<sup>2</sup>, ZHONGHENG FU<sup>2</sup>, RUIFENG ZHANG<sup>2</sup>, QIANFAN ZHANG<sup>2</sup>, HONGZHEN TIAN<sup>2</sup>, TIMOTH C. GERMAN<sup>3</sup>, YUANQI GUO<sup>2</sup>, SHIYU DU<sup>4</sup>, and JOSEPH S. FRANCISCO<sup>5</sup> — <sup>1</sup>IT4Innovations, VSB-TU Ostrava, Ostrava, Czech Republic — <sup>2</sup>School of Mat. Sci. and Eng., Beihang University, Beijing, China — <sup>3</sup>Theor. Div., Los Alamos National Laboratory, USA — <sup>4</sup>Eng. Lab. and Nucl. Ene. Mater., Chinese Acad. Sciences, Zhejiang 31520, China — <sup>5</sup>Dep. of Chem., Purdue University, USA

MXenes exhibit outstanding properties and therefore been considered as promising electrode material candidates. Taking 2D transition metal carbides (TMCs) as representatives, we systematically explored several influencing factors, including transition metal species, layer thickness, functional group, and strain on their mechanical properties (e.g., stiffness) and their electrochemical properties (e.g., ionic mobility). Considering potential charge-transfer polarization, we employed a charged electrode model to simulate ionic mobility and found that ionic mobility has a unique dependence on the surface atomic configuration influenced by bond length, valence electron number, functional groups, and strain. Under multiaxial loadings, electrical conductivity, high ionic mobility, low equilibrium voltage with good stability, excellent flexibility, and high theoretical capacity indicate that the bare 2D TMCs have potential to be ideal flexible anode materials, whereas the surface functionalization degrades the transport mobility and increases the voltage due to bonding between the nonmetals and Li.

DS 3.5 Mon 10:30 H39

**Photo-induced anomalous Hall effect in the type-II Weyl-semimetal WTe<sub>2</sub> at room-temperature** — PAUL SEIFERT<sup>1</sup>, FLORIAN SIGGER<sup>1,2</sup>, JONAS KIEMLE<sup>1</sup>, KENJI WATANABE<sup>3</sup>, TAKASHI TANIGUCHI<sup>3</sup>, CHRISTOPH KASTL<sup>4</sup>, ●PHILIPP BOOTZ<sup>1</sup>, URSULA WURSTBAUER<sup>1,2</sup>, and ALEXANDER HOLLEITNER<sup>1,2</sup> — <sup>1</sup>Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — <sup>2</sup>Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 München, Germany — <sup>3</sup>Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan — <sup>4</sup>Molecular Foundry, Lawrence Berkeley National Laboratory, One Cyclotron Road, 94720 Berkeley, California, United States

Using Hall photovoltage measurements, we demonstrate that an anomalous Hall (AH) voltage can be induced in few layer WTe<sub>2</sub> under circularly polarized light illumination. By applying a bias voltage along different crystal axes, we find that the photo-induced AH conductivity coincides with a particular crystal axis. Our results are consistent with the underlying Berry-curvature exhibiting a dipolar distribution due to the breaking of crystal inversion symmetry. We find that the decay time of the AH voltage exceeds the electron-phonon scattering time by orders of magnitude but is consistent with the comparatively long spin-lifetime of carriers in the momentum-indirect electron and hole pockets in WTe<sub>2</sub>. Our observation suggests, that a helical modulation of an otherwise isotropic spin-current is the underlying mechanism of the AHE.

DS 3.6 Mon 10:45 H39

**Local and correlated studies of humidity-mediated ferroelectric thin film surface charge dynamics** — ●IAROSLAV GAPONENKO<sup>1</sup>, NEUS DOMINGO<sup>2</sup>, NICOLAS STUCKI<sup>3</sup>, ALBERT VERDAGUER<sup>2</sup>, and PATRYCJA PARUCH<sup>1</sup> — <sup>1</sup>DQMP, University of Geneva, 1211 Geneva, Switzerland — <sup>2</sup>ICN2, Campus UAB, 08193 Bellaterra, Spain — <sup>3</sup>HES-SO/hepia, 1213 Geneva, Switzerland

Surface water is present on all materials exposed to ambient environmental conditions, modifying the ground state in fundamental studies as well as affecting the operation of bare-chip devices. Due to its polar nature, water strongly interacts with domains and domain walls in ferroelectric materials.

Here, we present a combined Kelvin probe force microscopy (KPFM) and near-ambient pressure x-ray photoelectron spectroscopy (AP-XPS) study of the relative humidity (RH) dependence of the formation and evolution of surface charges on oppositely polarised PZT thin films. AP-XPS measurements show chemical differences on surface adsorbates as well as significant changes in the bulk ionic distribu-

tion as a function of both the as-grown polarisation state and after switching. KPFM measurements tracking the dissipation of surface charges confirm that both the initial state of the samples and their switching history have an influence on the electrochemistry and surface charge dynamics as a function of RH. Through these two approaches, we demonstrate the complexity of surface water mediated chemistry and electrochemistry on ferroelectric materials.

15 min. break

DS 3.7 Mon 11:15 H39

**Impedance spectroscopy at tunnel junctions with adjacent solid-state electrolyte layer** — RICHARD MARQUARDT<sup>1</sup>, ●JÜRGEN CARSTENSEN<sup>2</sup>, GEORGE POPKIROV<sup>3</sup>, FINN ZAHARI<sup>1</sup>, HERMANN KOHLSTEDT<sup>1</sup>, and MARTIN ZIEGLER<sup>4</sup> — <sup>1</sup>Chair of Nanoelectronics, Faculty of Engineering, Kiel University, Germany — <sup>2</sup>Chair of Functional Nanomaterials, Faculty of Engineering, Kiel University, Germany — <sup>3</sup>Central Laboratory of Solar Energy and New Energy Sources, Bulgarian Academy of Sciences, Bulgarian — <sup>4</sup>Micro- and Nanoelectronic Systems, Electrical Engineering and Information Technology, Ilmenau University of Technology, Germany

Memristive devices for neuromorphic networks and non-volatile memories are getting a rapidly increased amount of attention in the last couple of years for neuromorphic applications, one promising candidate is the double barrier Nb/Al/Al<sub>2</sub>O<sub>3</sub>/NbOx/Au memristive device. Recent studies showed evidence, that the memristive character is based on a filamentary-free, homogenous interfacial switching mechanism. Here, mobile oxygen ions confined within the 2.5 nm thin NbOx layer alter the Schottky barrier of the top NbOx/Au interface. Therefore lead to the resistance change in the order of two magnitudes at 0.7V together with a change in the threshold voltage by a factor of five. In order to proof this model Impedance spectroscopy was applied to correlate the inner electronic and ionic process with the observed I-V characteristics. Evidence has been found that the Schottky interface is the active interface, which is responsive for the resistive switching of the device. The Al<sub>2</sub>O<sub>3</sub> tunneling barrier is modeled as a linear resistance.

DS 3.8 Mon 11:30 H39

**Binding mechanism of fluorine-containing ketones on zinc oxide surfaces for thin film transistor passivation** — ●JONAS KÖHLING, NATALIYA KALINOVICH, GERD-VOLKER RÖSCHENTHALER, and VEIT WAGNER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Solution processed metal-oxide thin film transistors are used in optical, mechanical and electrical applications. Oxygen and moisture induced surface traps cause instability and unreliability under electrical operation. For application purposes it is necessary to passivate surface traps. Tailored organic molecules can be effectively used for this task. For optimal functionality trap mechanisms and binding properties of these organic molecules have to be investigated.

In this work, the binding of fluorine-containing organic molecules on zinc oxide surfaces is monitored and the effect on electrical performance in thin film transistors was studied. Zinc oxide thin film transistors (12 nm thickness) were fabricated by aqueous spray pyrolysis. In order to overcome their instability against oxygen and moisture tailored organic fluorine-containing molecules with ketone groups as anchors sites were employed as passivation. Chemical binding of the molecules to hydroxide groups at the surface of zinc oxide is tracked by XPS and UV-Vis. The exact binding situation is elucidated by NMR. After passivation of the zinc oxide surface transistors exhibit almost vanished hysteresis, increased mobility and much better stability against electrical bias stress. Electrical results were correlated with the effective charge of the anchor atoms calculated by density functional theory.

DS 3.9 Mon 11:45 H39

**Visualization of Engineered Catalytic Hydrogen Evolution Sites on Molybdenum Dichalcogenides under Reaction Conditions** — ●BEATRICE SALA<sup>2</sup>, ELMAR MITTERREITER<sup>1,2</sup>, YUNCHANG LIANG<sup>3</sup>, MATTHIAS GOLIBRZUCH<sup>2</sup>, DAVID MCLAUGHLIN<sup>3</sup>, CHRISTOPH CSOKLICH<sup>3</sup>, ALEXANDER HOLLEITNER<sup>1,2</sup>, URSULA WURSTBAUER<sup>1,2</sup>, and ALLAKSANDR S. BANDARENKA<sup>1,3,4</sup> — <sup>1</sup>Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 München, Germany — <sup>2</sup>Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching, Germany — <sup>3</sup>Physik-Department ECS, Technische Universität München, James-Frank-Str. 1, 85748 Garching, Germany — <sup>4</sup>Catalysis Research Cen-



ter TUM, Ernst-Otto-Fischer-Straße 1, 85748 Garching, Germany

2D transition metal dichalcogenides are abundant and cost effective (co-)catalysts with tunable physical properties. In this respect, these materials are suitable for reactions related to energy provision, for instance hydrogen evolution reaction (HER). It is vital to understand which surface sites are highly active to improve the catalytic behavior of those materials. Here, we visualize catalytically active sites at the surface of molybdenum disulfide (MoS<sub>2</sub>) with lateral resolution on the nanometer scale by means of electrochemical STM. The edges of single MoS<sub>2</sub> flakes show high catalytic activity, whereas their surfaces are inactive. Furthermore, we demonstrate that the inert basal plane of these materials can be activated towards the HER with the focused beam of a helium ion microscope. Thus, we show the possibility to generate active sites with a spatial resolution below a few nanometer.

DS 3.10 Mon 12:00 H39

**High throughput investigation on the magnetic and electronic properties of out-of-plane ordered MXene** — ●XINRU LI and HONGBIN ZHANG — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

Two-dimensional (2D) MXene systems which can be obtained by etching MAX phases are considered as a breakthrough in synthesizing 2D functional materials. In this work, based on our previous high throughput screening of 14 Al-based MAXs out of 1080 MAX systems, we investigated 80 corresponding MXenes with ordered out-of-plane TM substitutions (o-MXene) in an extensive way. The magnetic ground states were determined by considering ferromagnetic (FM), one collinear antiferromagnetic (cAFM), and one noncollinear antiferromagnetic (nocAFM) orderings. It is observed that 25 out of 41 cases are with the FM ground states, 9 out of 41 cases are cAFM, while the rest are with intriguing nocAFM configurations. Furthermore, for the nocAFM o-MXenes, it is observed that the in-plane magnetization direction can induce significant changes on the electronic properties.

DS 3.11 Mon 12:15 H39

**Designing multifunctional i-MXene** — ●QIANG GAO, XINRU LI,

and HONGBIN ZHANG — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

MXene which can be obtained by etching the bulk MAX phase has attracted intensive attention, as a class of two-dimensional (2D) materials for potential applications as electrode materials, thermoelectric materials, and topological insulators.[1] Recently, the in-plane ordered MAX (i-MAX) compounds (Cr<sub>2/3</sub>M<sub>1/3</sub>)<sub>2</sub>AlC (M = Sc and Y), (V<sub>2/3</sub>Zr<sub>1/3</sub>)<sub>2</sub>AlC, and (Mo<sub>2/3</sub>Y<sub>1/3</sub>)<sub>2</sub>AlC have been reported.[2,3] Motivated by this, we have performed high-throughput screening for novel i-MXene (as derived from the i-MAX phase) systems, focusing particularly on the transport properties of magnetic cases. It is observed that systems with intriguing properties can be realized, such as 2D spin-gapless semiconductors, topological insulators, and candidates for thermoelectric applications. [1] G.R. Bhimanapati, *et al.*, ACS Nano **9**, 11509 (2015). [2] J. Lu, A. Thore, R. Meshkian, Q. Tao, L. Hultman, and J. Rosen, Crystal Growth & Design **17**, 5704 (2017). [3] M. Dahlqvist, J. Lu, R. Meshkian, Q. Tao, L. Hultman, and J. Rosen, Sci. Adv. **3**, e1700642 (2017).

DS 3.12 Mon 12:30 H39

**Superconductivity above 28 K in single unit cell FeSe films interfaced with GaO<sub>2-δ</sub> layer on NdGaO<sub>3</sub>(110)** — ●LILI WANG — Tsinghua University, Beijing, China

We prepared single unit cell FeSe films on GaO<sub>2-δ</sub> terminated perovskite NdGaO<sub>3</sub>(110) substrates and performed ex situ transport and scanning transmission electron microscopy measurements under protection of FeTe films. Our experimental measurements showed that the single unit cell FeSe films interfaced with GaO<sub>2-δ</sub> layer get electron doped with interface charge transfer. Most importantly, this kind of heterostructure exhibits a superconducting transition with onset temperature of ~28 K, significantly enhanced compared to the value of 8 K for bulk FeSe. Our work indicates that FeSe/GaO<sub>2-δ</sub> is another hetero-structure, after FeSe/TiO<sub>2-δ</sub>, that hosts interface enhanced superconductivity, providing a new platform for investigating the mechanism of interface high temperature superconductivity.

## DS 4: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge I (joint session O/TT/ CPP/DS)

First-principles electronic structure calculations have become an indispensable tool in many research areas where materials surfaces or interfaces play a central role. Corresponding calculations provide insight into catalytic mechanisms, interfacial ionic and charge transport in batteries or solar cells, materials degradation through corrosion or wear, and many other highly relevant application areas. Despite this prolific use, corresponding calculations face multiple issues. While the invited lectures will have a focus on this interface challenge, the symposium will also cover the general field of computational materials science and electronic-structure theory.

Organizers: Jens Nørskov (Technical University of Denmark), Karsten Reuter (Technical University Munich), and Matthias Scheffler (Fritz Haber Institute of the Max Planck Society, Berlin)

Time: Monday 10:30–13:00

Location: H9

### Topical Talk

DS 4.1 Mon 10:30 H9

**Scaling relations and beyond for kinetic Monte Carlo models in heterogeneous catalysis** — ●MIE ANDERSEN — Theoretical Chemistry, Technische Universität München, Germany

Heterogeneous catalysis typically operates at the interface between a gas or liquid and a solid catalytic material. In my talk, I will discuss mean-field and kinetic Monte Carlo models for the operating catalyst. These often rely on input data calculated using either first principles or more approximate methods, e.g. scaling relations, which use only selected adsorption energies as descriptors for the catalyst function [1,2]. I will also discuss recent work [3] where we used compressed sensing methods to identify new low-cost and accurate descriptors that allow to predict adsorption energies for a wide range of adsorbates, multi-metallic transition metal surfaces and facets. The descriptors are expressed as non-linear functions of intrinsic properties of the clean catalyst surface, e.g. coordination numbers and *d*-band moments. From a single DFT calculation of these properties, we predict adsorption energies at all potential surface sites, and thereby also the most stable geometry. Compared to previous approaches such as scaling relations, we find our approach to be both more general and more accurate for

the prediction of adsorption energies on alloys with mixed-metal surfaces, already when based on training data including only pure metals.

[1] M. Andersen *et al.*, Ang. Chem. Int. Ed. **55**, 5210 (2016)

[2] M. Andersen *et al.*, J. Chem. Phys. **147**, 152705 (2017)

[3] M. Andersen *et al.*, submitted

DS 4.2 Mon 11:00 H9

**The Teacher and the Student: Exchange-Correlation Energy Densities from Quantum Chemistry and Machine-Learning** — ●JOHANNES T. MARGRAF, CHRISTIAN KUNKEL, and KARSTEN REUTER — Chair for Theoretical Chemistry, Technische Universität München, Germany

(Semi-)local density functional approximations (DFAs) are the workhorse electronic structure methods in condensed matter theory and surface science. Central to defining such DFAs is the exchange-correlation energy density  $\epsilon_{xc}$ , a spatial function that yields the exchange-correlation energy  $E_{xc}$  upon integration.

Unlike  $E_{xc}$ ,  $\epsilon_{xc}$  is not uniquely defined. Indeed, there are infinitely many functions that integrate to the correct  $E_{xc}$  for a given electron density  $\rho$ . The challenge for constructing a useful DFA is to find a

systematic connection between  $\rho$  and  $\epsilon_{xc}$ . While several empirical and rigorous approaches to this problem are known, there has been little innovation with respect to the fundamental functional forms of DFAs in recent years.

Herein, we discuss two less explored routes to constructing DFAs. Specifically, a recipe for deriving  $\epsilon_{xc}$  directly from many-body wavefunctions is compared to a machine learning (ML) approach that infers the optimal  $\epsilon_{xc}$  for a given functional form. We find that local DFAs based on the many-body  $\epsilon_{xc}$  are not transferrable between systems because the underlying energy densities are inherently non-local. In contrast, the ML  $\epsilon_{xc}$  is by construction as local as possible. The extension of both approaches to non-local DFAs will be discussed.

DS 4.3 Mon 11:15 H9

**Self-Interaction Corrected SCAN for Molecules and Solids: All-Electron Implementation with Numerical Atom-Centered Basis Functions** — •SHENG BI, IGOR YING ZHANG, CHRISTIAN CARBOGNO, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Electronic self-interaction is the most severe cause of inaccuracies in all semilocal density-functional approximations (DFAs), including the promising meta-GGA “strongly constrained and appropriately normed” (SCAN) functional [1]. This error can be alleviated via localized orbital scaling corrections [2] or via self-interaction corrections (SIC) based on Fermi-orbitals [3]. In this contribution, we follow the latter concept which involves solving a set of SIC constraints. Here, we present an all-electron implementation of the self-consistent SIC for semilocal DFAs, including SCAN. We first validate our implementation by inspecting certain properties (HOMO and dissociation energies) for a molecular test set, showing that SIC improves SCAN calculations. Furthermore, we compare the performance of SCAN-SIC and SCAN $\alpha$ , i.e., SCAN with a fraction of exact exchange, in predicting the broken symmetry in pentacene – note that standard semilocal DFAs always favor symmetric solutions. Eventually, we discuss the extension of our SIC approach to periodic solids.

[1] J. Sun *et al.*, *Phys. Rev. Lett.* **115**, 036402 (2015).

[2] N. Q. Su *et al.*, *Proc. Natl. Acad. Sci.* **115**, 9678 (2018).

[3] Z. Yan *et al.*, *Phys. Rev. A* **95**, 052505 (2017).

DS 4.4 Mon 11:30 H9

**Progress in Fermi-Löwdin orbital self-interaction correction to DFT** — •TORSTEN HAHN, SEBASTIAN SCHWALBE, and JENS KORTJUS — Institute for Theoretical Physics, Freiberg, Germany

The accuracy of density functional theory (DFT) calculations is limited by the so called self-interaction error [1]. The recently proposed Fermi-Löwdin orbital based method [2,3,4] for self-interaction correction (FLO-SIC) is a unitary invariant and size extensive approach to overcome this error. We present the current state of the method and discuss selected applications. In addition we discuss strategies to improve the thermochemical and numerical performance of the FLO-SIC approach in combination with state-of-the-art exchange-correlation functionals.

[1] J. P. Perdew, A. Zunger, *Phys. Rev. B* **23**, 5048 (1981)

[2] M. R. Pederson *et al.*, *J. Chem. Phys.*, vol. 140, 121103 (2014)

[3] M. R. Pederson, *J. Chem. Phys.*, vol. 142, 064112 (2015)

[4] S. Schwalbe *et al.*, *J. Comp. Chem.*, vol. 39, 2463 (2018).

DS 4.5 Mon 11:45 H9

**Time evolution of the natural occupation numbers** — •CARLOS BENAVIDES-RIVEROS and MIGUEL A. L. MARQUES — Martin-Luther Universität Halle Wittenberg

Reduced density matrix functional theory (RDMFT) is based on the Gilbert theorem, which asserts that the ground-state wave function can be written as a functional of the one-body reduced density matrix. Since RDMFT accounts for fractional natural occupation numbers, it captures quite well static (strong) electron correlation (unlike DFT, RDMFT correctly predicts the insulating behavior of Mott-type insulators). Yet the time-dependent extension of RDMFT suffers from various shortcomings. Chief among them, the current status of the theory does not allow the fermionic occupation numbers to evolve in time. It is known that this deficiency is connected to the failure of RDMFT to account for relative phases at the level of the two-body reduced density matrix. Based on recent results on fermionic exchange symmetry, we propose a new equation for the time evolution of the fermionic occupation numbers.

DS 4.6 Mon 12:00 H9

**Nonempirical hybrid functionals constructed through adjustable potential probes for band gap predictions of extended systems** — •THOMAS BISCHOFF, IGOR RESHETNYAK, and ALFREDO PASQUARELLO — Chaire de Simulation à l’Echelle Atomique (CSEA), Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

We describe a nonempirical procedure for achieving accurate band gaps of extended systems through the insertion of suitably defined potential probes. By enforcing Koopmans’ condition on the resulting localized electronic states, we determine the optimal fraction of Fock exchange to be used in the adopted hybrid functional. As potential probes, we consider native defects, the extrinsic hydrogen impurity, and various adjustable potentials that allow us to vary the energy level of the localized state in the band gap and its degree of localization. By monitoring the delocalized screening charge, we achieve a measure of the hybridization with the band states, which can be used to improve the band gap estimate. Application of this methodology to AlP, C and MgO yields band gaps differing by less than 0.2 eV from experiment.

DS 4.7 Mon 12:15 H9

**Quantum-mechanical relation between atomic dipole polarizability and van der Waals radius** — •DMITRY FEDOROV, MAINAK SADHUKHAN, MARTIN STÖHR, and ALEXANDRE TKATCHENKO — University of Luxembourg, Luxembourg, Luxembourg

The atomic dipole polarizability  $\alpha$  and the van der Waals (vdW) radius  $R_{vdW}$  are two key quantities to describe the ubiquitous vdW forces important for the structure and dynamics of molecules and materials [1]. The commonly assumed relation between them,  $R_{vdW} \propto \alpha^{1/3}$ , is based on a classical picture of hard-sphere atoms. Employing the quantum Drude oscillator model [2], we reveal [3] the quantum-mechanical relation  $R_{vdW} = const. \times \alpha^{1/7}$  which is markedly different from its classical counterpart. Based on the accessible accurate reference data for  $\alpha$  and  $R_{vdW}$ , we demonstrate that the obtained formula can be used as a unified definition of the vdW radius solely in terms of the atomic polarizability for all chemical elements. Moreover, for vdW-bonded heteronuclear dimers consisting of atoms A and B, the simple combination rule  $\alpha = (\alpha_A + \alpha_B)/2$  provides a remarkably accurate way to calculate their equilibrium interatomic distance. These findings unveil a fundamental relationship between the geometric and electronic properties of atoms. From a practical point of view, they allow us to reduce the empiricism and improve the efficiency of computational models for vdW interactions.

[1] Hermann *et al.*, *Chem. Rev.* **117**, 4714 (2017)

[2] Jones *et al.*, *Phys. Rev. B* **87**, 144103 (2013)

[3] Fedorov *et al.*, *Phys. Rev. Lett.* **121**, 183401 (2018)

DS 4.8 Mon 12:30 H9

**impact of continuum electronic states on van der Waals dispersion interactions** — •MOHAMMAD REZA KARIMPOUR, DMITRY FEDOROV, and ALEXANDRE TKATCHENKO — University of Luxembourg, Luxembourg, Luxembourg

The ubiquitous van der Waals (vdW) forces play an important role for structure, stability, and dynamics of molecules and materials. Their description on atomistic level is important for molecular physics, crystal chemistry, surface science, structural biology, and pharmacy. To this end, the development of simple yet efficient models is of high importance. Normally, such models focus only on fluctuations to bound electron states, described via quantum harmonic oscillator potentials. However, the polarizability of real atomic and molecular systems has important contributions also from fluctuations to continuum states. To study their influence on the vdW dispersion interactions from a general point of view, here we consider models based on the Dirac delta-function potentials. In one-dimensional case, such a potential provides just one bound state whereas all excited states belong to the continuum electron spectrum. We apply both the atomistic method and the scattering picture representing the van der Waals and Casimir approaches for dispersion interactions, respectively. In the atomistic framework we compare our results to the ones of the quantum oscillator models. Within the other picture, we discuss an obtained new scaling law in comparison to the results known for excited atomic systems.

[1] Woods *et al.*, *Rev. Mod. Phys.* **88**, 045003 (2016)

[2] Hermann *et al.*, *Chem. Rev.* **117**, 4714 (2017)

DS 4.9 Mon 12:45 H9

**Relation between the van der Waals radius and higher-order atomic polarizabilities** — •ORNELLA VACCARELLI, DMITRY FEDOROV, and ALEXANDRE TKATCHENKO — University of Luxembourg,

Luxembourg, Luxembourg

The atomic polarizabilities and van der Waals (vdW) radii describe the electronic and geometric aspects of the ubiquitous vdW interactions [1, 2], respectively. Normally, these quantities are assumed to be independent. Therefore, they are determined separately from each other. Based on the quantum Drude oscillator model [3], recently we revealed [4] a remarkable direct relationship between the vdW radius and the dipole polarizability. This provides a unified determination of the vdW radius for all chemical elements solely in terms of their dipole polarizabilities. In addition, further relations between the vdW radius  $R_{\text{vdW}}$  and higher-order atomic polarizabilities  $\alpha_n$  ( $n = 1, 2, \dots$ ) were

found empirically. Here, we present a physical background for these results. The derivation of the corresponding scaling laws is performed by going beyond the dipole approximation for the Coulomb interaction to obtain higher-order contributions to attractive and repulsive forces acting on atoms in a vdW-bonded homonuclear dimer. We focus on the derivation of the proportionality constants  $C_n$  in the general relation  $R_{\text{vdW}}(\alpha_n) = C_n \alpha_n^{2/7(n+1)}$  unveiling their quantum nature.

- [1] Woods *et al.*, Rev. Mod. Phys. **88**, 045003 (2016)
- [2] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)
- [3] Jones *et al.*, Phys. Rev. B **87**, 144103 (2013)
- [4] Fedorov *et al.*, Phys. Rev. Lett. **121**, 183401 (2018)

## DS 5: Prize talk Selina Olthof (joint session PRV/DS/VA)

Time: Monday 12:30–13:00

Location: H32

### Prize Talk

DS 5.1 Mon 12:30 H32

**Absolute energy levels and interface energetics of halide perovskites** — ●SELINA OLTHOF — Institute of Physical Chemistry, University of Cologne, Luxemburger Strasse 116, 50939 Cologne, Germany — Laureate of the Gaede-Prize 2019

In recent years, the interest in halide perovskites rose at a rapid pace due to their tremendous success in the field of photovoltaics; but other fields, like light emitting diodes, show great potential as well. In such devices, the function and performance depend on the proper alignment of energy levels throughout the device, i.e. allowing for efficient charge transport across the various interfaces. Here, an advantage of these novel semiconductors is that the electronic structure and band gap can be readily tuned by changing the compositions of the perovskite.

In this talk, I will discuss recent findings regarding the variations in electronic structure of halide perovskites measured by a combination of UV-, inverse, and x-ray photoelectron spectroscopy (PES); in this extensive study, we cover all primary lead and tin based halide systems. Combining these results with DFT calculations and a tight binding model we are able to consistently describe variations found in the electronic structure. However, not only the absolute energy levels of these materials are of interest, but also their alignment to adjacent transport layers, as interface dipoles and band bending can significantly alter the electronic landscape within a device. We also performed interface resolved PES studies on the MAPbI<sub>3</sub> system. Comparing various bottom contacts we can show that chemical interactions, band bending, and interface dipole formation indeed play an important role in these perovskite systems.

## DS 6: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge II (joint session O/TT/DS/CPP)

Time: Monday 15:00–17:30

Location: H9

DS 6.1 Mon 15:00 H9

**Influence of structural deformations on the applicability of the Tamm-Dancoff approximation for organic molecules** — ●TOBIAS LETTMANN and MICHAEL ROHLFING — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

When calculating excited state properties of electronic systems within the many-body perturbation theory (MBPT), the Bethe-Salpeter equation (BSE) needs to be solved. This is often done within the Tamm-Dancoff approximation (TDA), neglecting the coupling of resonant and anti-resonant excitations.

It is generally accepted that the TDA is justified for large, extended systems e.g. bulk crystals. However it has been shown that the TDA may no longer hold for small organic molecules [1]. In this talk we discuss the applicability of the TDA for molecules of different sizes and show the transition between the two regimes. We then discuss how the applicability is influenced by deformations of the molecules, in particular by the related conjugation length of the  $\pi$ -system.

- [1] B. Baumeier *et al.*, J. Chem. Theory Comput. **8**, 997 (2012)

DS 6.2 Mon 15:15 H9

**Momentum-Resolved Electron Energy-Loss Spectroscopy in Oxides from Many-Body Perturbation Theory** — ●CHRISTIAN VORWERK<sup>1,2</sup>, CATERINA COCCHI<sup>1,2</sup>, and CLAUDIA DRAXL<sup>1,2</sup> — <sup>1</sup>Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — <sup>2</sup>European Theoretical Spectroscopy Facility

Electron energy-loss spectroscopy (EELS) is a powerful tool to investigate the local electronic and structural properties of crystalline materials. The accurate determination of these spectra from first principles requires a reliable description of the electron-hole interaction, screened by the surrounding many-electron system. We perform *ab initio* many-body perturbation theory calculations of EELS through the solution of the Bethe-Salpeter equation (BSE), including the screened non-local interaction between electron and hole. Employing an implementation in the all-electron full-potential package **exciting**, we show results for a wide range of energy loss, from the optical to the hard x-ray region.

We study EELS at finite momentum loss  $\mathbf{q}$ , from small  $\mathbf{q}$  close to the dipole limit to large  $\mathbf{q}$  well beyond the first Brillouin zone. This momentum resolution of EELS reveals dipole-forbidden excitations that are invisible in absorption spectroscopy. Our calculations also yield insight into the excitonic dispersion, *i.e.* the excitonic bandstructure. We discuss the effects of momentum loss in the EELS spectra of oxide materials, including CaO, CeO<sub>2</sub>, and the wide-gap transparent oxide Ga<sub>2</sub>O<sub>3</sub>, considering both the optical and x-ray energy-loss range.

DS 6.3 Mon 15:30 H9

**Electron-magnon scattering in elementary ferromagnets from first principles: implementation and results** — ●CHRISTOPH FRIEDRICH, MATHIAS C.T.D. MÜLLER, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute of Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Propagating electrons and holes can scatter with spin fluctuations and form quasiparticles as a result or more complex many-body states. To calculate this effect, a  $\mathbf{k}$ -dependent self-energy describing the scattering of electrons and magnons is constructed from the solution of a Bethe-Salpeter equation for the  $T$  matrix. Partial self-consistency is achieved by the alignment of the chemical potentials. We discuss details of the implementation and illustrative results. The renormalized electronic band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy, which are strongest in Fe. The renormalization gives rise to a band anomaly at large binding energies in iron, which results from a coupling of the quasihole with Stoner excitations.

DS 6.4 Mon 15:45 H9

**Dielectric function of homogeneous electron gas from Bethe-Salpeter equation** — ●JAAKKO KOSKELO<sup>1,2</sup>, MARTIN PANHOLZER<sup>2,3</sup>, LUCIA REINING<sup>1,2</sup>, and MATTEO GATTI<sup>1,2,4</sup> — <sup>1</sup>Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA, Université Paris-Saclay, F-91128 Palaiseau, France — <sup>2</sup>ETSF — <sup>3</sup>Institute for Theoretical Physics, Johannes Kepler University, Linz, Austria — <sup>4</sup>Synchrotron SOLEIL, France

The homogeneous electron gas (HEG) is one of the most important

model systems in condensed matter physics, and it has been subject of a great number of studies. Some properties of HEG such as total energy and static correlation functions can be obtained from quantum Monte Carlo simulations with great accuracy, but for dynamical correlation functions only very few results are available.

Methods based on the Bethe-Salpeter equation (BSE) have been very successful in semiconductors and insulators, but metals have been less studied. In this contribution, we use the BSE in its standard approximations, including a statically screened electron-hole interaction, to study the dielectric function of HEG. We find significant differences in static screening and spectra compared to other approaches. In particular, the BSE in its current approximations fails to reproduce the negative static screening in the low-density HEG, which is related to a so-called ghost exciton. We also use the time-dependent mean-density approximation [1] in order to compare our results to experimental loss spectra of sodium.

[1] M. Panholzer et al, Phys. Rev. Lett. **120**, 166402 (2018).

DS 6.5 Mon 16:00 H9

**DFT study of electronic and optical properties of SrTiO<sub>3-δ</sub> including many-body effects** — ●VIJAYA BEGUM, MARKUS E GRUNER, and ROSSITZA PENTCHEVA — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg.

The electronic and optical properties of SrTiO<sub>3</sub> (STO), a perovskite material of key importance in the field of oxide electronics, are explored in the framework of density functional theory including many-body effects within the GW approximation and excitonic corrections by solving the Bethe-Salpeter equation (BSE). We further analyse the origin of the strong excitonic effects, in particular a peak at  $\approx 6.5$  eV, by decomposing the BSE eigenvectors obtained from GW+BSE to extract the leading electron-hole pair contribution for the particular BSE eigenstate following the approach of Bokdam *et al.* [Scientific Reports **6**, 28618 (2016)]. Alternatively, we use the model-BSE (mBSE) which utilises a parametrised analytical model for the static screening. For STO, the mBSE spectrum closely reproduces the one from GW+BSE, which allows to reduce the computational effort by circumventing the intermediate time-consuming GW step. We further proceed to describe the effect of oxygen defects on the electronic and optical properties in STO.

Funding by DFG- SFB1242, project C02 is gratefully acknowledged.

DS 6.6 Mon 16:15 H9

**Second-order Møller-Plesset perturbation theory and beyond for the band gap and single-particle excitations of solids** — ●MARIA DRAGOMI<sup>1</sup>, SERGEY V. LEVCHENKO<sup>2,1,3</sup>, IGOR YING ZHANG<sup>4,1</sup>, and MATTHIAS SCHEFFLER<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, DE — <sup>2</sup>Skolkovo Innovation Center, Moscow, RU — <sup>3</sup>NUST MISIS, Moscow, RU — <sup>4</sup>Fudan University, Shanghai, CN

Calculations of the fundamental band-gap and the low-energy excitations of solids are still a challenge for electronic-structure theory. The computationally efficient Kohn-Sham (KS) density functional theory (DFT) with the widely used local or semi-local approximations provides a KS band gap which is much smaller than the fundamental gap. Many-body perturbation theory, on the other hand, addresses the fundamental gap directly. We present here an efficient scalable implementation of Møller-Plesset second order perturbation theory (MP2) for quasi-particle energies [1,2]. By solving the Dyson equation of the single-particle Green's function, considering self-energy up to second order, we go beyond MP2. The new approach shows a competitive or even superior performance in comparison to the current state-of-the-art methods such as hybrid functionals and GW approximation, where second order exchange is missing. We present numerical results for the band-gap of a wide range of semiconductors and insulators.

[1] J. Sun and R. J. Bartlett, J. Chem. Phys. **104**, 8553 (1996).

[2] A. Grüneis, et.al, J. Chem. Phys. **133**, 074107 (2010).

DS 6.7 Mon 16:30 H9

**Accelerating GW Calculations within the LAPW Framework** — ●SVEN LUBECK, ANDRIS GULANS, and CLAUDIA DRAXL — Humboldt-Universität zu Berlin, Germany

The GW approach of many-body perturbation theory is an indispensable method for calculating the electronic band structure of solids. Its implementation in computer programs using the linearized augmented plane-wave + local orbital (LAPW+LO) method allows for obtaining numerically precise results. Unfortunately, high precision comes at

the price of a large number of LAPWs and LOs. In this work, we accelerate GW calculations by optimizing the use of LAPWs and LOs in the computer package **exciting** [1]. On the one hand, we introduce a systematic way of obtaining a minimal set of LOs. On the other hand, we perform a basis transformation from the plane-wave part of the LAPWs to different types of basis functions, exploring the efficiency of numeric atom-centered orbitals, Gaussian type orbitals, and Kohn-Sham orbitals. Presenting band gaps of two exemplary materials, zincblende ZnO and hexagonal monolayer BN, we illustrate that our optimization schemes reduce the computational cost down to values as low as 15% without compromising the precision.

[1] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, and C. Draxl, J. Phys.: Condens. Matter **26**, 363202 (2014).

DS 6.8 Mon 16:45 H9

**Ab-initio description of transient ion formation of NO on Au(111)** — DANIEL CORKEN, NICHOLAS D. M. HINE, and ●REINHARD J. MAURER — Departments of Physics and Chemistry, University of Warwick, United Kingdom

Gaining a fundamental understanding of the interactions of molecules on metal surfaces is essential for the development of novel heterogeneous catalysts. An interesting feature of gas-surface reactions at metal surfaces is that the Born-Oppenheimer approximation breaks down. Vibrationally excited and translationally hot molecules can transfer energy to the electrons of a metal via excitation of electron-hole pairs (EHP). In case of NO on Au(111), [1] this nonadiabatic energy loss is believed to stem from the transient generation of charged ion species at the surface. A computationally feasible and accurate description of such a molecule-metal charge-transfer state represents a challenge and several methods have been proposed. Upon a review of existing experimental evidence, we will present our approach to this problem. We use linear expansion-Delta-Self-Consistent-Field Density Functional Theory (le $\Delta$ SCF-DFT) [2] to model the anionic resonance of NO on Au(111). The le $\Delta$ SCF-DFT method enforces the electronic configuration of reference molecular states while solving the Kohn-Sham equations self-consistently. By comparison to experiment and other models, we assess the methods' ability to describe the ground- and excited-states during molecular scattering. We further explore avenues to extract nonadiabatic couplings and to construct model Hamiltonians based on this method. [1] JCP **130**, 174716, [2] JCP **139**, 014708;

DS 6.9 Mon 17:00 H9

**Luminescence of  $\beta$ -SiAlON:Eu<sup>2+</sup> phosphors: DFT study** — ●SALEEM AYAZ KHAN<sup>1</sup>, ONDREJ ŠÍP<sup>1</sup>, ROBIN NIKLAUS<sup>2</sup>, WOLFGANG SCHNICK<sup>2</sup>, and JAN MINAR<sup>1</sup> — <sup>1</sup>University of West Bohemia, Pilsen, Czech Republic — <sup>2</sup>LMU Munich, Germany

Highly efficient phosphor-converted light-emitting diodes (pc-LEDs) are popular in lighting and high-tech electronics applications [1]. Among them  $\beta$ -SiAlON:Eu<sup>2+</sup> stands out as a promising narrow-band green phosphor for white-LEDs applications exhibiting good thermal and chemical stabilities. Photoluminescent properties of this material can be tuned by introducing the disorder at various sublattices. To understand the mechanism behind this effect, we performed a systematic study of electronic structure and photoluminescence properties of  $\beta$ -SiAlON:Eu<sup>2+</sup>. The calculations were done within the *ab-initio* fully relativistic full-potential framework. The disorder was treated by employing both the supercell approach and the coherent potential approximation (CPA). The Stokes shifts were calculated from differences of total energies of the ground and excited states of  $\beta$ -SiAlON:Eu<sup>2+</sup>. The main focus is on monitoring how the Al and O content and Eu<sup>2+</sup> activator concentrations influence the local  $\beta$ -Si<sub>3</sub>N<sub>4</sub> electronic structure and how this may be used to tune photoluminescence properties.

[1] Z. Wang, W. Ye, Iek-H. Chu, and S. P. Ong, Chem. Mater., **28**, 8622 (2016).

DS 6.10 Mon 17:15 H9

**Spin fluctuations in itinerant ferromagnets: Computing the dynamic transverse spin susceptibility with TDDFT and PAW** — ●THORBJØRN SKOVHUS and THOMAS OLSEN — Technical University of Denmark

We present a numerical scheme for computing the dynamic transverse spin susceptibility using time-dependent density functional theory which allows us to study magnons in itinerant ferromagnets. The scheme is based on a real-space grid implementation of the projected augmented wave method and use a simple plane wave representation of

the response function. Employing the adiabatic local density approximation for the exchange-correlation kernel, calculations of the magnon spectra in bulk transition metals iron and nickel are presented. In the

context of the present implementation, the influence from the choice of numerical scheme on the violation of the Goldstone theorem is investigated.

## DS 7: Optical Analysis of Thin Films II (Reflection, Ellipsometry, Raman, IR-DUV Spectroscopy, ...)

Time: Monday 15:00–16:15

Location: H32

DS 7.1 Mon 15:00 H32

**Topology Related Phenomena in Anisotropic Organic Microcavities** — ●OTA KUNT, MARKAS SUDZIUS, HARTMUT FRÖB, and KARL LEO — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Dresden, Germany

We investigate planar microcavities consisting of two dielectric Bragg reflectors and an optically anisotropic uniaxial cavity layer with its optical axis tilted with respect to the growth direction of the structure. The optical properties of these devices are thoroughly investigated by angular and polarization resolved spectroscopic measurements and simulated using transfer matrix technique, which is extended to account for the optical anisotropy. Both experiment and simulations show polarization splitting of the cavity modes due to anisotropy. The modes are in general elliptically polarized, non-orthogonal and differ in both energy and spectral broadening. Points in the photon in-plane momentum space are found where the modes coalesce in both energy and energy broadening, are circularly polarized and are cores of polarization vortices. These points represent non-Hermitian degeneracies or exceptional points of a non-Hermitian system. We investigate in detail the analogy between the system's optical response and that of a biaxial absorbing crystal and investigate the influence of organic gain material in the cavity.

DS 7.2 Mon 15:15 H32

**Structural Color Sensors: Tracking the Thermal History of Materials** — ●HENNING GALINSKI<sup>1</sup>, VOLKER SCHNABEL<sup>1</sup>, MAX DÖBEL<sup>2</sup>, and RALPH SPOLENAK<sup>1</sup> — <sup>1</sup>Laboratory for Nanometallurgy, Department of Materials, ETH Zurich Vladimir-Prelog-Weg 1-5/10, 8093 Zurich, Switzerland — <sup>2</sup>Ion Beam Physics, ETH Zurich, Otto-Stern-Weg 5, 8093 Zurich, Switzerland

The engineering of non-destructive, low footprint optical sensors has attracted significant interest in research in recent years. Such devices can enable real-time and spatiotemporal tracking of materials properties even in secluded applications, such as offshore wind turbines, or extreme environments, as found in thermal solar collectors. Here, we demonstrate a novel thermal sensor based on structural color that provides direct optical feedback of materials properties such as hardness, wear and resistivity [1]. The sensor can be used at high temperatures (1000 °C) and allows the continuous detection of changes in refractive index larger than 1%. The monitoring concept relies on a lossy Gires-Tournois interferometer configuration using thermally induced detuning of a highly absorbing state in the optical spectrum as sensor feedback. The displacement of the absorbing state is directly proportional to thermally induced changes in hardness and resistivity in the material. Using the specific case of TiAlN coatings we show that such detuning is due to a symmetry-breaking structural phase transition, which is accompanied by the formation of saturated structural colors.

[1] V. Schnabel, R. Spolenak, M. Döbeli, H. Galinski, *Advanced Optical Materials* 2018, 6, 1800656.

DS 7.3 Mon 15:30 H32

**The influence of deposition conditions on the continuous broad sub-bandgap-absorption of the High Entropy Oxide: MgCoNiCuZn-O** — ●LARS WENNING and EMELINE MICHEL — I. Institute of Physics (IA), RWTH Aachen University, Germany

Introducing entropy as a competing factor to synthesize and engineer new materials has been shown to be a promising way to discover new materials like high entropy alloys, which exhibit astonishing mechanical properties, e.g. combining high fracture toughness and high yield strength. Advancing the idea of entropy stabilized alloys to High Entropy Oxides is expected to lead to novel materials for industrial appli-

cations and scientific research. Some high entropy oxides have already shown astounding properties like colossal dielectric constant or room temperature superionic conductivity. This work investigates the extraordinary optical behavior of MgCoNiCuZn-oxide thin films and the influence of processing conditions during the reactive sputter deposition. To this end the films are characterized employing a variety of techniques including X-ray diffraction as well as optical characterization using ellipsometric spectroscopy and FT-IR spectroscopy.

DS 7.4 Mon 15:45 H32

**Optical properties along the pseudo-binary line between Bi<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>Se<sub>3</sub>** — ●LUDOVICA GUARNERI, STEFAN MAIER, and MATTHIAS WUTTIG — I.Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

A unique bonding mechanism, coined metavalent bonding (MVB), has recently been introduced. It is characterized by set of unique properties including large optical dielectric constants, high Born effective charges and soft optical modes. It has been identified in a class of inorganic materials including Phase Change Materials, Thermoelectrics and Topological Insulators. In addition, a unique bond breaking mechanism has been found, where MVB materials are characterized by a high probability of multiple events, i.e. several fragments being dislodged by a single laser pulse in atom probe tomography. Such a behavior is not found in materials which utilize ordinary covalent, metallic or ionic bonding. Bi<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>Se<sub>3</sub> show respectively high and low probability of multiple events, which indicates that Bi<sub>2</sub>Se<sub>3</sub> employs MVB, while Sb<sub>2</sub>Se<sub>3</sub> does not. We have thus studied the pseudo-binary line Bi<sub>2</sub>Se<sub>3</sub>:Sb<sub>2</sub>Se<sub>3</sub> to investigate how MVB breaks down. To this end, we measure the optical properties using FT-IR spectroscopy between 30 meV and 0.80 eV. In this range, the dielectric function is governed by the electronic polarizability of the valence electrons, allowing to probe chemical bonding. In a narrow stoichiometry range on the Bi-rich side, a significant increase in the dielectric constant upon crystallization is observed. This finding is evidence for the formation of MVB, which confirms that MVB is a distinctive bonding mechanism.

DS 7.5 Mon 16:00 H32

**Tailoring the optical properties of atomically-thin tungsten disulfide via ion irradiation** — ●LINAN MA<sup>1</sup>, YANG TAN<sup>1</sup>, MAHDI GHORBANI-ASL<sup>2</sup>, SHENGQIANG ZHOU<sup>2</sup>, ARKADY V KRASHENINNIKOV<sup>2</sup>, and FENG CHEN<sup>1</sup> — <sup>1</sup>School of Physics, Shandong University, Jinan, China — <sup>2</sup>Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam and Materials Research, Dresden, Germany

Two-dimensional transition metal dichalcogenides exhibit excellent optoelectronic properties. However, the large band gaps in many semiconducting transition metal dichalcogenides make optical absorption in the near-infrared wavelength regime impossible, which prevents applications of these materials in optical communications. In this work, we demonstrate that Ar ion irradiation is a powerful post-synthesis technique to tailor the optical properties of the semiconducting tungsten disulfide by creating S-vacancies and thus controlling material stoichiometry. First-principles calculations reveal that the S-vacancies give rise to deep states in the band gap, which determine the near-infrared optical absorption of the tungsten disulfide monolayer. As the density of the S-vacancies increases, the enhanced near-infrared linear and saturable absorption of tungsten disulfide is observed, which is explained by the results of first-principles calculations. We further demonstrate that by using the irradiated tungsten disulfide as a saturable absorber in a waveguide system, the passively Q-switched laser operations can be optimized, thus opening new avenues for tailoring the optical response of transition metal dichalcogenides by defect-engineering through ion irradiation.

## DS 8: Instrumentation Micro-/Nano-Analysis and Lithography/Structuring (joint session KFM/DS/O)

Time: Monday 15:00–16:30

Location: PHY 5.0.21

**Invited Talk** DS 8.1 Mon 15:00 PHY 5.0.21

**On-surface synthesis by atomic manipulation studied with AFM** — ●LEO GROSS — IBM Research - Zurich, Säumerstr. 4, 8003 Rüschlikon, Switzerland

Elusive molecules can be created using atomic manipulation with a combined atomic force/scanning tunneling microscope (AFM/STM). Molecules that are highly reactive and short-lived under ambient conditions can be stabilized at low temperature on inert surfaces. Employing high-resolution AFM with functionalized tips provides insights into the structure, geometry, aromaticity and bond orders of the molecules created and into the reactions performed [1].

We created radicals, diradicals [2], non-Kekulé molecules [3], antiaromatics [4], and polyynes [5] and studied their structural and electronic properties. We recently showed that the reorganization energy of a molecule on an insulator can be determined [6]. In addition, we expanded the toolbox for the synthesis of molecules by atomic manipulation, demonstrating reversible cyclisation reactions [2], skeletal rearrangements [5] and controlled reactions on insulating substrates by electron attachment/detachment [7].

References: [1] L. Gross et al. *Angew. Chem Int. Ed* 57, 3888 (2018). [2] B. Schuler et al. *Nat. Chem.* 8, 220 (2016). [3] N. Pavlíček et al. *Nat. Nano.* 12, 308 (2017). [4] Z. Majzik et al. *Nat. Commun.* 9, 1198 (2018). [5] N. Pavlíček et al. *Nat. Chem.* 10, 853 (2018). [6] S. Fatayer et al. *Nat. Nano.* 13, 376 (2018). [7] S. Fatayer et al. *Phys. Rev. Lett.* 121, 226101 (2018).

DS 8.2 Mon 15:30 PHY 5.0.21

**Additive laser fabrication of silver and silver-composite 3D micro-structures** — ●ERIK H. WALLER<sup>1</sup> and GEORG VON FREYMAN<sup>1,2</sup> — <sup>1</sup>Physics department and State Research Center OPTIMAS, Technische Universität Kaiserslautern, Kaiserslautern — <sup>2</sup>Fraunhofer Institute for Industrial Mathematics (ITWM), Kaiserslautern

We present direct laser writing (DLW) of silver and silver-composite microstructures via photoreduction in liquid resists. Several photore-sist compositions are compared based on visual inspection of 2D and 3D test structures complemented by EDS and spectral resonance measurements.

Compared to common approaches for additive manufacturing of 3D metallic structures, e.g., selective laser melting or sintering, DLW is a very precise fabrication technology allowing sub-micrometer feature sizes. However, structures fabricated by DLW are usually made of polymers. Renewed interest in DLW of metallic microstructures has emerged due to their potential, e.g., in plasmonics. The underlying principle of metal DLW is photo-induced reduction of a precursor to neutral metal within the laser focus. The metal particles subsequently agglomerate to form the building block of a structure. Adverse effects are mainly heating of and scattering by the evolving structure as well as low quantum yield and slow speed of the reaction. Thus, we here test different photore-sist compositions with respect to the above mentioned criteria and identify key parameters to best control these photoreactions.

DS 8.3 Mon 15:50 PHY 5.0.21

**Hard X-ray Photoelectron Diffraction in Graphite** — ●OLENA FEDCHENKO<sup>1</sup>, SERGEY CHERNOV<sup>1</sup>, KATERINA MEDJANIK<sup>1</sup>, SERGEY BABENKOV<sup>1</sup>, DMITRY VASILYEV<sup>1</sup>, AIMO WINKELMANN<sup>2</sup>, HANS-JOACHIM ELMERS<sup>1</sup>, and GERD SCHÖNHENSE<sup>1</sup> — <sup>1</sup>JGU, Institut für Physik, Mainz — <sup>2</sup>Laser Zentrum, Hannover

A new high-energy momentum microscope (kinetic energies up to >7 keV) allows full-field imaging of the ( $k_x$ - $k_y$ ) photoelectron distribution with a large field of view (up to 20 Å<sup>-1</sup> dia.) in momentum space and ToF energy recording. Avoiding symmetry-varying rotation of sample and/or analyser, "full-field k-imaging" provides an ideal means for X-ray photoelectron diffraction (XPD) studies. High-resolution (< 0.1°) diffractograms can be recorded within minutes thanks to the high brilliance of beamline P22 at PETRA III [1]. We present an XPD study for electrons from the C 1s core level in graphite in a wide energy range from 2840 to 7283 eV. Fine details in the diffractograms reflect the large number of scatterers (10<sup>5</sup>-10<sup>6</sup>) due to the large inelastic mean free path. A calculation based on the Bloch wave approach to electron diffraction by lattice planes [2] shows excellent agreement. The short photoelectron wavelength (10% of the interatomic distance) "amplifies" phase differences and turns hard X-ray XPD into a very sensitive structural tool. The results are important for valence band XPD [3].

[1] C. Schlueter et al., *Synchr. Radiation News* 31, 29 (2018); [2] A. Winkelmann et al., *New J. of Phys.* 10, 113002 (2008); [3] G. Schönhense et al., arXiv 1806.05871 (2018).

DS 8.4 Mon 16:10 PHY 5.0.21

**High-Resolution High-Sensitivity Characterization using SIMS based Correlative Microscopy** — ●SANTHANA ESWARA, ALISA PSHENOVA, JEAN-NICOLAS AUDINOT, and TOM WIRTZ — Advanced Instrumentation for Ion Nano-Analytics, MRT, Luxembourg Institute of Science and Technology, L-4422 Belvaux, Luxembourg

Technological materials are being increasingly engineered by optimizing the structure at the nanometer-level and the chemical composition at the dopant-level. Therefore, analytical techniques capable of both high-resolution and high-sensitivity are indispensable. Transmission Electron Microscopy (TEM) offers excellent lateral resolution down to atomic scale, but the analytical techniques typically available in a TEM such as EDX or EELS do not have the sensitivity to analyze trace elements (e.g. dopants). In comparison, Secondary Ion Mass Spectrometry (SIMS) is well-known for high-sensitivity analysis of materials down to the ppm level. However, the lateral resolution of SIMS is fundamentally limited by the ion-solid interaction volume to ~ 10 nm. Recently we developed SIMS in a Helium Ion Microscope (HIM) and demonstrated a SIMS lateral resolution of ~ 15 nm[1]. While this is a remarkable breakthrough, it is still 2 to 3 orders-of-magnitude poorer in comparison to high-resolution techniques such as TEM imaging. To overcome this limitation, we developed correlative microscopy methods combining SIMS imaging with high-resolution techniques such as TEM and HIM (SE mode). We will discuss the HIM-SIMS and in-situ TEM-SIMS correlative techniques[2]. [1] D. Dowsett et al, *Anal. Chem.*, 89, 8957-8965, 2017 [2] L. Yedra et al, *Sci. Rep.* 6, 28705, 2016

## DS 9: Layer Deposition (ALD, MBE, Sputtering, ...)

Time: Monday 15:00–16:30

Location: H39

DS 9.1 Mon 15:00 H39

**MBE growth of  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> by using a Sn catalyst-layer** — ●ALEXANDER KARG<sup>1</sup>, MAX KRACHT<sup>2</sup>, SEBASTIAN BENZ<sup>2</sup>, FABIAN MICHEL<sup>2</sup>, MARCUS ROHNKE<sup>3</sup>, STEPHAN FIGGE<sup>1</sup>, JÖRG SCHÖRMANN<sup>2</sup>, MARCO SCHWALTER<sup>1</sup>, JÜRGEN JANEK<sup>3</sup>, ANDREAS ROSENAUER<sup>1</sup>, and MARTIN EICKHOFF<sup>1</sup> — <sup>1</sup>Institute of Solid State Physics, University of Bremen, Bremen, Germany — <sup>2</sup>Institute of Experimental Physics 1, Justus Liebig University, Giessen, Germany — <sup>3</sup>Physical-Chemical Institute, Justus Liebig University, Giessen, Germany

MBE-growth of  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> on c-plane Al<sub>2</sub>O<sub>3</sub> by MBE is only possible in metal-rich growth conditions, which normally leads to the formation and subsequent desorption of the volatile suboxide Ga<sub>2</sub>O, thus hampering layer-growth. Additional supply of Sn during growth expands the growth window and enables the formation of  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> in this regime.

To further investigate the role of Sn during growth we significantly reduced the Sn exposure time and deposited an ultrathin (<1 ML) Sn layer before Ga<sub>2</sub>O<sub>3</sub> growth.

We found that this Sn layer is sufficient to enable the formation of  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> thin films without Sn incorporation, demonstrating the catalytic role of Sn in the growth process. The impact of this technique for processing technology of  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> devices will also be discussed.

DS 9.2 Mon 15:15 H39

**Influence of surface modification on electrochemical performance of Ni-rich NCM cathodes for Lithium ion batteries** — ●RAJENDRA SINGH NEGI and MATTHIAS T. ELM — Center for Materials Research, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen

Ultrathin Al<sub>2</sub>O<sub>3</sub> coatings were applied to Ni-rich NCM powder using atomic layer deposition (ALD) in order to create a protective barrier layer at electrode-electrolyte interface. The results of FIB-scanning electron microscopy and transmission electron microscope images show a homogeneous and conformal Al<sub>2</sub>O<sub>3</sub> coating on the surface of Ni-rich NCM powder. C-rate and cycling tests show that the Al<sub>2</sub>O<sub>3</sub> coating improves the electrochemical performance with a higher capacity retention as compared to pristine cathodes at room temperature under 0.5C. The superior performance is attributed due to the suppression of side reactions at the interface between the active cathode powder and the electrolyte.

DS 9.3 Mon 15:30 H39

**Epitaxial growth of SrTiO<sub>3</sub> thin films by MOVPE** — ●AYKUT BAKI, JULIAN STÖVER, KLAUS IRMSCHER, TONI MARKURT, MARTIN ALBRECHT, and JUTTA SCHWARZKOPF — Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2 12489 Berlin, Germany

SrTiO<sub>3</sub> represents a prototype of complex perovskites. It provides a high dielectric constant and a switchable/tunable resistivity, which makes it potentially interesting for resistive switching memories (ReRAM). A large number of studies exists about physical thin film deposition by pulsed laser deposition (PLD). However, SrTiO<sub>3</sub> thin films are rarely deposited by metal-organic vapor phase epitaxy (MOVPE), although this method provides the epitaxy of smooth and defect-poor thin films since growth takes place near the thermodynamic equilibrium. The approach of our study is to grow defect-free epitaxial SrTiO<sub>3</sub> films and to fundamentally investigate on the correlation between deposition conditions and film properties. Well-ordered SrTiO<sub>3</sub> thin films are epitaxially grown by MOVPE on (100) SrTiO<sub>3</sub>, (110)<sub>o</sub> DyScO<sub>3</sub> and (110)<sub>o</sub> NdGaO<sub>3</sub> substrates under different strain conditions by the use of Sr(tmhdh)<sub>2</sub>-tetraglyme and Ti(iso-propoxid)<sub>2</sub>(tmhdh)<sub>2</sub> precursors. The structural properties of SrTiO<sub>3</sub> thin films grown under a wide range of growth parameters by MOVPE and PLD are analyzed by high-resolution X-ray diffraction, transmission electron microscopy, atomic force microscopy and their impact on electrical properties are shown by resistivity and capacitance-voltage measurements.

DS 9.4 Mon 15:45 H39

**Cu- and Mn-doping in ferroelectric K<sub>0.5</sub>Na<sub>0.5</sub>NbO<sub>3</sub> epitaxial films grown by PLD** — ●DANIEL PFÜTZENREUTER, MARTIN SCHMIDBAUER, JULIAN STÖVER, KLAUS IRMSCHER, DETLEF KLIMM, and JUTTA SCHWARZKOPF — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin

(K,Nb)NbO<sub>3</sub> is a lead-free ferro- and piezoelectric material potentially

used for e.g. sensor or memory applications. Pulsed laser deposition (PLD) of K<sub>0.5</sub>Na<sub>0.5</sub>NbO<sub>3</sub> thin films with reproducible high crystalline quality requires the use of phase pure and dense targets. Therefore, an optimized target preparation routine based on solid-state sintering was developed. Raw materials are ground to a mean grain size of 10  $\mu$ m and pressed into a target applying an isostatic pressure of 2000 bar. Subsequently, a two-step sinter routine ensures the formation of a pure perovskite phase. Here, a calcination step at 850 °C and a subsequent sinter step at 1050 °C are executed. Besides pure K<sub>0.5</sub>Na<sub>0.5</sub>NbO<sub>3</sub> also the impact of Cu- and Mn-doping on the sinter procedure has been studied. Aliovalent doping on K<sub>x</sub>Na<sub>1-x</sub>NbO<sub>3</sub> ceramics has been reported to have a significant impact on electrical properties of the material, however, studies on thin films are rarely published. Therefore, doped K<sub>0.5</sub>Na<sub>0.5</sub>NbO<sub>3</sub> targets were prepared and applied for thin film growth with PLD. Under optimized growth conditions, deposition of K<sub>0.5</sub>Na<sub>0.5</sub>NbO<sub>3</sub> thin films resulted in well-ordered epitaxial films. The impact of Cu- and Mn-doping on thin films has been studied with respect to structural and electrical properties of the films.

DS 9.5 Mon 16:00 H39

**Ion-beam sputtered oxide buffer layers as a viable alternative to thin films grown with atomic layer deposition** — ●MARTIN BECKER, FLORIAN KUHL, PHILIP KLEMENT, ANGELIKA POLITY, JÖRG SCHÖRMANN, PETER J. KLAR, and SANGAM CHATTERJEE — Institute of Experimental Physics I and Center for Materials Research, Heinrich-Buff-Ring 16, Justus Liebig University Giessen, D-35392 Giessen, Germany

Sputtering deposition techniques are well suited to fabricate polycrystalline oxide thin-films on different substrates as they reliably offer homogeneous and reproducible layer growth at high deposition rates. Conventional RF and DC sputtering, however, are subject to limitations based on substrate heating and impurity incorporation. Ion-beam sputter-deposition (IBSD) tackles these issues and yields thin films of high compactness and adherence. Therefore, in many applications, IBSD has become a viable alternative to conventional plasma-based deposition.

Here, we report on a system for the ion beam processing of semiconductors with the focus on buffer layer growth. Its task is to increase the quality of the growth of the functional layer itself by creating a smoother surface or providing a surface triggering a preferential crystal orientation of the functional layer. We discuss different oxide-based model systems. Further, we will compare the results with buffer layers grown with atomic layer deposition (ALD), since in most cases ALD is the method of choice when it comes to the ability to produce accurate thicknesses and uniform surfaces.

DS 9.6 Mon 16:15 H39

**Correlation between sputter deposition parameters and I-V curves in memristive devices** — ●FINN ZAHARI<sup>1</sup>, SVEN GAUTER<sup>2</sup>, JULIAN STROBEL<sup>3</sup>, JULIA CIPO<sup>2</sup>, FELIX GEORG<sup>2</sup>, THOMAS MUSSENBROCK<sup>4</sup>, LORENZ KIENLE<sup>3</sup>, HOLGER KERSTEN<sup>2</sup>, and HERMANN KOHLSTEDT<sup>1</sup> — <sup>1</sup>Nanoelectronics, Faculty of Engineering, Kiel University, Germany — <sup>2</sup>Plasma Technology, Department of Physics, Kiel University, Germany — <sup>3</sup>Synthesis and Real Structure, Faculty of Engineering, Kiel University, Germany — <sup>4</sup>Electrodynamics and Physical Electronics, Electrical Engineering and Information Science, BTU Cottbus-Senftenberg, Germany

Neuromorphic analogue systems are recently highly investigated to realize novel bio-inspired computing architectures which may have advantages in power dissipation and scalability over traditional transistor technologies. Double barrier memristive devices (DBMD) with the layer sequence Nb/Al/Al<sub>2</sub>O<sub>3</sub>/NbO<sub>x</sub>/Au are promising candidates to emulate synaptic behavior in analog circuits. Selector-device free crossbar-arrays based on DBMDs have been already realized for pattern recognition tasks. The recognition performance of such systems strongly depends on the individual electrical I-V characteristics of the DBMDs. In this contribution we show evidence that crucial parameters of the process plasma, such as floating potential of the substrate, electron temperature and energy influx, are strongly correlated with the I-V characteristics of the individual devices. These results are supported by transmission electron microscopy (TEM). Our findings enable a new pathway for the development of plasma engineered memristive devices.

## DS 10: Thermoelectric and Phase Change Materials

Time: Monday 16:45–18:00

Location: H39

DS 10.1 Mon 16:45 H39

**Switching behaviour of epitaxial Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> thin films** — ●MARIO BEHRENS, ANDRIY LOTNYK, JÜRGEN W. GERLACH, and BERND RAUSCHENBACH — Leibniz Institute of Surface Engineering (IOM), Permoserstraße 15, 04318 Leipzig, Germany

Phase change materials represent a promising material class with applications in various fields such as photonics, data storage and neuromorphic computing. The unique characteristic of these materials is a pronounced electrical and optical property contrast between different phases combined with the possibility to switch between these phases fast and reversibly. One of the most prominent phase change materials is the Te-based chalcogenide Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> which has been intensively studied due to its well-balanced switching properties. A promising approach to gain deeper knowledge of the material properties is to employ epitaxially grown thin films, since it enables precise control of the structure and the phase and furthermore allows studies presupposing single-crystalline orientation. In this work, the switching behaviour of epitaxial Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> thin films grown on Si(111) substrates by pulsed laser deposition is investigated. X-ray diffraction and aberration-corrected high-resolution scanning transmission electron microscopy studies of the thin films before and after switching demonstrate that phase transitions between different crystalline phases can be achieved without losing the epitaxial framework of the structures. These results therefore offer valuable insights into the switching processes of epitaxial phase change materials and might help to advance the design of phase change memories by employing highly textured structures.

DS 10.2 Mon 17:00 H39

**Controlling Disorder and Disorder-Related Physical Properties in the Phase Change Material Sn<sub>1</sub>Sb<sub>2</sub>Te<sub>4</sub>** — ●NIKITA POLIN, STEFAN MAIER, BRIGITTE BAUMKÖTTER, and MATTHIAS WUTTIG — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

Phase-change materials (PCMs) possess physical properties suited for a wide range of applications from non-volatile data storage, data processing to thermoelectrics. The recently investigated PCM-material Sn<sub>1</sub>Sb<sub>2</sub>Te<sub>4</sub> (SST) displays a high amount of atomic disorder attributed to intrinsic vacancies. From the fundamental research perspective SST is one of the few experimentally observed realizations of an Anderson insulator. From the applicational point of view the vacancy disorder plays an important role in shaping electronic properties. These observations make SST a promising candidate for a multilevel data storage device.

The microscopic understanding of the underlying physical phenomena is therefore of interest. The aim of this work is to get insights into interplay between disorder, transport and bonding. For this purpose optical, structure determination and electronic transport measurements shall be employed.

DS 10.3 Mon 17:15 H39

**Phonon modes and thermal conductivity in Si/SiO<sub>2</sub> multishell nanotubes** — C. I. ISACOVA<sup>1</sup>, A. I. COCEMASOV<sup>1</sup>, D. L. NIKA<sup>1</sup>, O. G. SCHMIDT<sup>2</sup>, and ●V. M. FOMIN<sup>1,2</sup> — <sup>1</sup>E. P. Pokatilov Laboratory of Physics and Engineering of Nanomaterials, Moldova State University, Chisinau MD-2009, Republic of Moldova — <sup>2</sup>Institute for Integrative Nanosciences, Leibniz IFW Dresden, Dresden D-01069, Germany

Theoretical atomistic study of thermal transport is conducted for Si/SiO<sub>2</sub> multishell nanotubes, which model rolled-up Si/SiO<sub>2</sub> nano-

structures. Phonon modes are obtained within Lattice Dynamics Theory. Thermal conductivity in Si/SiO<sub>2</sub> nanotubes, as calculated using Boltzmann Transport Equation within the relaxation-time approximation, is lower than that in Si nanowires with the same lateral dimensions due to the acoustical mismatch of the materials and a stronger phonon confinement. A large number of phonon modes are scattered on Si/SiO<sub>2</sub> interfaces, what enhances the effect of the boundary scattering mechanism on thermal conductivity of multishell nanotubes. Thermal conductivity is found to decrease almost linearly as a function of the number of Si/SiO<sub>2</sub> bilayers in multishell nanotubes. The present work is supported by the DFG grant no. FO 956/4-1.

DS 10.4 Mon 17:30 H39

**Resistive switching in optoelectronic III-V materials based on deep traps** — ●MICHAEL SCHNEEDLER, VERENA PORTZ, ULRICH SEMMLER, MARCO MOORS, RAINER WASER, RAFAL E. DUNIN-BORKOWSKI, and PHILIPP EBERT — Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Jülich, 52425, Germany

Resistive switching random access memories (ReRAM) are promising candidates for energy efficient, fast, and non-volatile universal memories that unite the advantages of RAM and hard drives. Unfortunately, the current ReRAM materials are incompatible with optical interconnects and wires. Optical signal transmission is, however, inevitable for next generation memories in order to overcome the capacity-bandwidth trade-off. Thus, we present here a proof-of-concept of a new type of resistive switching realized in III-V semiconductors, which meet all requirements for the implementation of optoelectronic circuits. This resistive switching effect is based on controlling the spatial positions of vacancy-induced deep traps by stimulated migration, opening and closing a conduction channel through a semi-insulating compensated surface layer. The mechanism is widely applicable to opto-electronically usable III-V compound semiconductors.

DS 10.5 Mon 17:45 H39

**Absolute Seebeck coefficient of thin platinum films and individual silver nanowires** — ●MAXIMILIAN KOCKERT<sup>1</sup>, DANNY KOJDA<sup>1</sup>, RÜDIGER MITDANK<sup>1</sup>, ANTON ZYKOV<sup>2</sup>, STEFAN KOWARIK<sup>2,3</sup>, JOHANNES RUHAMMER<sup>4</sup>, ZHI WANG<sup>4</sup>, MICHAEL KRÖNER<sup>4</sup>, PETER WOIAS<sup>4</sup>, TONI MARKURT<sup>5</sup>, and SASKIA F. FISCHER<sup>1</sup> — <sup>1</sup>Novel Materials Group, Humboldt-Universität zu Berlin, D-10099 Berlin — <sup>2</sup>Nanoscale processes and growth, Humboldt-Universität zu Berlin, D-10099 Berlin — <sup>3</sup>Bundesamt für Materialforschung und -prüfung (BAM), D-12203 Berlin — <sup>4</sup>Laboratory for Design of Microsystems (IMTEK), University of Freiburg, D-79110 Freiburg — <sup>5</sup>Leibniz-Institute for Crystal Growth (IKZ), D-12489 Berlin

Thermoelectric properties of as sputtered and tempered thin platinum films and single crystalline silver nanowires were investigated and compared to bulk. Structural properties like film thickness, grain size and nanowire diameter were correlated with the thermoelectric properties. Furthermore, we present a model to describe the temperature dependence of the absolute Seebeck coefficient  $S$  of thin films, nanowires and bulk, which consists of a thermodiffusion and phonon drag part.  $S$  of thin platinum films is reduced compared to the bulk and we find that the film thickness and grain size by means of the electron mean free path influence  $S$ . Silver nanowires exhibit a reduction of the thermodiffusion part and a shift of the phonon drag peak towards higher bath temperatures compared to the bulk, but without changing the maximum value of  $S$ . In addition, a discussion of the influence of the electron-phonon and phonon-phonon interaction on  $S$  is given.



## DS 11: PhD-Symposium: Photoluminescence of halide perovskites: What does it tell us and what not? (joint session DS/AKJDPG/HL)

Perovskite Solar Cells (PSCs) have recently emerged as a new research field due to their rapid increase in power conversion efficiency. Many research groups formerly working in other fields such as in DSSC, organic solar cells and thin film solar cells, quantum dots, single molecules have jointly created a new research field. Photoluminescence spectroscopy is a technique used rather widely in all of these fields as a simple standard method. Applying specific models and theory, photoluminescence can however be converted into an advanced characterization technique. The models and analysis tools used for this have been unique to the specific fields so far and now tend to collide when PSCs are measured and analysed.

This symposium therefore aims to give a brief overview of advanced models and analysis tools which allow a more nuanced interpretation of photoluminescence emission of perovskite solar cell materials. In a mix of introductory talks, invited expert talks and contributed talks we will explore how certain models have been used to analyse PSCs and argue why and under what conditions a certain model can or cannot be applied to perovskite solar cells.

### Organizers:

- Juliane Borchert, Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom
- Klara Suchan, Lund University, Kemicentrum, Naturvetarvägen 16, 22362 Lund, Sweden
- Tobias Seewald, Department of Physics, University of Konstanz, Universitätsstr. 10, 78457 Konstanz, Germany

Time: Tuesday 9:30–13:15

Location: H32

**Invited Talk** DS 11.1 Tue 9:30 H32  
**Photoluminescence Analysis of Thin Films: What can it tell us about (Perovskite) Solar Cells?** — •THOMAS UNOLD — Helmholtz-Zentrum Berlin für Materialien und Energie

Photoluminescence analysis has been an important analytical tool in semiconductor characterization, and depending on the experimental conditions can reveal detailed information about various optical and electronic properties such as radiative recombination, non-radiative recombination, defects, carrier trapping and the quasi-Fermi level splitting[1-4]. The technique can be applied to thin films as well as to complete solar cell devices, but may require additional analysis to consider the presence of either free surfaces or built-in electrical fields, additional recombination processes as well as partial charge extraction. In the ideal case different types of luminescence measurements yield a consistent picture of the material properties and the limitations of device performance. Different aspects of such photoluminescence analyses will be discussed with a special focus on how results obtained on (hybrid) perovskites comply with the state-of-the-art knowledge on more common inorganic semiconductor materials. [1] T. Unold, L. Gütay, in *Advanced Characterization Techniques for Thin Film Solar Cells*, Wiley VCH (2011) 151-175. doi.org/10.1002/9783527636280.ch7 [2] F. Staub et al., *Phys. Review Applied* 6 (2016) 044017 [3] C. Hages et al., *Adv. Energy Mater.* 7(2017) 1700167 [4] M. Stolterfoht et al., *Nature Energy* 3 (2018) 847.

DS 11.2 Tue 10:00 H32  
**In-situ film formation studies of metal-halide perovskite layers** — •KATRIN HIRSELANDT<sup>1,2</sup>, RAHIM MUNIR<sup>1</sup>, FLORIAN MATHIES<sup>1</sup>, ABOMA MERDASA<sup>1</sup>, EMIL J. W. LIST-KRATOCHVIL<sup>2</sup>, and EVA UNGER<sup>1,2</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Kekuléstraße 5, 12489 Berlin, Germany — <sup>2</sup>Institut für Physik, Institut für Chemie & IRIS Adlershof, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 6, 12489 Berlin, Germany

By optimizing the perovskite fabrication process during spin-coating by introduction of complex solvent blends and quenching steps, solar cells with power conversion efficiencies above 22% have been realized on small active areas. Reproducing published fabrication procedures is not trivial as process conditions vary from place to place and adapting methodologies developed for small-area devices based on spin-coating to larger area devices even less so. Understanding the film formation during different stages of processing allows for a more rational approach to translate deposition strategies to scalable processing methods.

In this study we compared the temporal evolution of MAPbI<sub>3</sub> and Cs<sub>0.05</sub>(FA<sub>0.83</sub>MA<sub>0.17</sub>)<sub>0.95</sub>Pb(I<sub>0.83</sub>Br<sub>0.17</sub>)<sub>3</sub> (3CAT) covered substrates during spin-coating using a fibre-optic based photolumines-

cence and reflection spectroscopy setup. Varying the time of a crystallization-inducing anti-solvent drip, we identified a much narrower process window for MAPbI<sub>3</sub>, compared to 3CAT corroborated with scanning electron microscope images of annealed samples. We here present insight into the difference in crystallization kinetics of these different standard formulations for perovskite processing.

**Invited Talk** DS 11.3 Tue 10:15 H32  
**Defect activity in lead halide perovskite semiconductors** — •SILVIA MOTTI — Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, OX1 3PU, Oxford, United Kingdom

Perovskite semiconductors have recently emerged as promising materials for optoelectronic applications, with photovoltaic efficiencies that have now reached over 23%. Great research effort has been employed towards understanding how the perovskite crystalline and electronic structure relates to their remarkable defect tolerance and surprisingly long carrier lifetimes and high open circuit voltages. At the same time, the material instability often interferes with experimental observations, besides posing a major challenge for commercial application. A comprehensive investigation of defect activity in lead halide semiconductors was conducted by combining computational studies with experimental evidences from optical spectroscopy. It was possible to identify the most predominant charge-trapping point defects in MAPbBr<sub>3</sub> and MAPbI<sub>3</sub> and their role in recombination dynamics, explaining the defect tolerance in these semiconductors. Moreover, the reactivity of such defects under external stimuli could be associated with the photoinstabilities observed in these materials, allowing for the development of successful strategies to control them. This understanding opens the possibility of developing intelligent fabrication methods and further optimizing performance and stability of perovskite optoelectronic devices.

DS 11.4 Tue 10:45 H32  
**The impact of lead iodide on the recombination kinetics in metal halide perovskites** — •ABOMA MERDASA<sup>1</sup>, ALEXANDROS KILIGARIDIS<sup>2</sup>, CAROLIN REHERMANN<sup>1</sup>, MOJTABA ABDI-JALEBI<sup>3</sup>, JONAS STÖBER<sup>2</sup>, BORIS LOUIS<sup>2</sup>, MARINA GERHARD<sup>2</sup>, SAMUEL D. STRANKS<sup>3</sup>, EVA L. UNGER<sup>1,2</sup>, and IVAN G. SCHEBLYKIN<sup>2</sup> — <sup>1</sup>Young Investigator Group Hybrid Materials Formation and Scaling, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — <sup>2</sup>Chemical Physics and NanoLund, Lund University, Lund, Sweden. — <sup>3</sup>Cavendish Laboratory, Department of Physics, University of Cambridge, Cambridge, United Kingdom.

Metal halide perovskites are promising semiconductor materials for photovoltaic devices with solar cell efficiencies soaring over 20%, but

understanding the fundamental operational principles are lagging behind. One example is the role and influence of lead iodide (PbI<sub>2</sub>) reportedly being both beneficial and detrimental for a device. Herein, we present a study on the impact of lead iodide on the charge-carrier recombination kinetics in methylammonium lead triiodide (MAPbI<sub>3</sub>) thin films. We simultaneously acquire spectrally-resolved photoluminescence quantum yield and time-resolved photoluminescence lifetime at excitation wavelengths ranging from 450 nm to 780 nm during hours of light-soaking, and identify a unique radiative recombination mechanism occurring at the PbI<sub>2</sub>/MAPbI<sub>3</sub> interface when charge carriers are generated in PbI<sub>2</sub>. We thereby provide important insight into the long-debated question of whether excess PbI<sub>2</sub> is beneficial or detrimental for charge carrier dynamics in perovskite solar absorber materials.

### 15 min. break

**Invited Talk** DS 11.5 Tue 11:15 H32  
**Beyond traditional use of photoluminescence: Assessing halide perovskites quantitatively and qualitatively** — ●CAROLIN SUTTER-FELLA — Lawrence Berkeley National Laboratory, Berkeley, California, US

Hybrid metal halide perovskites have recently transformed the landscape of light harvesting solar energy materials while showing promise in a range of other optoelectronic applications. These materials do not only show exceptional optoelectronic properties and apparent defect tolerance but are also easy to synthesize via solution processing. Nevertheless, there are non-radiative recombination losses which have to be characterized and ideally tied back to synthesis conditions.

In the first part of this talk I will cover our work on quantitative photoluminescence quantum yield measurements under variation of the halide as well as cation. This quantity will be related to the device relevant open circuit voltage (V<sub>oc</sub>) by comparing the electrically measured Voc to the optically implied Voc. In the second part I will show how in situ photoluminescence spectroscopy can be used to monitor perovskite film and nanoparticle formation. I will reveal the onset of semiconducting properties during synthesis and the correlation to other material characteristics such as morphology and crystal phase. The work provides guidance to a fast screening of the synthetic parameter space and ultimately controlled experimental procedures that yield high device efficiencies.

DS 11.6 Tue 11:45 H32  
**Temperature dependent charge carrier transport in MAPI single crystal thin films** — ●ALEXANDER BIEWALD<sup>1</sup>, RICHARD CIESIELSKI<sup>1</sup>, NADJA GIESBRECHT<sup>1</sup>, KATHRIN HANDLOSER<sup>1</sup>, PABLO DOCAMPO<sup>2</sup>, THOMAS BEIN<sup>1</sup>, and ACHIM HARTSCHUH<sup>1</sup> — <sup>1</sup>Department Chemie und (CeNS), LMU München, Deutschland — <sup>2</sup>School of Electrical and Electronic Engineering, Newcastle, UK

Methylammonium lead iodide (MAPI)-based thin-film solar cells today reach power conversion efficiencies of more than 20% [1]. The material is prototypical for the large class of perovskite semiconductor materials for photovoltaic applications and is therefore at the focal point of research interest to a global community. Here, we present an all-optical study of the charge carrier diffusion properties in large-crystal MAPI thin films using photoluminescence microscopy [2]. We vary the temperature between 170 K and room temperature, thus remaining in the tetragonal crystal phase [2]. We probe the local material properties of individual crystal grains within a PMMA-coated MAPI thin film and find a steady increase of the diffusion constant towards lower temperatures. In a previous paper we found that grain boundaries in such thin films act as solid walls for diffusing charge carriers [2], which we also see at low temperatures.

- [1] M. A. Green, et al., Solar cell efficiency tables (version 52), 2018.  
 [2] R. Ciesielski, et al., ACS Appl. Mat. & Interfaces. 10 (9), 7974-7981 (2018).  
 [3] N.O. Yamamuro, et al., J. Phys. Chem. Solids 53 (7), 935-939

(1992).

**Invited Talk** DS 11.7 Tue 12:00 H32  
**Photophysics of Sn-based hybrid perovskites** — ●MARIA ANTONIETTA LOI — Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands

Thanks to the intensive research efforts of a large scientific community over the past years, lead (Pb)-based hybrid perovskite solar cells have reached impressive (>23%) power conversion efficiency. Against the initial criticism about their instability, also large improvements in the thermal and photo stability of this kind of solar cells were obtained in the last years. Despite these outstanding accomplishments, the toxicity of lead causes concerns about the possible large-scale utilization of this new type of solar cell. Among the various alternatives to lead, Sn has been recognized to have a great potential, as the Sn-based hybrid perovskites display excellent optical and electrical properties such as high absorption coefficients, very small exciton binding energies and high charge carrier mobilities. Recently solar cells with efficiencies approaching 10% have been reported. In my presentation I will report about important features of the photophysical properties of formamidinium tin triiodide. Photoluminescence spectra are highly asymmetric at the high-energy edge. This is accompanied by the unusually large blue shift of the time-integrated photoluminescence with increasing of the excitation power. These phenomena are associated with very slow hot carrier relaxation and state-filling of band edge states. Most importantly, the hot carrier photoluminescence is evident not only upon pulsed excitation but also with continuous wave one.

DS 11.8 Tue 12:30 H32  
**Metastable defects in perovskite semiconductors reveal microscopic insight into non-radiative processes** — ●MARINA GERHARD<sup>1</sup>, BORIS LOUIS<sup>1,2</sup>, RAFAEL CAMACHO<sup>2</sup>, ABOMA MERDASA<sup>3</sup>, ALEXANDER KILIGARIDIS<sup>1</sup>, JUN LI<sup>1</sup>, ALEXANDER DOBROVOLSKY<sup>1</sup>, JOHAN HOFKENS<sup>2</sup>, and IVAN G. SCHEBLYKIN<sup>1</sup> — <sup>1</sup>Division of Chemical Physics and NanoLund, Lund University, Box 124, 22100 Lund, Sweden — <sup>2</sup>KU Leuven, Molecular Imaging and Photonics, Celestijnenlaan 200f, Box 2404, 3001 Leuven, Belgium — <sup>3</sup>Helmholtz-Zentrum für Materialien und Energie GmbH, Kekulestraße 5, 12489 Berlin, Germany

Metal halide perovskites are an interesting model system for fundamental studies of non-radiative processes due to their photoluminescence (PL) fluctuations on a timescale of milliseconds to seconds, also referred to as 'blinking'. This phenomenon is attributed to the presence of metastable defects, able to switch between a passive (not quenching) and an active (quenching) configuration. Here, we study temperature dependent blinking of methylammonium lead iodide nanocrystals using PL microscopy. Monitoring the behavior of individual defects allows us to understand their concerted contribution to macroscopic quantities, such as the temperature dependent PL quantum yield. We find that both the quenching efficiency and the switching rate of the metastable defects decrease with decreasing temperature. Based on a simple mechanistic picture, we estimate activation barriers for the switching on the order of 200-800 meV. This energy range suggests that the switching mechanism could be related to ion migration.

DS 11.9 Tue 12:45 H32  
**Panel Discussion (with invited speakers)** — ●THOMAS UNOLD<sup>1</sup>, SILVIA MOTTI<sup>2</sup>, CAROLIN SUTTER-FELLA<sup>3</sup>, and MARIA ANTONIETTA LOI<sup>4</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin für Materialien und Energy — <sup>2</sup>Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, OX1 3PU, Oxford, United Kingdom — <sup>3</sup>Lawrence Berkeley National Laboratory, Berkeley, California, US — <sup>4</sup>Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands

Do pre-existing models hold? Or do we need novel approaches to fully understand perovskite photoluminescence?

## DS 12: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge III (joint session O/ CPP/ DS/ TT)

Time: Tuesday 10:30–13:00

Location: H9

**Topical Talk**

DS 12.1 Tue 10:30 H9

**Addressing the structure and dynamics of weakly-bonded interfaces** — ●MARIANA ROSSI — Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin

Interfaces between different materials constitute the basis of technological devices. Incorporating organic components within different architectures opens the path for creating more versatile interfaces with a wide range of properties at a reduced cost. However, the large conformational space that organic components can explore at finite temperatures and the inherent anharmonicity of their intra and intermolecular interactions brings further challenges to first-principles simulations. In this talk, I will discuss our recent efforts to address these challenges, based on developments within density functional theory an *ab initio* (path integral) molecular dynamics. I will present strategies for conformational space sampling of organic/inorganic interfaces, discuss the relationship between atomic and electronic structure including the effect of different functionals, present techniques to include anharmonicity in vibrational fingerprints and machine learning tools to calculate these at reduced costs, and our recent methodological developments that allow the inclusion of quantum nuclear effects in high-dimensional systems (especially weakly bonded interfaces) using path integral molecular dynamics.

DS 12.2 Tue 11:00 H9

**Elucidating the Nuclear Quantum Dynamics of Intramolecular Double Hydrogen Transfer in Porphycene** — ●YAIR LITMAN<sup>1</sup>, JEREMY O. RICHARDSON<sup>2</sup>, TAKASHI KUMAGAI<sup>1</sup>, and MARIANA ROSSI<sup>1</sup> — <sup>1</sup>Fritz Haber Institute of the Max Planck Society, Berlin, Germany — <sup>2</sup>ETH, Zurich, Switzerland

We address the double hydrogen transfer (DHT) dynamics of the porphycene molecule: A complex paradigmatic system where the making and breaking of H-bonds in a highly anharmonic potential energy surface requires a quantum mechanical treatment not only of the electrons but also of the nuclei[1]. We combine density-functional theory calculations, employing hybrid functionals and van der Waals corrections, with recently proposed and optimized path-integral ring-polymer methods for the calculation of vibrational spectra and reaction rates. Our simulations predict the position and width of the N-H stretching band of porphycene and DHT rates in excellent agreement with experiments, thus confirming our determination of the tunneling pathways and the anharmonic mode couplings that play a role in this reaction. They also provide quantitative information about the usually ignored competition between concerted and stepwise DHT pathways at different temperature. These results show that our theoretical approach can describe hydrogen transfer dynamics in different environments, for example when porphycenes are adsorbed on surfaces in prototype molecular switch architectures[2]. [1] Y. Litman, Richardson, J. O., Kumagai, T., Rossi, M. *arXiv:1810.05681*. [2] T. Kumagai, et al., *J. Chem. Phys.*, **148**, 102330 (2018).

DS 12.3 Tue 11:15 H9

**Interplay of quantum nuclear fluctuations and the electronic structure of the cyclohexane/Rh(111) interface** — ●KAREN FIDANYAN and MARIANA ROSSI — Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, Berlin

Cyclohexane (C<sub>6</sub>H<sub>12</sub>) adsorbed on metal surfaces can participate in catalytic dehydrogenation reactions, which show good potential for hydrogen storage. It has been observed experimentally that C<sub>6</sub>H<sub>12</sub> adsorbed on the Rh(111) surface shows an isotope effect on the work function change and the adsorption energy upon deuteration [1]. The physical origin of this puzzling isotope effect on the electronic structure has not been fully resolved. We employ density-functional theory (PBE functional with van der Waals corrections) and *ab initio* path-integral molecular dynamics at 150 K to characterize the underlying physics of this phenomenon. We perform these simulations almost at classical-nuclei cost by making use of the spatially-localized ring-polymer contraction scheme proposed in Ref. [2]. The harmonic approximation to zero-point-energy in the adsorption energy is not able to capture the isotope effects observed experimentally. We thus include anharmonic corrections through the dynamics and identify the temperature-dependent electronic level broadening and renormaliza-

tion due to the interaction with phonons in this system.

- [1] T. Koitaya and J. Yoshinobu, *Chem. Rec.* **14** 848-856 (2014).  
 [2] Y. Litman, D. Donadio, M. Ceriotti and M. Rossi, *J. Chem. Phys.* **148** 102320 (2018).

DS 12.4 Tue 11:30 H9

**Quantum-Nuclear Effects in Anharmonic Thermal Transport of Organic Materials** — ●HAGEN-HENRIK KOWALSKI, MARIANA ROSSI, MATTHIAS SCHEFFLER, and CHRISTIAN CARBOGNO — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

To date, an accurate computational assessment of thermal transport in organic compounds still constitutes a considerable challenge for first principles theory, since the vibrations in such compounds are to a large extent governed by quantum-nuclear (QN) *and* strongly anharmonic (SA) effects [1]. Perturbative approaches account for QN, but not for SA effects, whereas Molecular Dynamics (MD) approaches [2] with classical nuclei account for SA, but neglect QN effects. To overcome this limitation, we here present a framework capable of accounting for both QN and SA effects by sampling the vibrational motion via Thermostatted Ring Polymer Molecular Dynamics (TRPMD). The lattice thermal conductivity is assessed through the Green-Kubo formalism and the auto-correlation of the heat flux. To obtain this quantity, we extend the *ab initio* heat-flux definition proposed in Ref. [2] from MD to TRPMD, in order to include QN effects. We critically discuss the approach, its accuracy, and numerical cost for several materials, ranging from toy-models, e.g., solid Argon, to recently discussed organic materials, in which both QN and SA effects are non-negligible.

- [1] M. Rossi, P. Gasparotto, M. Ceriotti, *Phys. Rev. Lett.* **117**, 115702, (2016).  
 [2] C. Carogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901, (2017).

DS 12.5 Tue 11:45 H9

**Electronic Conduction in Metal Junctions with Multi-Heme Proteins** — ●ZDENEK FUTERA<sup>1</sup>, XIUYUN JIANG<sup>1</sup>, JAN ELSNER<sup>2</sup>, and JOCHEN BLUMBERGER<sup>1,3</sup> — <sup>1</sup>Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom — <sup>2</sup>University of Cambridge, Robinson College, Grange Road, Cambridge CB3 9AN, United Kingdom — <sup>3</sup>Institute for Advanced Study, Technische Universität München, Lichtenbergstrasse 2 a, D-85748, Garching, Germany

Multi-heme proteins such as STC or MtrF are membrane proteins facilitating long-range electron transfer (ET) across cell membrane in metal-reducing bacteria. We have used classical molecular dynamics (MD) together with electronic-structure calculations based on density functional theory (DFT) to show that in native environment the conducted electrons are transferred by incoherent hopping between the heme cofactors. However, recent experimental measurements of current-voltage (I-V) curves suggested that the ET mechanism changes to coherent electron tunneling in vacuum when the protein is electronically coupled with metal electrodes. To investigate such conditions, we performed MD simulations in accurate gold/protein interaction force field to identify adsorption of STC and MtrF between two gold electrodes. By large-scale DFT calculations of the whole interfacial structure we identified the conduction channels formed predominantly by delocalized heme iron states. Finally, we apply Landauer formalism to compute I-V curves on STC junction using the DFT electronic states corrected for band alignment and discuss the ET mechanism.

DS 12.6 Tue 12:00 H9

**Elastic and lattice-dynamical properties of titanium-based compounds** — ●PETER WEBER, PASQUALE PAVONE, and CLAUDIA DRAXL — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Germany

Titanium is the basic element of a variety of compounds with very different electronic, mechanical, and thermal properties. While, for instance, the rocksalt crystals TiC and TiN are well known for their hardness, allotropes of TiO<sub>2</sub> show much softer elastic behaviour. In this work we present the results of an *ab-initio* investigation of the elastic and lattice-dynamical properties of these compounds under pressure. The elastic-constant tensor is calculated up to the third order. Pres-

sure effects on the lattice-dynamical properties of these compounds are evaluated in terms of the mode Grüneisen parameter at the Brillouin zone center. The calculations are performed using density-functional theory as implemented in the full-potential all-electron software package **exciting** [1]. Linear and nonlinear elastic constants are obtained using the **ElaStic** tool [2].

- [1] A. Gulans *et al.*, *J. Phys.: Condens. Matter* **26** (2014) 363202  
 [2] R. Golezorkhtabar *et al.*, *Comp. Phys. Commun.* **184** 1861 (2013)

DS 12.7 Tue 12:15 H9

**Understanding the electron transport through NiSi<sub>2</sub>-Si interfaces** — •FLORIAN FUCHS<sup>1,2,3,4</sup>, SIBYLLE GEMMING<sup>1,2,3</sup>, and JÖRG SCHUSTER<sup>2,4</sup> — <sup>1</sup>Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — <sup>2</sup>Center for Advancing Electronics Dresden (cfaed), Dresden, Germany — <sup>3</sup>Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — <sup>4</sup>Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Metal-semiconductor interfaces are of huge importance for applications and can be found in various field-effect transistors. We study the interface between NiSi<sub>2</sub> and silicon on the basis of density functional theory and the NEGF formalism. Different crystal orientations and strain states are investigated systematically.

We focus on the tunneling phenomena of carriers through the Schottky contact at the interface, which are crucial for the on-current in transistors. The on-current is found to be strongly dependent on strain and orientation. It will be shown that the height of the Schottky barrier determines the tunneling current. However, not all changes in the current can be traced back to the barrier height. The modification of the electronic structure matter as well, which can be modeled based on the effective mass of the tunneling carriers. We have also extracted work functions of the isolated materials which we relate to the extracted Schottky barrier heights. It will be shown that the Schottky-Mott model fails for this material system. Better approaches will be discussed in our contribution.

DS 12.8 Tue 12:30 H9

**Impact of Lattice Screening on Wannier-Mott Excitons** — •CLAUDIA RÖDL — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Optical properties of materials are most relevant for a large variety of technological applications, ranging from photovoltaics over various spectroscopy techniques to LEDs and displays. In optical spec-

tra, microscopic quantum many-body effects like excitons, i.e. coupled electron-hole-pair excitations, are measurable at a macroscopic scale and crucially determine the materials properties. Hence, a deep understanding of exciton physics constitutes an indispensable driving force for innovation in optics and optoelectronics.

The state-of-the-art parameter-free theoretical description of excitons is based on the Bethe-Salpeter equation of many-body perturbation theory. The present theoretical standard approach takes only the static electronic screening of the electron-hole-pair interaction into account. The coupling of excitons to phonons and, hence, polaronic screening contributions are omitted. However, the exciton-phonon coupling is crucial for the qualitative and quantitative understanding of exciton spectra in materials with strong polaronic effects, such as many technologically highly relevant oxides. We will tackle this problem and explore routes towards the inclusion of the polaronic screening contributions into the Bethe-Salpeter framework. As test systems, we study simple two-atomic bulk semiconductors and insulators.

DS 12.9 Tue 12:45 H9

**Discovering a novel nanometric cubic phase in monochalcogenide semiconductors - Theory meets experiment** — •GUY MAKOV<sup>1,2</sup>, URI ARGAMAN<sup>1</sup>, ELAD SEGEV<sup>2</sup>, RAN ABUTBUL<sup>1,2</sup>, and YUVAL GOLAN<sup>1,2</sup> — <sup>1</sup>Dept. of Materials, Ben-Gurion University, Beer-Sheva, Israel — <sup>2</sup>Ilse Katz Institute of nanoscience, Ben-Gurion University, Beer-Sheva, Israel

A new nanometric cubic binary phase with a low-symmetry 64-atom cubic structure was recently discovered in tin monosulfide. Subsequently, this phase was synthesized and identified in tin monoselenide and posited to exist in germanium monosulfide and monoselenide based on density functional theory total energy calculations. A series of computational and experimental studies have identified promising optical properties due to the larger bandgap and non-centrosymmetric structure of the crystal. The structure, atomic positions, band gaps and vibrational spectra of these phases were determined by ab-initio density functional calculations and found to be in very good agreement with experimental measurements. The phases were determined to be mechanically stable from ab-initio phonon spectra and energetically close to competing structures such as rhombohedral and orthorhombic. Surface energy calculations indicate that the particles must be stabilized by ligand adsorption. Ligand surface properties are explored to explain the nanocrystal growth mechanisms. This talk will focus on the results of our calculations on surface and bulk properties and their interplay with experimental studies.

## DS 13: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge IV (joint session O/CPP/DS/TT)

Time: Tuesday 14:00–16:45

Location: H9

### Topical Talk

DS 13.1 Tue 14:00 H9

**The Data Revolution in Materials Science, Through the Lens of the Materials Project** — •KRISTIN PERSSON — University of California, Berkeley, USA

Advanced materials are essential to economic and societal development, with applications in multiple industries, from clean energy, to national security, and human welfare. Historically, novel materials exploration has been slow and expensive, taking on average 18 years from concept to commercialization. Due to the tremendous improvements in computational resources, coupled with software development during the last decades, real materials properties can now be calculated from quantum mechanics much faster than they can be measured. A new era of computational materials prediction and design has been born. A result of this paradigm change are databases like the Materials Project which is harnessing the power of supercomputing together with state of the art quantum mechanical theory to compute the properties of all known inorganic materials and beyond, design novel materials and offer the data for free to the community together with online analysis and design algorithms. We leverage the rich data from the Materials Project for machine learning; accelerating materials design, characterization and finally synthesis of materials. This talk will survey this rapidly evolving and exciting paradigm in science, showcasing the possibilities and iteration between ideas, computations, insight and new materials development.

DS 13.2 Tue 14:30 H9

**High-throughput simulations of complex band structure** — •EMANUELE BOSONI and STEFANO SANVITO — School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2

The Complex Band Structure (CBS) generalizes the conventional band structure of a material by considering wave-vectors with complex components. The CBS extends the description of the allowed states of a material beyond the bulk propagating states, including in the picture the evanescent wave-functions that grow or decay from one unit cell to the next. Even though these latter states are forbidden by translational symmetry, they become important when this is broken via, for example, an interface. In the past, many studies made use of CBS calculations in order to confirm or motivate experimental findings, but only recently we see some efforts to give a unified perspective to the study of this quantity [1]. Moreover, the growth in recent years of high-performance computational resources available at relatively low cost opens the possibility to make a systematic, high-throughput, study of the CBS within the Density Functional Theory (DFT) framework.

In this contribution we will present our implementation of the Transfer Matrix Method [1] for the calculation of the CBS within the DFT code Siesta [2] and we will explain challenges and benefits of the high-throughput approach. We will present a proof of concept example in which we calculated the CBS for a set of materials and we will conclude explaining the relevance of our project in the field of spintronics.

- [1] Reuter M. G., *J. Phys.: Condens. Matter.* **29**, 053001 (2017)

[2] J. M. Soler et al., J. Phys.: Condens. Matt. 14, 2745 (2002)

DS 13.3 Tue 14:45 H9

**Computational Screening of 2D Materials for Solar Cells Application** — ●ANDERS CHRISTIAN RUIS-JENSEN and KRISTIAN SOMMER THYGESEN — Institute for Physics, Technical University of Denmark

Two-dimensional (2D) materials have attracted great attention in recent years, not least due to their extremely strong coupling to light and pronounced excitonic effects. This makes 2D materials an ideal playground for studying light-matter interaction in nano-scale materials for applications within e.g. solar cells and photo-detectors. In this work, we present a large-scale computational study of a wide variety of 2D materials with the aim of identifying novel candidates with strong light-matter interaction. Specifically, we calculate the absorption spectrum of almost 2000 materials at the level of the Random Phase Approximation (RPA) and/or by solving the Bethe-Salpeter Equation (BSE). This enables us of calculating the Power Conversion Efficiency (PCE) for all these materials fully ab-initio. Based on this we identify specific 2D semiconductors for both single- and tandem solar cells. The best candidates present power densities (PCE per unit mass) of several orders of magnitude larger than both Si and GaAs. Lastly, we also show a detailed analysis of a few 2D materials, in which we find exciton states with exceptionally strong coupling to light and large exciton binding energies.

DS 13.4 Tue 15:00 H9

**First-principles Modelling of Solid-Solid Interfaces in all Solid-State Batteries** — ●BORA KARASULU<sup>1</sup>, JAMES P. DARBY<sup>1</sup>, CLARE P. GREY<sup>2</sup>, and ANDREW J. MORRIS<sup>3</sup> — <sup>1</sup>Dept. of Physics, Univ. of Cambridge, UK — <sup>2</sup>Dept. of Chemistry, Univ. of Cambridge, UK — <sup>3</sup>School of Metallurgy and Materials, Univ. of Birmingham, UK

All solid-state batteries (ASSBs) can potentially mitigate the safety issues known for conventional Li-ion batteries, and provide enhanced energy densities, by replacing the organic electrolyte solutions with solid inorganic equivalents. Mechanical and (electro)chemical incompatibilities between the ASSB solid components, however, lead to high resistances, curtailing the Li-ion transport at their interfaces. In this talk, we introduce a high-throughput ab initio modelling approach towards the rational design of electrolyte/electrode interfaces in ASSBs. First, we obtain phase diagrams of sulfide-based electrolytes with diverse compositions, phases, vacancies and doping using the Ab Initio Random Structure Searching (AIRSS) method. Next, the stable and low-lying metastable phases are screened for their ionic conductivity using ab initio molecular dynamics simulations. Finally, diverse surfaces of the selected electrolyte phases are interfaced with the surfaces of electrodes or other interfacial (e.g. solid electrolyte interphase, SEI) layers to determine the stable combinations using an automated procedure (INTERFACER). The devised approach will be demonstrated in action for a collection of interfaces, e.g. Li-P-S electrolytes with LiCo<sub>2</sub>, Li-metal electrodes and alike.

DS 13.5 Tue 15:15 H9

**New Insights into Amorphous Materials and their Surfaces by Combining Machine Learning and DFT** — ●VOLKER DERINGER — University of Cambridge, Cambridge, UK

Understanding links between atomic structure, chemical reactivity, and physical properties in amorphous solids is a long-standing challenge. DFT-based atomistic simulations have played important roles in this, but come at high computational cost. Novel interatomic potentials based on machine learning (ML) achieve close-to DFT accuracy, but require only a small fraction of the cost. In this talk, I will argue that such ML-based potentials are particularly useful for studying amorphous solids.

First, I will describe a Gaussian Approximation Potential (GAP) for amorphous carbon, which we recently used to simulate the deposition of tetrahedral amorphous carbon (*ta-C*) films, one atom at a time. These simulations reproduced the experimentally observed count of sp<sup>3</sup> atoms and gave new insight into the microscopic growth mechanism. I will then discuss how ML-based potentials can be combined with density-functional methods to yield new insights into surface functionalization (specifically, hydrogenation and oxidation) of *ta-C*. Finally, I will present recent work on amorphous silicon, another prototypical non-crystalline material that ML-driven simulations can describe with high accuracy. Looking ahead, these studies suggest that ML-based potentials may become more widespread tools for the realistic modelling and understanding of the amorphous state.

DS 13.6 Tue 15:30 H9

**Harvesting from unbiased sampling of open systems: phase diagrams and property maps of surfaces and clusters in reactive atmosphere** — ●YUANYUAN ZHOU, MATTHIAS SCHEFFLER, and LUCA M. GHIRINGHELLI — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Numerous processes that occur at surfaces of materials play a critical role in the manufacture and performance of functional materials, e.g., electronic, magnetic, and optical devices, sensors, catalysts, and coatings. A prerequisite for analyzing and understanding the electronic properties and the function of surfaces is detailed knowledge of the atomic structure, i.e., the surface composition and geometry under realistic condition. We introduce a Replica-Exchange (RE) Grand-Canonical (GC) Monte-Carlo algorithm. By means of the coupled sampling at several chemical potentials (i.e., partial pressures) of a reactive gas atmosphere and temperatures, the REGC scheme enables the unbiased calculation of (*p*, *T*) phase diagrams of surfaces, nanoparticles, or clusters in contact with reactive atmosphere, where all anharmonic contributions are included. Moreover, the multi-canonical sampling yields the temperature-pressure dependence (map) of all equilibrium observables that can be measured within the given model Hamiltonian. For instance, structural parameters such as the radial distribution function, or the fundamental electronic gap. This allows for rational design, where *operando* condition are taking fully into account. We demonstrate the approach for model Lennard-Jones surfaces as well as Si clusters and surfaces in a hydrogen atmosphere.

DS 13.7 Tue 15:45 H9

**Crystal structure prediction for high capacity battery materials** — ●ANGELA F HARPER<sup>1</sup> and ANDREW J MORRIS<sup>2</sup> — <sup>1</sup>Department of Physics, University of Cambridge, JJ Thomson Ave, Cambridge CB3 0HE, UK — <sup>2</sup>School of Metallurgy and Materials, University of Birmingham, Edgbaston, Birmingham, UK

The future of large-scale energy storage relies heavily on the ability of Li-ion batteries to have high capacity and long-term stability. At present, graphite anodes limit the overall capacity of Li-ion batteries to a theoretical maximum of 372 mAh/g, and thus there is a need for higher capacity anodes such as phosphorus. We have studied lithiation in phosphorus using a combination of *ab initio* random structure searching (AIRSS) and density-functional theory calculations. In the Li-P system we found a novel phase of P<sub>21</sub>2<sub>1</sub>2<sub>1</sub> Li<sub>4</sub>P<sub>3</sub>, which showed stable 0K phonon modes [1]. We further showed, using defect AIRSS searches, that doping the known Li-P phases with aluminium improved their electronic density of states at the Fermi level, and could improve conductivity in phosphorus anodes. To improve the cyclability of these phosphorus anodes, which break down after several cycles due to volume expansion of over 200%, in this talk we will investigate the phase diagrams and voltage profiles of several ternary compounds of Li-P-M where M is a metallic element which maintains the conductivity of aluminium doping and adds stability to the anode.

[1] Mayo, M. et al. Chem. Mater. 2016, 28, 2011\*2021

DS 13.8 Tue 16:00 H9

**Constructing Accurate Machine Learning Force Fields for Flexible Molecules** — ●VALENTIN VASSILEV-GALINDO, IGOR POLTAVSKY, and ALEXANDRE TRATCHENKO — Physics and Material Science Research Unit, University of Luxembourg, Luxembourg

State-of-the-art machine learning (ML) models can reproduce potential energy surfaces (PES) for molecules containing up to a few tens of atoms with the accuracy comparable to the most exact ab initio methods. This provides a unique tool for computing different thermodynamic properties that would require millions of CPU years otherwise. For instance, a recently developed sGDML[1,2] model predicts forces and energy with CCSD(T) accuracy using just a few hundreds of configurations for training. However, up to now ML has been mainly applied to rather rigid molecules. In this regard, our objective is to test ML for flexible molecules and out-of-equilibrium configurations along transition paths. For this, we select molecules (e.g. azobenzene, stilbene) with relatively complex transition paths, which result from an interplay between long- and short-range interactions. Then, different paths connecting PES minima are tested using sGDML. This allows us to define optimal descriptors and the most appropriate strategies for choosing the training sets, which is crucial for ML models relying on a limited number of training points. Our results open an avenue for efficiently calculating transport pathways, transition rates and other out-of-equilibrium properties with previously unattended accuracy.

- [1] Chmiela, S. et al., *Sci. Adv.* 3, e1603015 (2017).  
 [2] Chmiela, S. et al., *Nat. Commun.* 9, 3887 (2018).

DS 13.9 Tue 16:15 H9

**Calculating critical temperatures for magnetic order in two-dimensional materials** — ●DANIELE TORELLI — CAMD, Department of Physics, Technical University of Denmark, 2820 Kgs. Lyngby, Denmark

Recent observation of ferromagnetic out-of-plane order in two-dimensional (2D) CrI<sub>3</sub> highlights the importance of a microscopic understanding of magnetic anisotropy (MA) in ground state magnetic systems. Single-ion anisotropy and anisotropic exchange coupling comprise crucial ingredients to escape the Mermin-Wagner theorem which implies that rotational symmetry cannot be spontaneously broken at any finite temperature in 2D and thus prevents magnetic order.

In the present work we investigate the variation of critical temperature in Heisenberg model systems using classical Metropolis Monte Carlo simulations. A fit for square, hexagonal and honeycomb lattices leads to a simple expression for the critical temperatures as a function of MA and exchange coupling constants.

Based on a new developed computational 2D materials database, we predict 2D structures with high critical temperatures and high thermodynamic and dynamic stability for future experimental investigations. As testing system, relevant Heisenberg exchange couplings and MA energies in mono-layer CrI<sub>3</sub> are obtained from first principle calculations and energy mapping analysis, yielding to an estimation of Curie

temperature in good agreement with experimental results.

DS 13.10 Tue 16:30 H9

**Amino-acids on metallic surfaces: searching conformational space** — ●DMITRII MAKSIMOV, CARSTEN BALDAUF, and MARIANA ROSSI — Fritz-Haber-Institut der Max-Planck- Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Organic-inorganic interfaces are challenging for computational modeling, in particular regarding the prediction of stable configurations at the interface, which determine the electronic properties of the system as a whole. The amino acid arginine is a flexible molecule in the gas phase and experiments show its self-assembly into dimers, rings, and chains on Ag(111) and Au(111) surfaces. For two protonation states (neutral Arg and charged ArgH<sup>+</sup>), we perform systematic structure searches by placing known gas-phase minima in different orientations on top of the surfaces, followed by full relaxation within long-range dispersion corrected density-functional theory (DFT). In the analysis, we aim at understanding the alterations of the conformational space from the gas phase to surface adsorption by means of a dimensionality-reduced representation based on a combination of the Smooth Overlap of Atomic Positions (SOAP) and the Sketchmap techniques [1]. The favorable interaction with the metallic surface reduces the number of accessible conformations for neutral Arg. For the adsorption of charged ArgH<sup>+</sup>, the number of local minima increases due to surface-dependent partial charge screening. [1] S. De et al., *J. Cheminform.*, **9:6** (2017)

## DS 14: Poster

Time: Tuesday 17:00–20:00

Location: Poster E

DS 14.1 Tue 17:00 Poster E

**Grain Boundaries Act as Solid Walls for Charge Carrier Diffusion in Large Crystal MAPI Thin Films** — ●FRANK SCHÄFER<sup>1</sup>, RICHARD CIESIELSKI<sup>1</sup>, NICOLAI HARTMANN<sup>1</sup>, NADJA GIESBRECHT<sup>1</sup>, THOMAS BEIN<sup>1</sup>, PABLO DOCAMPO<sup>2</sup>, and ACHIM HARTSCHUH<sup>1</sup> — <sup>1</sup>Department Chemie und Center for Nanoscience (CeNS), LMU München, Deutschland — <sup>2</sup>School of Electrical and Electronic Engineering, Newcastle University, United Kingdom

Micro- and nanocrystalline methylammonium lead iodide (MAPI)-based thin-film solar cells today reach power conversion efficiencies of over 20%. We investigate the impact of grain boundaries on charge carrier transport in large crystal MAPI thin films using time-resolved photoluminescence (PL) microscopy and numerical model calculations. Crystal sizes in the range of several tens of micrometers allow for the spatially and time resolved study of boundary effects. Whereas long-ranged diffusive charge carrier transport is observed within single crystals, no detectable diffusive transport occurs across grain boundaries. The observed PL transients are found to crucially depend on the microscopic geometry of the crystal and the point of observation. In particular, spatially restricted diffusion of charge carriers leads to slower PL decay near crystal edges as compared to the crystal center. In contrast to many reports in the literature, our experimental results show no quenching or additional loss channels due to grain boundaries for the studied material, which thus do not negatively affect the performance of the derived thin-film devices.

DS 14.2 Tue 17:00 Poster E

**2D Fluorescence Spectroscopy for Monitoring Photo-induced Degradation in Metal Halide Perovskite** — ●ALEXANDROS KILIGARIDIS<sup>1</sup>, ABOMA MERDASA<sup>2</sup>, CAROLIN REHERMANN<sup>2</sup>, MOJTABA ABDI-JALEBI<sup>3</sup>, JONAS STÖBER<sup>1</sup>, BORIS LOUIS<sup>1</sup>, MARINA GERHARD<sup>1</sup>, SAMUEL D. STRANKS<sup>3</sup>, EVA L. UNGER<sup>1,2</sup>, and IVAN G. SCHEBLYKIN<sup>1</sup> — <sup>1</sup>Chemical Physics and NanoLund, Lund University, PO Box 118, 22100 Lund, Sweden. — <sup>2</sup>Young Investigator Group Hybrid Materials Formation and Scaling, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein Strasse 16, 12489 Berlin, Germany — <sup>3</sup>Cavendish Laboratory, Department of Physics, University of Cambridge, JJ Thomson Avenue, Cambridge CB3 0HE, United Kingdom

One of the vital factors in one day achieving long-lifetime perovskite devices is tackling the obstacle of chemical instability observed in halide perovskites upon illumination and in combination with the presence of oxygen and/or water.

In a recent series of studies we employ a novel 2D fluorescence

method to shed light to underlying degradation mechanisms and their correlation to external environmental factors. We use this method to spatially probe thin films as well as micro/nano-sized single perovskite crystals to produce excitation-emission matrices and utilize them as a type of degradation fingerprints. The diffraction limited resolution of the measurements enables the comparison between different morphological surface structures on thin perovskite film and their tendency to photo-degrade in various environments.

DS 14.3 Tue 17:00 Poster E

**Electric field induced quenching of photoluminescence in individual CH<sub>3</sub>NH<sub>3</sub>PbX<sub>3</sub> (X=I, Br) nanocrystals** — RUIYUN CHEN<sup>1,2</sup>, ●JUN LI<sup>1</sup>, ALEXANDER DOBROVOLSKY<sup>1</sup>, SORANYEL GONZÁLEZ-CARRERO<sup>3</sup>, MARINA GERHARD<sup>1</sup>, VLADIMIR CHIRVONY<sup>3,4</sup>, JULIA PÉREZ-PRieto<sup>3</sup>, and IVAN SCHEBLYKIN<sup>1</sup> — <sup>1</sup>Division of Chemical Physics and NanoLund, Lund University, Lund 22362, Sweden — <sup>2</sup>State Key Laboratory of Quantum Optics and Quantum Optics Devices, Institute of Laser Spectroscopy, Shanxi University, Taiyuan 030006, China — <sup>3</sup>Instituto de Ciencia Molecular, Universidad de Valencia, c/Catedrático J. Beltrán, 2, Paterna 46980, Spain — <sup>4</sup>UMDO (Unidad de Materiales y Dispositivos Optoelectrónicos), Instituto de Ciencia de los Materiales, Universidad de Valencia, Valencia 46071, Spain

Metal halide perovskites have attracted lots of attention because of extraordinary performance of these solution-processed materials in optoelectronics. However, the even higher efficiency and much better stability are wanted for their practical applications. Therefore, a deeper physical understanding of the charge carrier dynamics and the ion migration in the perovskite semiconductors are required to overcome these limitations. Here, we found that the external alternating electric field (EF) quenches the photoluminescence (PL) of individual CH<sub>3</sub>NH<sub>3</sub>PbX<sub>3</sub> (X=I, Br) nanocrystals. After switching off the alternating EF, the PL intensity recovered within several minutes. However, constant EF showed very little quenching effect compared with alternating. The physical mechanism behind this will be discussed.

DS 14.4 Tue 17:00 Poster E

**Compositional Variation in Inkjet-Printed Lead Halide Perovskite** — ●HAMPUS NÄSSTRÖM<sup>1</sup>, FLORIAN MATHIES<sup>1</sup>, THOMAS UNOLD<sup>2</sup>, and EVA UNGER<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Young Investigator Group Hybrid Materials Formation and Scaling, Berlin, Germany — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Department Structure and Dynamics of Energy Materials, Berlin, Germany

Lead halide perovskites, APbX<sub>3</sub>, have recently proved an excellent absorber material for photovoltaic devices. Through variation of the cation, A, and halide, X, as well as mixing two or more of these, a huge variety of absorber materials are achievable. In this work, we present how controlled compositional variations within a sample of lead halide perovskite can be obtained via inkjet printing. Furthermore, we show how the variation in absorption, absolute photoluminescence and mobility throughout the sample can be correlated to the power conversion efficiencies of photovoltaic devices with the corresponding composition. This correlation provides us with a method for fast screening of potential absorber materials for photovoltaic applications without device manufacturing.

DS 14.5 Tue 17:00 Poster E

**Lecker im Licht, Wie beeinflusst die Beleuchtung das Aussehen unserer Supermarktwaren?** — CAROLIN MANTSCH und •THOMAS GRILLENBECK — Ignaz-Günther Gymnasium Rosenheim

Mit allen möglichen Tricks versuchen Supermärkte die Kunden zum Kauf zu animieren. Das Licht wird an den Supermarkttheken gezielt eingesetzt, sodass Obst und Gemüse besonders frisch, knackig aussehen oder Fleisch besonders saftig, frisch erscheint. Frischwaren welken/reifen im Laufe der Zeit. Meine innovative Idee ist deshalb, die LEDs jederzeit genau an die Warenfarbe anzupassen. Tomaten, die mit der Zeit reifen, werden demnach zu Beginn stärker beleuchtet, als die gereiften Tomaten. Dafür habe ich einen LED-Lichtmischer (RBG) nachgebaut, damit sich daraus ein, auf den Reifegrad der Frischwaren, regelbarer Lichtmischer entwickeln kann. In meiner Arbeit wird gezeigt, wie ein Reflexionsspektrum entsteht und dass dieses in verschiedenen Methoden gemessen werden kann. Außerdem wurde mit einer aufgestellten Formel veranschaulicht, wie der Sinneseindruck im Auge entsteht und an einem Rechenbeispiel verdeutlicht, dass diese Formel im Rahmen kleiner Fehlerquellen ausführbar ist.

DS 14.6 Tue 17:00 Poster E

**Fabrication of nanostructured oxides by focused electron beam induced processing** — •ELIF BILGILISOY, CHRISTIAN PREISCHL, FLORIAN VOLLNHALS, and HUBERTUS MARBACH — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen, Germany

We explored techniques employing a highly focused electron beam in UHV for the controlled fabrication of nanostructured oxide surfaces. This can be done by electron beam induced local modification of the substrate such that it becomes active towards the decomposition of subsequently dosed precursor molecules, referred to as electron beam induced surface activation (EBISA)[1]. The initial deposits might grow autocatalytically upon prolonged precursor dosage already at room temperature in our UHV instrument. EBISA requires a surface that can be correspondingly activated by the electron beam. We could identify oxides like Si<sub>x</sub>O<sub>y</sub> and TiO<sub>2</sub> as suitable candidates [2, 3]. Thereby EBISA worked successfully with Fe(CO)<sub>5</sub> and Co(CO)<sub>3</sub>NO depending on the actual substrate partially with chemical selectivity. As activated sites we could identify reactive oxygen vacancies created through electron beam induced stimulated oxygen desorption. Along with the presentation of these results, we will also demonstrate first successful results on Cobalt oxide generalizing the EBISA process on oxides.

[1] Marbach, H., Applied Physics A, 117(3): p. 987-995 (2014).

[2] Drost, M., et al., Small methods, 1(6): p. 1700095 (2017).

[3] Walz, M.-M., et al., Physical Chemistry Chemical Physics, 13(38): p. 17333-17338 (2011).

DS 14.7 Tue 17:00 Poster E

**Thin film investigations on the ferroelectric organic charge transfer salt TTF-Chloranil** — •LUKAS KELLER and MICHAEL HUTH — Institute of Physics, Goethe University, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

Tetrathiafulvalene-chloranil (TTF-CA) is an organic ferroelectric below  $T_C = 81$  K [1] whose bulk properties have been studied in some detail [2]. However, very limited research has been done on thin films despite the strong dependence of the paraelectric to ferroelectric phase transition on strain which can most easily be tailored in thin film structures [3]. Moreover, the ferroelectric phase coexists with a dimerized spin chain for which it is so far unclear whether it shows long-range order.

Here we present recent results of the electrical and dielectric properties of TTF-CA thin films grown by molecular beam deposition. In particular we focus on the influence of the ferroelectric state of the layers on nearby metallic electrodes by way of surface scattering modi-

fications. Furthermore, we present results on the dielectric screening effect caused by the TTF-CA layer on the charge transport in a nano-granular metal layer in close proximity.

[1]: Torrance et al., Phys. Rev. Lett. 47, 24 (1981). [2]: Horiuchi et al., Chem. Lett. 43, 26 (2014). [3]: Huth et al., Mater. Res. Express 1, 046303 (2014)

DS 14.8 Tue 17:00 Poster E

**Direct Write, Free Form 3D Nanomagnetism** — •LUKAS KELLER and MICHAEL HUTH — Institute of Physics, Goethe University, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

3D nano-printing by focused electron beam induced deposition (FEBID) has matured to a level that highly complex and functional deposits are becoming available for nanomagnetism [1] and plasmonics.

Our pattern file generator program [2], which defines the electron beam movement at any time during the deposition, handles precursor dynamic related issues like proximity effects and corrects for height-dependent precursor coverage. The target geometry can be defined by hand or using powerful 3D software tools like "blender" [3].

Here we present a selection of successfully deposited magnetic 3D nano-structures, generated with our implementation of a pattern file generator, and some measured hysteresis loops of their magnetic stray field. We demonstrate that also 3D mixed material structures are available by combining ferromagnetic with paramagnetic 3D elements.

[1]: Scientific Reports 8, 6160 (2018)

[2]: Beilstein J. Nanotechnol., 9, 2581-2598 (2018)

[3]: <https://youtu.be/v8s24WvGj9E>

DS 14.9 Tue 17:00 Poster E

**Magnetization Reversal of Individual Three Dimensional (3D) Fe-Co Nanostructures** — •MOHANAD AL MAMOORI<sup>1</sup>, LUKAS KELLER<sup>1</sup>, MICHAEL HUTH<sup>1</sup>, CHRISTIAN SCHRÖDER<sup>2</sup>, and JENS MÜLLER<sup>1</sup> — <sup>1</sup>Institute of Physics, Goethe University Frankfurt — <sup>2</sup>Institute for Applied Materials Research, Bielefeld University of Applied Sciences

Three dimensional (3D) magnetic nanostructures are promising for future magnetic memory and sensing applications, in particular since more complex magnetic configurations become possible when expanding 2D nanomagnets to the third dimension. In [1,2], we have employed focused electron beam induced deposition (FEBID) to grow 3D nanomagnets in combination with a micro-Hall sensor acting as substrate and high-resolution detection device of small magnetic stray fields. We find that the magnetisation reversal propagates by multi-domain switching scenarios. In this presentation, firstly, systematic measurements of the magnetic stray fields of Fe-Co nano-cubes and -trees as a function of temperature and magnetic field applied at different angles, will be reported. Secondly, in order to gain further insights in the hysteresis loops, (irreversible) magnetic interaction effects and coercivity distributions, first-order-reversal curves (FORC) of these 3D nanomagnets supported by simulations of a simple macro-spin model, will be shown. Finally, an outlook to the future design of such structures towards the realization of 3D artificial spin ice architectures will be given. [1] L.Keller et al., *Sci. Rep.* **8**, 6160 (2018). [2] M. Al Mamoori et al., *Materials* **11**, 289 (2018).

DS 14.10 Tue 17:00 Poster E

**The microscopic structure of ballistic graphene nanoribbons** — •MARKUS GRUSCHWITZ, THI THUY NHUNG NGUYEN, HERBERT SCHLETTER, STEFFEN SCHULZE, and CHRISTOPH TEGENKAMP — Institut für Physik, TU Chemnitz, Germany

Epitaxial graphene nanoribbons on SiC were shown to host ballistic transport channels, even under ambient conditions [1]. Thereby, the transport of these 40nm wide ribbons, which are grown via self-assembly on sidewalls of SiC(0001) mesa structures, depends crucially on atomistic details of the structure [2]. Here we present high resolution STM and TEM investigations done on such ribbons.

For ribbons along the [1100]-direction STM reveals a continuous graphene layer with a zig-zag edge structure. Thereby, the lower edge merges into the SiC(0001) terrace giving rise to hybridization and formation of an edge state. This growth mode is confirmed by S/TEM investigations. Cross sectional STEM reveals freestanding graphene separated from the facet by more than three times the distance of graphene on SiC(0001). Moreover, the EDX and EELS capabilities of the HRTEM were used to characterize the surface near areas in detail. Upon growth of graphene by desorption of silicon by high temperature annealing, the first 6H-SiC unit cell reveals sp<sup>2</sup>-hybridization coming along with Si deficiency. Compared to the facets, it turns out that

these residual imperfections in SiC are more frequent at terraces, which supports higher Si-evaporation rate at the mesas in order to grow selectively graphene nanoribbons. References: [1] J. Aprozanz et al., Nat. Comm. 9, 4426, (2018). [2] A.A Zakharov et al., arXiv:1809.10001

DS 14.11 Tue 17:00 Poster E

**Tunable 2D electron gas at the LaAlO<sub>3</sub>/SrTiO<sub>3</sub>(001) interface** — IGOR MAZNICHENKO<sup>1</sup>, SERGEY OSTANIN<sup>1</sup>, ARTHUR ERNST<sup>2,3</sup>, and INGRID MERTIG<sup>1,2</sup> — <sup>1</sup>Institute for Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany — <sup>2</sup>Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — <sup>3</sup>Institute for Theoretical Physics, Johannes Kepler University, Altenberger Straße 69, 4040 Linz, Austria

Currently, the formation of a two-dimensional electron gas (2DEG) at the TiO<sub>2</sub>/LaO-terminated interface of LaAlO<sub>3</sub>/SrTiO<sub>3</sub> (LAO/STO) is well understood. The LAO critical thickness of four unit cells needed to measure the 2DEG was established. Here, we show how 2DEG can be tuned externally by changing electronic balance at the LAO(001) surface or, alternatively, at the intrinsically hole-doped AlO<sub>2</sub>/SrO interface of LAO/STO heterostructures. The effects of liquid gating at LAO(001) and imperfect AlO<sub>2</sub>/SrO were simulated in the framework of the first-principles Green function method within a coherent potential approximation. We evaluated the Fermi surface cross sections and effective masses of the 2DEG carriers, which were computed upon the degree of external chemical disorder. These findings may be extremely important for applications of 2DEG.

DS 14.12 Tue 17:00 Poster E

**Impact of long-range disorder on the 2D electron gas formation at a LaAlO<sub>3</sub>/SrTiO<sub>3</sub> interface** — IGOR MAZNICHENKO<sup>1</sup>, SERGEY OSTANIN<sup>1</sup>, ARTHUR ERNST<sup>2,3</sup>, and INGRID MERTIG<sup>1,2</sup> — <sup>1</sup>Institute for Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany — <sup>2</sup>Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — <sup>3</sup>Institute for Theoretical Physics, Johannes Kepler University, Altenberger Straße 69, 4040 Linz, Austria

A two-dimensional electron gas (2DEG) can be formed at an interface between two insulators such as LaAlO<sub>3</sub> and SrTiO<sub>3</sub> without any additional doping. Nevertheless, structural imperfections or defects at the interface, which may arise during the growth process or be of another origin, can definitely affect 2DEG properties either increasing or reducing the 2DEG density. In this work, we study 2DEG formation at both perfect and imperfect interfaces of LaAlO<sub>3</sub>/SrTiO<sub>3</sub> heterostructures in the framework of the density functional theory. Using a first-principles Green function method within a coherent-potential approximation, we investigate consistently the development of the 2DEG density starting from a defectless interface and introducing sequentially various kinds of long-range disorder such as cation intermixing and oxygen vacancies. Finally, we evaluate the 2DEG carrier density from the Fermi surface cross sections and effective masses of the carriers, which may be directly related to the multiple transport phenomena in the system [1].

[1] I. V. Maznichenko et al, Phys. Rev. Materials 2, 074003 (2018).

DS 14.13 Tue 17:00 Poster E

**Characterization of electron emission from diamond-coated tungsten tips** — ALEXANDER TAFEL<sup>1</sup>, MINGJIAN WU<sup>2</sup>, ERDMANN SPIECKER<sup>2</sup>, PETER HOMMELHOFF<sup>1</sup>, and JÜRGEN RISTEIN<sup>1</sup> — <sup>1</sup>Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen — <sup>2</sup>Institute of Micro- and Nanostructure Research & Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

Coating metal needle tips with diamond promises a robust high brightness photocathode useful for dielectric laser acceleration and time resolved electron microscopy and diffraction. The chemical and structural properties of tungsten tips coated with nanocrystalline diamond are thoroughly characterized. Electron diffraction and electron energy loss spectroscopy (EELS) confirm the presence of diamond with 20 nm sized columnar grains. Transmission electron microscopy and STEM-EELS reveal graphitic paths between diamond grains. The graphitic grain boundaries provide sufficient conductivity for the feedback of emitted electrons from the surface and - in case of surface hydrogen termination - the negative electron affinity of diamond substantially increases the electron yield. We present first experimental results of electron emission from diamond coated tips both in continuous field emission and femtosecond laser-triggered mode.

DS 14.14 Tue 17:00 Poster E

**Temperaturabhängige Untersuchung des spezifischen elektrischen Widerstandes von Schichten aus MoN<sub>x</sub>** — SABINE STÜCK<sup>1</sup>, MARTIN KOMMER<sup>2</sup>, MARTIN BALZER<sup>2</sup>, MARTIN FENKER<sup>2</sup> und FRANK SCHMIDL<sup>1</sup> — <sup>1</sup>Friedrich-Schiller Universität Jena, Physikalisch-Astronomische Fakultät, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena — <sup>2</sup>Forschungsinstitut Edelmetalle+Metallchemie, Katharinenstraße 17, 73525 Schwäbisch Gmünd

Wir untersuchen Schichten aus Molybdänitrid (MoN<sub>x</sub>), die mittels HiPIMS und PLD hergestellt wurden, auf ihre strukturellen und elektrischen Eigenschaften. Besonderes Augenmerk liegt auf der Temperaturabhängigkeit des spezifischen elektrischen Widerstandes.

Neben der stöchiometrischen Zusammensetzung der Schichten, werden die aufgefundenen Phasen und die Kristallinität gezeigt und diskutiert. Für die strukturellen Untersuchungen kommen hier unter anderem AES und Röntgenbeugungsmethoden zum Einsatz. Schwerpunkt der Untersuchung stellt die temperaturabhängige Messung des spezifischen elektrischen Widerstandes dar. Dessen ungewöhnliche Temperaturabhängigkeit wird hier erörtert. Die Schichten werden bis in den einstelligen Kelvinbereich vermessen, sodass sich ein Übergang in die supraleitende Phase einstellt. Die kritischen Temperaturen ( $T_C$ ) sowie die kritischen Stromdichten ( $j_C$ ) der Schichten werden bestimmt.

DS 14.15 Tue 17:00 Poster E

**Ultrafast energy transport in nanoscopic metal-insulator multilayers - Electrons vs. phonons** — MARC HERZOG<sup>1</sup>, JAN-ÉTIENNE PUDELL<sup>1</sup>, ALEXANDER VON REPPERT<sup>1</sup>, ALEXEI MAZNEV<sup>2</sup>, MATTHIAS KRONSEDER<sup>3</sup>, CHRISTIAN BACK<sup>3,4</sup>, GREGORY MALINOWSKI<sup>5</sup>, and MATIAS BARGHEER<sup>6</sup> — <sup>1</sup>Institut für Physik und Astronomie, Universität Potsdam — <sup>2</sup>Dept. of Chemistry, MIT — <sup>3</sup>Institut für Experimentelle und Angewandte Physik, Universität Regensburg — <sup>4</sup>Fakultät für Physik, TU München — <sup>5</sup>Institut Jean Lamour, Université Lorraine — <sup>6</sup>Helmholtz-Zentrum Berlin

The transport of heat (or energy in general) in nanoscopic heterostructures is of great interest on a fundamental as well as a technological level, e.g. in the context of thermal management in devices or heat-assisted magnetic recording. In metal-insulator metastructures heat can be conducted by diffusion of electrons and/or lattice vibrations. Using time-resolved x-ray diffraction, we recently observed a surprisingly large thermal equilibration time between two ultrathin films of Au and Ni of more than 80 ps [1]. A detailed analysis revealed a significant contribution of lattice heat transport although electrons typically dictate the thermophysical properties in these metals. Here, we extend such experiments to metallic multilayers with an incorporated few-nm insulating MgO layer to suppress electron transport and calibrate the heat transport by phonon diffusion. At length scales smaller than the phonon mean free path ballistic transport is expected to efficiently contribute. We thus discuss the possibility of ballistic phonon transport in such systems. [1] Pudell et al. Nat. Commun. 9, 3335 (2018).

DS 14.16 Tue 17:00 Poster E

**Spatiotemporal control of surface acoustic waves (SAW), surface skimming longitudinal wave (SSLW) and static surface deformation** — JAN-ÉTIENNE PUDELL<sup>1</sup>, MARC HERZOG<sup>1</sup>, MATTHIAS SANDER<sup>2</sup>, DANIEL SCHMIDT<sup>3</sup>, MATIAS BARGHEER<sup>1,4</sup> und PETER GAAL<sup>3</sup> — <sup>1</sup>Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — <sup>2</sup>ESRF - The European Synchrotron CS40220 38043 Grenoble Cedex 9 France — <sup>3</sup>Institut für Nanostruktur und Festkörperphysik, Universität Hamburg, 20355 Hamburg, Germany — <sup>4</sup>Helmholtz Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany

We present control of coherent and incoherent deformations in solids on sub-nanosecond timescales using a temporal and spatial sequence of optical excitation pulses. For this purpose, we introduce an experimental setup that exerts control of the spatial overlap of subsequent excitations via the polarization of the optical excitation pulse. Specific exemplary coherent control cases are discussed theoretically and compared to experimental data. As application we show the characterization of SAW and SSLW modes by suppressing the other mode respectively. Therefore, we use a thin film yttrium trioxomanganate on Ytria-stabilized zirconia substrate.

DS 14.17 Tue 17:00 Poster E

**Effects of screening on the optoelectronic properties of 2D materials** — ABDERREZAK TORCHE, JENS HÜHNERT, and GABRIEL BESTER — University of Hamburg, Hamburg, Germany



2D materials represent nowadays a promising route for new technologies due to their exceptional optical and electronic properties. These properties are highly dependent on the surrounding environment, consequently, one can modify a desired property such as the band gap or the doping simply by changing the environment. Despite the fact that 2D materials have been studied since the discovery of graphene in 2004, both at the experimental and the theoretical levels, the understanding of the effects of screening (e.g. substrate effects) is still not complete although some general rules are well established.

From a theoretical point of view, the study of screening in 2D materials is computationally heavy. Standard approaches to study the optical properties of materials, such as the BSE formalism, have several limitations because the inclusion of the environment hinders the calculation of quasi-particle energies in 2D.

The goal of our research is to go beyond these limitations and treat larger systems (i.e. thousands of atoms) which are more relevant from an experimental (and/or industrial) point of view. For that goal, we propose a hybrid approach combining density functional theory and configuration interaction methods to predict the binding energies of excitations in 2D materials (excitons, trions, ...) taking the effect of the environment into account via screening.

DS 14.18 Tue 17:00 Poster E

**Origin of Ferrimagnetic Properties in Disordered Spinel Ferrite Thin Films** — ●VITALY ZVIAGIN<sup>1</sup>, PAULA HUTH<sup>2</sup>, CHRIS STURM<sup>1</sup>, JÖRG LENZNER<sup>1</sup>, ANNETTE SETZER<sup>1</sup>, REINHARD DENECKE<sup>2</sup>, PABLO ESQUINAZI<sup>1</sup>, MARIUS GRUNDMANN<sup>1</sup>, and RÜDIGER SCHMIDT-GRUND<sup>1</sup> — <sup>1</sup>Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstr. 5, Germany — <sup>2</sup>Universität Leipzig, Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Linnéstr. 2, Leipzig

Spinel ferrite thin films,  $Zn_xFe_{3-x}O_4$  ( $0 \leq x \leq 1.26$ ) and  $ZnFe_2O_4$  (ZFO), were deposited on  $TiN/(100)MgO$  and  $(100)SrTiO_3$  substrates by pulsed laser deposition. The bulk as well as surface cation distribution was estimated from the relative strength of O 2p to Fe 3d and 4s electronic transitions in the dielectric function (DF) as well as analysis of Fe 3p and 2p XPS core level spectra, respectively. As the predominant cation configuration becomes less inverse with Zn increase from  $x = 0$  to 1.26, the surface becomes less deficient (abundant) in tetrahedral (octahedral)  $Fe^{3+}$  occupation, as compared to the bulk. The net magnetic response was related to the antiphase boundary and inhomogeneous composition defect formation. Bulk tetrahedral  $Fe^{3+}$  occupation in ZFO films was found to increase with the decrease in deposition temperature and was directly correlated to the increase in net magnetic response. The change in the ferrimagnetic order in the ZFO films was related to the bulk Fe distribution and is examined as a function of deposition as well as annealing temperature and atmosphere.

DS 14.19 Tue 17:00 Poster E

**Single-source, metalorganic, low-temperature growth of carbon nanowalls: the role of precursor dissociation** — ●SEBASTIAN TIGGES, AXEL LORKE, and NICOLAS WÖHRL — University of Duisburg-Essen and CENIDE, Faculty of Physics, 47057 Duisburg, Germany

Carbon nanowalls (CNWs) exhibit exceptional thermal as well as electrical conductivity and adjustable surface area. This makes them especially attractive for energy technologies (such as fuel cells) and application in sensors. Here, we investigate different CNW structures deposited at remarkably low temperatures (ca. 350°C). In an inductively coupled plasma-enhanced chemical vapour deposition system, specific morphologies are obtained by tuning essential process parameters such as flow rate of precursor gas and process pressure. Scanning electron microscopy reveals three distinct CNW structures of varying morphology and inter-wall distance. Raman spectroscopy shows significant variation in both defect density and defect type, depending on morphology. Additionally, X-ray photoelectron spectroscopy and Auger microscopy is used to determine the overall and spatially resolved chemical composition of different morphologies. Plasma characterization, specifically determination of the number density of light-emitting species in the plasma, is done by optical emission actinometry. It is illustrated, how the formation of individual morphologies is depending on the residence time of the complex precursor molecule, which is used as the carbon source in the process. From these observations a simple growth model is derived.

DS 14.20 Tue 17:00 Poster E

**Sputter Deposition of Chalcogenide Superlattices with Varying Interfacial Diffusion** — ●PETER KERRES, HENNING HOLLER-MANN, KAI SCHEUVENS, MATTHIAS DÜCK, and MATTHIAS WUTTIG — I. Institute of Physics (IA), RWTH Aachen University

Superlattices consisting of thin layers of germanium telluride (GeTe) and antimony telluride ( $Sb_2Te_3$ ) are currently considered as energy efficient phase-change memory devices. In order to unravel the detailed switching mechanism, the determination of the superlattice structure is crucial. Sputter deposition of the constituents offers a broad parameter window, thereby enabling a systematic investigation of samples with varying structure and morphology. This study focusses on the interdiffusion at adjacent GeTe/ $Sb_2Te_3$  heterointerfaces employing X-Ray Diffraction (XRD). A series of superlattice samples has been deposited on a mica substrate, while the amount of interdiffusion is varied with the applied deposition temperature. Structural changes in the samples are monitored with  $\theta - 2\theta$  XRD scans. The significant changes in the measurements are then compared with simulations, which take the disorder into account.

DS 14.21 Tue 17:00 Poster E

**Ion-beam sputtering of tungsten oxide** — ●MARIO GIES, MARTIN BECKER, FABIAN MICHEL, and ANGELIKA POLITY — Institute for Exp. Physics I and Center for Materials Research (LaMa), Justus Liebig University Giessen, Germany

Tungsten oxide films were prepared on glass substrates coated with fluorine-doped tin oxide (FTO) by ion-beam sputtering from a metallic tungsten target using different gas mixtures of argon and oxygen. The films were deposited at various growth temperatures between 100 and 400°C. The different growth temperatures allow the systematic adjustment of crystallinity between amorphous and polycrystalline tungsten oxide. At those temperatures a series of samples were created in which the oxygen flow rate was varied between 5 and 10 sccm. The results show that the choice of different oxygen flows during the deposition permits the creation of thin films with varying optical properties. Out of this, the various compositions of the films could be estimated. Besides those main series, hydrogen-doped films were deposited under the use of hydrogen as additional reactive gas during the sputtering process. All samples were investigated regarding different aspects like crystallinity, composition, morphology, optical properties and electrochromic behavior.

DS 14.22 Tue 17:00 Poster E

**Hydrophobic and hydrophilic silica shells on metal nanoparticles via plasma-enhanced in-flight coating process** — LISA WURLITZER<sup>1,2</sup>, PATRICK POST<sup>3</sup>, ●SIMON HOMANN<sup>1,2</sup>, WOLFGANG MAUS-FRIEDRICHS<sup>1,2</sup>, and ALFRED WEBER<sup>3</sup> — <sup>1</sup>Institute of Energy Research and Physical Technology, Leibnizstraße 4, 38678 Clausthal-Zellerfeld, Germany — <sup>2</sup>Clausthal Centre of Material Science, Agricolastraße 2, 38678 Clausthal-Zellerfeld, Germany — <sup>3</sup>Institute of Particle Technology, Leibnizstraße 19, 38678 Clausthal-Zellerfeld, Germany

Coated nanoparticles have a wide variety of applications in modern material science because of their interesting properties.  $TiO_2$ -nanoparticles for example are used in sunscreen, because of their photocatalytic activity. The goal of this work is to produce silica shells with metal and  $TiO_2$  as core-materials for a targeted creation of hydrophilic and hydrophobic layers.  $SiO_2$  is the here desired shell material because of its chemical inertness and optical transparency. This is archived with a modified method of an in-flight plasma-enhanced-chemical-vapor-deposition (PECVD) using a non-thermal dielectric barrier discharge. Tetraethyl orthosilicate (TEOS) and hexamethyldisiloxane (HMDSO) were used as precursors. The coated particles are studied via x-ray photoelectron spectroscopy (XPS). Results show a hydrophilic coating of silica-organic material on platinum using HMDSO, while the deposition of TEOS on  $TiO_2$  results in a hydrophobic, inorganic silica shell.

DS 14.23 Tue 17:00 Poster E

**Unraveling the interplay of structure and electronic properties in the phase-change material compound family of GST** — ●CARL-FRIEDRICH SCHÖN, MATTHIAS DÜCK, and MATTHIAS WUTTIG — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

Phase-change materials (PCM) are a promising candidate for universal memory, as their optical reflectivity and electrical resistivity change considerably between the amorphous and the crystalline state. Devices utilizing that transition have recently been realized in the form of the

Micron/Intel Optane Memory. It is even more intriguing that some PCMs of the GeTe-SbTe compound family (GST) show the transition from insulating to metallic behavior (MIT) within the crystalline phase. Interlinked with disorder effects, this MIT's nature is unprecedentedly Anderson-like. While the understanding of the electronic properties is paramount, assumptions regarding band shape, effective mass and degeneracy at the L-point have yet to be proven. In this work, film thickness and the degree of disorder in terms of vacancy type, quantity and arrangement of GST thin films are varied. Growth control and structural characterization are employed to map the properties across the MIT, which is induced by the redistribution of randomly distributed vacancies to vacancy layers. The goal is to unravel the interplay of structure, morphology, band structure and electronic properties to gain insights into the mechanisms driving the MIT. The findings of this work are aimed to support the development of analogue neural computing units and multi-state memory devices.

DS 14.24 Tue 17:00 Poster E

**External C-ERDA and RBS analysis setup** — ●FELIX JUNGE<sup>1</sup>, MASAHIRO SAITO<sup>1,3</sup>, KIM HOLM<sup>1,2</sup>, FELIPE LIPP BREGOLIN<sup>1</sup>, and HANS HOFSSÄSS<sup>1</sup> — <sup>1</sup>II. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen Germany — <sup>2</sup>Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — <sup>3</sup>Toray Research Center Inc., 3-3-7, Sonoyama, Otsu, Shiga 520-0842, Japan

In this work we describe the new construction of the external analysis setup at the University of Göttingen, which is used to perform Rutherford backscattering (RBS) simultaneously to coincidence elastic recoil detection analysis (C-ERDA) under atmospheric pressure. In addition, thin layers of titanium were deposited to a Si<sub>3</sub>N<sub>4</sub> membrane and the RBS and C-ERDA spectra were recorded. Furthermore, polyamide and Mylar foils were measured as reference samples. The aim is to measure a depth profile of the hydrogen concentration in thin films and self supporting foils and thus to enable a quantitative elemental analysis of the light elements. Moreover, it is planned to load the titanium films with hydrogen and produce hydrogen containing amorphous carbon layers on Si<sub>3</sub>N<sub>4</sub> membranes.

DS 14.25 Tue 17:00 Poster E

**Depth profiling of PEALD-AlN films based on Al2p XPS peak decomposition** — ●ALI MAHMOODINEZHAD<sup>1,2</sup>, EMILIA POZAROWSKA<sup>1</sup>, KARSTEN HENKEL<sup>1,2</sup>, DIETER SCHMEISSER<sup>1</sup>, and JAN INGO FLEGE<sup>2</sup> — <sup>1</sup>Applied Physics and Sensor Technology, BTU Cottbus-Senftenberg — <sup>2</sup>Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg

AlN has remarkable properties (wide band gap, low electrical and thermal conductivity, high dielectric constant, piezoelectricity) and is attractive for (opto)electronic and sensor applications. However, high oxygen content within nitride films is always a critical issue due to the thermodynamically favorable oxidation against nitridation resulting in deteriorated materials properties. In order to clarify whether the oxidation is a surface-limited or a bulk process elemental depth profiling is essential. In this work XPS in combination with Ar<sup>+</sup> sputtering is applied to carry out depth profiling of AlN films prepared by plasma-enhanced atomic layer deposition using different parameters (plasma source, power and pulse duration). Particularly, the Al2p core levels are analyzed where the signals are decomposed into four components, representing weaker contributions of pure AlN and aluminum oxide phases as well as stronger signals of mixed oxygen-rich and nitrogen-rich phases. After sputtering (providing access to the deeper part of the film) the pure AlN phase content increases while the pure aluminum oxide content stays relatively constant. These issues are discussed with regard to the preparation parameters employed and accompanying XRD and electrical measurements.

DS 14.26 Tue 17:00 Poster E

**Formation and characterization of Si-QDs in annealed Si/SiNx and Si/SiO<sub>2</sub> multilayers** — ●ROSTISLAV MEDLÍN, PAVEL CALTA, PAVOL ŠUTTA, and MARIE NETRALOVÁ — New Technologies Research Centre, UWB Pilsen, Univerzitní 8, 306 14, Czech Republic Si quantum dots (Si-QDs) embedded in dielectric matrix have attracted much attention for the applications in fields such as data storages or optoelectronics. In this work we performed a detailed comparative study of the structural, optical and photoluminescent properties of Si-QDs formed in annealed Si/SiNx and Si/SiO<sub>2</sub> multilayers. Samples have been grown by means of PECVD with a substrate temperature of 250°C using silane, nitrogen and nitrous oxide as precursor

gases and post-annealed between 600-1100°C. TEM, XRD, Raman, FT-IR, UV-Vis and PL techniques were used to characterize the prepared superlattices. The dependences of the photoluminescence, structural and chemical bonding characteristics of Si-QDs on the dielectric barrier material and thickness were investigated. The cross-section TEM, XRD and Raman measurements confirms the formation of Si-QD in the range 3-20 nm. It was found that the size of the formed Si-QDs was dependent on the annealing temperature as well as the sublayer thickness. Columnar growth and evolution of wavy interface morphology was discussed.

DS 14.27 Tue 17:00 Poster E

**B20-type FeGe on Ge (100) grown by pulse laser melting** — ●ZICHAO LI<sup>1,2</sup>, YUFANG XIE<sup>1,2</sup>, MAO WANG<sup>1,2</sup>, CHI XU<sup>1,2</sup>, YE YUAN<sup>1,2</sup>, SLAWOMIR PRUCNAL<sup>1</sup>, and SHENGQIANG ZHOU<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany — <sup>2</sup>Technische Universität Dresden, D-01062 Dresden, Germany

B20-type FeGe is one of the noncentrosymmetric materials hosting skyrmions. Due to its nanoscale helical spin textures that only need extremely low spin-polarized currents to be moved, this material is one promising candidate for ultra-dense information storage and spintronics. In this work, we propose a simple method to prepare B20-type FeGe, which only includes a room temperature deposition of 10 nm Fe layer on Ge (100) substrates and a following process by pulse laser melting. The formation of B20 phase is confirmed by X-ray Diffraction With a preferential orientation of FeGe(111)//Ge(001). The FeGe samples show superparamagnetic properties and their blocking temperatures increase with increasing laser power. We conclude that this phenomenon is due to the increased grain size of B20 FeGe phase with increasing laser energy. This work provides a path of obtaining different B20-type transition metal germinides which can be magnetic-Skyrmion hosting materials for spintronics.

DS 14.28 Tue 17:00 Poster E

**Investigation of ultra-low energy ion implanted graphene by RBS and NRA** — ●MANUEL AUGE and HANS HOFSSÄSS — II. Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany

Dopant introduction into both graphene and transition metal dichalcogenides (TMDs) in a controllable manner is highly desirable. Hence, electronic doping other than electric gauging or chemical functionalization would be a major breakthrough. In our study, a unique mass selected ion beam deposition system is used to incorporate low energy ions into 2D-lattices. Therefore, a 30 keV ion beam is decelerated in a UHV-chamber down to energies as low as 10 eV. A beam sweep ensures a uniform profile over an area of 1 cm<sup>2</sup> up to 2.5 cm<sup>2</sup>. At the present time, sources are available for B, C, N, F, P, S, Mn, Fe, Se, W and Au ions. In this work, we show the successful incorporation of B, Mn and Au into graphene. In order to proof the implanted areal concentration as well as the elemental composition, Rutherford backscattering measurements were performed on tetrahedral amorphous carbon films doped with Mn and Au, respectively. For this purpose, we use a 860 keV He<sup>2+</sup>-beam and detect the backscattering events caused by the interaction between the high energetic projectile and the coulomb potential of atomic nuclei of the sample. Light elements in low concentrations are only hard to detect analytically. Nevertheless, implanted B can be investigated by a nuclear reaction analysis. We irradiate implanted test samples with a 430 keV proton beam generating the <sup>11</sup>B(p, 2α)α nuclear reaction with a detection limit of about 5 · 10<sup>13</sup> B/cm<sup>2</sup>.

DS 14.29 Tue 17:00 Poster E

**Towards multimodal measurements on printed thin films** — ●MICHAEL BUCHHORN<sup>1</sup>, CHRISTOPHER GREVE<sup>1</sup>, FABIAN PANZER<sup>2</sup>, and EVA HERZIG<sup>1</sup> — <sup>1</sup>Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany — <sup>2</sup>Lehrstuhl für Optoelektronik weicher Materie - Herzig Group, Universität Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany

The performance of many novel material systems heavily depends on their nanoscale structure. The structure on the other hand can be to some extent controlled by the way the material is processed, which allows a certain tunability of the functionality of the materials.

For this reason, it is of interest to understand structure formation processes in detail. Using a slot die printing system with various en-

environmental control parameters [1] we therefore wish to examine as many structural parameters during processing as possible to obtain a detailed picture of the formation process. To achieve this, we have extended our printing chamber with various simultaneous measurement capabilities [2] and demonstrate here the capabilities for sample quality and structural analysis of organic solar cell materials.

[1] Pröller, Stephan; Moseguí González, Daniel; Zhu, Chenhui; Schaible, Erik; Wang, Cheng; Müller-Buschbaum, Peter; Hexemer, Alexander; Herzig, Eva M. *Rev. Sci. Inst.*, 88 (6), 066101, 2017

[2] Buchhorn, Michael; Wedler, Stefan; Panzer, Fabian, *J. Phys. Chem. A*, 122 (46), 9115, 2018

DS 14.30 Tue 17:00 Poster E

**Investigations of LaVO<sub>3</sub> and PrVO<sub>3</sub> thin films by Raman spectroscopy and ellipsometry** — SIMON BREHM<sup>1</sup>, ●CAMELIU HIMCINSCHI<sup>1</sup>, IONELA LINDFORS-VREJOU<sup>2</sup>, KUMAR DEEPAK<sup>3</sup>, WILFRID PRELLIER<sup>3</sup>, and JENS KORTUS<sup>1</sup> — <sup>1</sup>Institute of Theoretical Physics, TU Bergakademie Freiberg, 09596 Freiberg, Germany — <sup>2</sup>II. Physikalisches Institut, Universität zu Köln, D-50937, Germany — <sup>3</sup>Laboratoire CRISMAT, CNRS-ENSICAEN, F-14050 Caen, France

In this work, 3d transition metal vanadates (LaVO<sub>3</sub> and PrVO<sub>3</sub>) thin films grown by pulsed-laser deposition on different crystalline substrates (DyScO<sub>3</sub>, LSAT, LaGaO<sub>3</sub>, SrTiO<sub>3</sub>) were investigated. The phase transition to orbital ordering of the films was evaluated by Raman spectroscopy. For this purpose, temperature-dependent measurements were carried out in a range of 90 K to 300 K using 633 nm laser line as excitation. The dependence of the orbital ordering on the film orientation on the different substrates was addressed. Additionally, spectroscopic ellipsometry was used to determine the optical constants of the LaVO<sub>3</sub> and PrVO<sub>3</sub> thin films at room temperature.

DS 14.31 Tue 17:00 Poster E

**Superradiant and transport lifetimes of the cyclotron resonance in the topological insulator HgTe** — ●JAN GOSPODARIC<sup>1</sup>, VLAD DZIOM<sup>1</sup>, ALEXEY SHUVAEV<sup>1</sup>, ANDREI PIMENOV<sup>1</sup>, ALENA DOBRETSOVA<sup>2</sup>, NIKOLAY NIKOLAEVICH MIKHAILOV<sup>2</sup>, and ZE DON KVON<sup>2</sup> — <sup>1</sup>Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — <sup>2</sup>Rzhanov Institute of Semiconductor Physics and Novosibirsk State University, Novosibirsk 630090, Russia

In this work, we investigated the phenomenon of collective radiative decay, or superradiance, in three-dimensional topological insulator HgTe with conducting surface states. Specifically, by utilizing an approach of a continuous-wave spectroscopy we examined the cyclotron resonance of the surface electrons in the terahertz frequency range. Due to the quasi-classical regime of the cyclotron resonance at terahertz frequencies, the results can be well explained via classical electrodynamic approach. This allowed us to separate the energy losses in the system into intrinsic and radiation losses, respectively. We showed experimentally that a semi-transparent gate on the top of HgTe quantum well allows us to switch the sample to a regime where the superradiance, i.e. coherent emission, dominates the losses.

DS 14.32 Tue 17:00 Poster E

**In-situ investigation of electrochromic coloration processes in tungsten trioxide thin films by optical spectroscopy** — ●ALEXANDER G. STRACK<sup>1,2</sup>, JAN L. DORNSEIFER<sup>1,2</sup>, SIMON BURKHARDT<sup>1,2</sup>, LIMEI CHEN<sup>1,2</sup>, MATTHIAS T. ELM<sup>1,2,3</sup>, and PETER J. KLAR<sup>1,2</sup> — <sup>1</sup>Institut of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — <sup>2</sup>Center for Materials Research (LaMa), Heinrich-Buff-Ring 16, 35392 Giessen, Germany — <sup>3</sup>Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Giessen, Germany

Smart-windows with thin films of tungsten trioxide are helpful for an efficient heat management, since heat transfer through windows may be very high. A well insulated building may save costs. For decreasing heat transfer, it is desirable to understand the microscopic switching properties of the tungsten trioxide film and to be able to control the process. With various experimental techniques it is possible to investigate the electrochromic coloring process in thin tungsten trioxide films. Raman spectroscopy reveals the different vibrational modes of WO<sup>6+</sup>, WO<sup>5+</sup> and WO<sup>4+</sup> in poly-crystalline tungsten films. We employ a principal component analysis to correlate the evolution of Raman modes with the coloration process. Corresponding results will be shown and discussed.

DS 14.33 Tue 17:00 Poster E

**Surface dead layer in thin manganite films studied by Surface-Enhanced Raman Spectroscopy** — SEBASTIAN MERTEN, ●JONAS

WAWRA, and VASILY MOSHNYAGA — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Half-metallic mixed-valence manganites are promising materials for spintronic applications. However, extrinsic effects, like surface dead layer or chemical segregation, prevent that they unfold their true potential. Here, we present a Surface-Enhanced Raman (SER) spectroscopy study of the surface dead layer in doped La<sub>0.7</sub>(Ca or Sr)<sub>0.3</sub>MnO<sub>3</sub> thin films, grown by MAD technique. The required Au nanoparticles have been grown with the same technique. The SER spectra of the free manganite surface reveal an electron-enrichment, manifested by the appearance of strong Jahn-Teller stretching modes. To manipulate this electron-rich surface layer, we have modified the manganite surface by deposition of 1-2 monolayers of SrO, MgO and TiO<sub>2</sub>, and compared the obtained SER spectra with those from the free surface. Financial support of the Deutsche Forschungsgesellschaft via SFB TP A02 is acknowledged.

DS 14.34 Tue 17:00 Poster E

**Sum-frequency generation vibrational spectroscopy of 4-Nitrothiophenole and 4-Aminothiophenole adsorbed on gold surfaces** — ●MATTHIAS LINKE, DAMIAN FIRLA, and ECKART HASSELBRINK — Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen, Germany

Self-assembled molecular films and their characterization has attracted much interest over the last decades, especially in the field of nanotechnology. The application of such films relies on controlling of their topological as well as their chemical properties. An extensively studied system consists of gold as a substrate and thiol molecules as the molecular layer which is formed easily by self-assembly. Sum-frequency generation vibrational spectroscopy (SFGVS) is a useful tool for characterization of surfaces. Different vibrational modes could be observed although the ones of aromatic compounds in the range of 1200 to 1650 cm<sup>-1</sup> typically show only moderate IR- and/or Raman-activity which both are a necessity for SFGVS. 4-Nitrothiophenole (NTP) and 4-Aminothiophenole (ATP), which differ in the substituent and the electronic effects caused by these, have been adsorbed on gold surfaces and studied by SFGVS. The ring mode 8a and the symmetrical stretching mode for the NO<sub>2</sub>-group for NTP and the mode 19a for ATP have been observed and were used to characterize the layers.

DS 14.35 Tue 17:00 Poster E

**The dependence of piezoelectric performance of AlN thin films on Si(111) on post-growth annealing treatment** — ●DMYTRO SOLONENKO<sup>1</sup>, CONSTANCE SCHMIDT<sup>1</sup>, CHRIS STOECKEL<sup>2</sup>, KARLA HILLER<sup>2</sup>, and DIETRICH R.T. ZAHN<sup>1</sup> — <sup>1</sup>Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — <sup>2</sup>Zentrum für Mikrotechnologie, Chemnitz University of Technology, 09107 Chemnitz, Germany

Aluminum nitride (AlN) is a material well-suited for microelectromechanical systems (MEMS) due its relatively high piezoelectric coefficients as well as high physical and chemical stability. Thin AlN films, used in the production of MEMS, are often fabricated by reactive magnetron sputtering, which, despite its efficiency and low cost, is known to produce films of mediocre quality and thus tolerable piezoelectric performance. The effect of post-growth annealing, which is usually performed to improve the crystallinity of semiconductors, was investigated for sputtered AlN films by X-ray diffraction, Raman and IR spectroscopies, spectroscopic ellipsometry, and atomic force microscopy. The results show that the strain built in the films during the growth starts to effectively relax at around 1000 °C, which is related to a dewetting of the AlN crystallites from the silicon substrate surface under formation of O-containing species such as SiO<sub>2</sub> and AlON. Up to 800 °C, the average grain size enlarges and the film porosity is reduced, which positively affects the piezoelectric coefficient, d<sub>33</sub>, determined using piezoresponse force microscopy.

DS 14.36 Tue 17:00 Poster E

**Functionalization of Silicon Nanoribbons on Ag(110)** — ●ALEXANDER EHM, DMYTRO SOLONENKO, DIETRICH R.T. ZAHN, and PATRICK VOGT — Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Silicon nanoribbons (SiNRs) are quasi one-dimensional one-atom thin Si structures, forming under ultra-high vacuum conditions on well-ordered Ag(110) surfaces. These SiNRs have a width of 1.6 nm, a length of several 100 nm and are well aligned parallel to each other,

along the Ag[-110] direction [1]. The atomic structure of the SiNRs is explained by inter-connected Si pentagons [2], a structure unique among all Si-related materials, leading to distinct properties when e.g. to diamond like Si. Oxidation of the SiNRs by exposure to molecular oxygen, for example, proceeds along the ribbons, starting from their extremities, while their edges and top are stable [3].

We used in situ Raman spectroscopy to get further insight into the vibrational properties of SiNRs and investigate their modification through oxygen and hydrogen adsorption. Our results confirmed the "burning match" effect [3], suggesting a higher stability of SiNRs when compared to other 2D Si materials. Oppositely, the hydrogenation of SiNRs fails, the reasons of which will be discussed.

[1] C. Leandri et al., *Surface Science* 574, L9-L15 (2005)

[2] J. I. Cerda et al., *Nat. Comm.* 13076 (2016)

[3] P. De Padova et al., *Nano Lett.*, Vol. 8, No. 8, 2299-2304 (2008)

DS 14.37 Tue 17:00 Poster E

**Understanding the Limits of Plasmonic Sensitivity and Tip-Enhanced Raman Spectroscopy** — ●LU HE, MAFUHJUR RAHAMAN, TERESA ISABEL PICOTO PENA MADEIRA, and DIETRICH R.T. ZAHN — Reichenhainerstraße 70 P181 Chemnitz Germany

Tip-Enhanced Raman Spectroscopy has attracted growing interest over the last decades. Due to the confined electric field at the metallic tip apex, one can both enhance the Raman sensitivity, and reduce the probing area significantly. The enhancement factor can be large enough to enable this technique to be sensitive to detailed structures[1] and orientation of surface species[2] well beyond the diffraction limit of light reaching a spatial resolution of about 2 nm[1,2]. For a metal-metallic tip-sample system, the full width at half maximum (FWHM) of the local electric field is estimated by  $2\sqrt{Rd}$ , with R is the radius of the tip and d is the tip-sample distance[3]. However, the situation can be different if the substrate structure is smaller than the tip radius R. In this contribution we will address this issue by calculating the local electric field using finite element method simulations and varying the substrate dimensions. Our simulations will not only provide a deeper understanding of the TERS mechanism of such structures, but also help in realizing highly efficient TERS experiments using similar systems.

DS 14.38 Tue 17:00 Poster E

**Active optical metasurfaces based on defect engineered phase-change and phase-transition materials** — JURA RENSBERG, MARTIN HAUFERMANN, ●KEVIN WOLF, and CARSTEN RONNING — Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Energetic ion beams are widely used to modify the electronic and structural properties of solids by introducing impurity atoms into the crystal lattice. Commonly, the inevitable formation of irradiation damage during ion bombardment is described as disadvantageously for ion beam doping and subsequent post-implantation annealing procedures are required. Since the electronic structure of both, phase-change materials, such as chalcogenide glasses, and phase-transition materials, such as vanadium dioxide, are very sensitive to small amounts of lattice defects, area selective ion irradiation can be used to locally adjust either the phase and/or the phase transition temperature of these materials. Using this robust technique, optical metasurfaces including tunable absorbers based on thermally triggered dichroism and reconfigurable polarizers based on artificially induced phase coexistence are demonstrated.

DS 14.39 Tue 17:00 Poster E

**A squeezable tunneling junction setup for the measurement of thermoelectricity in nanojunctions** — ●MATTHIAS POPP and HEIKO B. WEBER — Friedrich-Alexander-Universität Erlangen-Nürnberg

Motivated by experiments on epitaxial graphene-graphene nanojunctions [Kis17] we built a setup which is capable of adjusting the distance between two silicon carbide (SiC) plates on the picometer scale. Thereby we can bring electrodes which are patterned on top of the SiC plates into close vicinity. By adjusting the distance between the plates we can adjust the (tunneling) resistance of the so formed nanocontact within a wide range. The observed stability is such that single-molecule junctions can be established. As a remarkable feature, we can induce temperature gradients across the junction, allowing for thermoelectrical measurements. On our poster we present first results of thermoelectricity measurements on gold-gold and gold-molecule-gold nanojunctions.

[Kis17] F. Kisslinger, *et al.*, *Charge-carrier transport in large-area epitaxial graphene*. *Annalen der Physik* 1700048 (2017)

DS 14.40 Tue 17:00 Poster E

**Using Tunnelling Spectroscopy to Monitor Changes in the Electronic Structure of Chalcogenide Thin Films Occurring by Tuning their Electronic Properties** — ●LISA METZNER<sup>1</sup>, JOHANNES REINDL<sup>1</sup>, and MATTHIAS WÜTTIG<sup>1,2</sup> — <sup>1</sup>I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — <sup>2</sup>JARA - FIT, RWTH Aachen University, Germany

Phase change materials (PCM) possess some unique physical properties, which make them well suited candidates for the integration in novel data storage technology, like the recently presented 3D XPoint memory. In such devices, the large contrast in electrical resistivity between stable amorphous and crystalline phases, switched by electrical pulses on a nanosecond timescale, is exploited.

In addition to this extraordinary mechanism, in the material class of chalcogenides, to which the PCM belong, many compounds with other interesting physical properties such as good thermoelectrics, topological insulators or superconductors can be found. In these materials, methods like alloying or thermal annealing provide means for tuning their electronic structure and properties, such as n-p transitions or band gap engineering.

In order to quantify these changes in the electronic structure of the materials, the electronic density of states (DOS) around the Fermi level is a crucial physical property. This quantity can be determined by tunnelling spectroscopy. Therefore, here we present measurements performed on tunnel junctions of PbXTe components, which were produced by in-situ sputter deposition.

DS 14.41 Tue 17:00 Poster E

**Investigation of bipolar resistive switching mechanisms in amorphous and crystalline Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> using different electrode materials** — ●HAGEN BRYJA, MARIO BEHRENS, ANDRIY LOTNYK, and BERND RAUSCHENBACH — Leibniz Institute of Surface Engineering (IOM), Permoserstraße 15, 04318 Leipzig, Germany

Electric-field-induced resistive random-access memory has received much attention as candidate for next-generation non-volatile memory applications due to its fast switching, simple structure and low power consumption. Chalcogenide-based phase change alloy Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> (GST) has shown promising properties for such memory devices, since its switching mechanism relies on either ionic migration or pure electronic effects.

Here, the influence of the electrode material and solid phase of GST on bipolar resistive switching was investigated. For this, Pt/GST/Cr and Ag/GST/Cr memory cells were both prepared using pulsed laser deposited amorphous or crystalline GST. Transmission electron microscopy investigations and detailed analysis of the current-voltage characteristics are presented. In the case of Pt/GST/Cr the resistive switching arises from a pure space-charge limited conduction (SCLC) mechanism, whereas Ag/GST/Cr shows a combination of SCLC with electrochemical metallization effects. For both cells it was found that the magnitude of the resistance and the high/low resistance ratio are significantly affected by the solid phase of GST. Furthermore, application-related properties such as multi-state capability, endurance and retention time were compared.

DS 14.42 Tue 17:00 Poster E

**Microstructuring of rf-sputtered VO<sub>2</sub> thin films for improved transmittance properties** — ●HANNES GIESE, FLORIAN KUHL, and ANGELIKA POLITY — Institute of Experimental Physics I and Center for Materials Research (ZfM/LaMa), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen

Vanadiumdioxide (VO<sub>2</sub>) is a material which changes its transmittance properties due to a temperature induced metal-to-insulator phase transition (MIT). The transmittance for infrared light in the monoclinic low temperature phase is much higher than in the tetragonal high temperature phase, thus VO<sub>2</sub> is predestined for use as a smart window coating for an improved climate control in buildings. To gain a better optical impression and a higher transmittance in the visible range, one attempts to reduce the VO<sub>2</sub> covered area by microstructuring but on the other hand to maintain the switching effect.

The VO<sub>2</sub> thin films were deposited by radio-frequency sputtering (rf sputtering). Microstructuring was carried out by photolithography with different patterns and both, positive and negative photoresists. As last step ion beam etching (IBE) was used for structuring the samples to obtain different patterns in the VO<sub>2</sub> thin film. The samples

were characterized by UV/Vis spectroscopy for optical properties and light microscopy for determining the pattern sizes. The influence of different patterns, variation of covered area, etching parameters and size of the structures on the optical parameters was investigated to gain the best compromise between enhancing the transmittance in visible light and still a good switching efficiency for the MIT in the infrared range.

DS 14.43 Tue 17:00 Poster E

**Structural and electrical properties of layered FeGe<sub>2</sub> thin films** — ●SAMUEL GAUCHER, BERND JENICHEN, and JENS HERFORT — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The solid-phase epitaxy (SPE) of Ge thin films over Fe<sub>3</sub>Si surfaces was investigated recently as a solution to create lattice-matched heterojunctions. A persistent challenge in this field had been to grow epitaxial semiconductors over metals by MBE, a limiting factor for a number of envisaged applications in the field of spintronics. In order to solve this issue, amorphous Ge was deposited on ferromagnetic quasi-Heusler compound Fe<sub>3</sub>Si and crystallized slowly by annealing. Instead of pure Ge, the resulting single-crystalline films were shown to be a new 2D polymorph of FeGe<sub>2</sub> with space group P4mm. TEM studies reveal a layered structure with monolayer Fe planes sitting between tetragonal Ge bilayers.<sup>1</sup> The material does not exist in a bulk form, its creation being interpreted as an ordering phenomenon induced by minimization of the elastic energy of the epitaxial film.<sup>1</sup> It is possible to isolate the material on an insulating GaAs substrate by first growing a few monolayers of crystalline Fe<sub>3</sub>Si, and then thicker amorphous Ge in a ratio such as to obtain the right stoichiometry for FeGe<sub>2</sub> (with some Si atoms sitting on Ge sites). Electrical measurements conducted on FeGe<sub>2</sub> films of 8 to 12 nm indicate a thickness dependence of their resistivity. Magnetotransport at low temperature reveal a strong anomalous Hall effect.

<sup>1</sup>Jenichen et al., Phys. Rev. Mater. **2**, 051402 (2018).

DS 14.44 Tue 17:00 Poster E

**Electronic Noise in Hafnium and Yttrium Oxide-Based RRAM Devices** — ●MARTIN LONSKY<sup>1</sup>, ESZTER PIROS<sup>2</sup>, STEFAN PETZOLD<sup>2</sup>, ERIC JALAGUIER<sup>3</sup>, EMMANUEL NOLOT<sup>3</sup>, CHRISTELLE CHARPIN<sup>3</sup>, CHRISTIAN WENGER<sup>4</sup>, LAMBERT ALFF<sup>2</sup>, and JENS MÜLLER<sup>1</sup> — <sup>1</sup>Institute of Physics, Goethe-University Frankfurt, Frankfurt am Main, Germany — <sup>2</sup>Institute of Materials Science, Technical University Darmstadt, Darmstadt, Germany — <sup>3</sup>CEA, LETI, Minnatec Campus, Grenoble, France — <sup>4</sup>IHP GmbH, Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany

Resistive random access memory (RRAM) devices have attracted great attention due to their potential to be applied as a reliable, fast and high-density non-volatile data storage solution. Here, we present a study on transition metal oxide-based devices, in which the mechanism of resistive switching is related to the formation and rupture of oxygen-deficient conducting filaments in the oxide layer. Up until today, the exact mechanisms of charge transport and their dependence on various parameters are not yet fully understood. In this context, a better and more detailed physical picture would yield strong benefits with regard to the fabrication of more reliable and efficient devices. Therefore, we compared HfO<sub>2</sub>- and Y<sub>2</sub>O<sub>3</sub>-based memory cells by employing fluctuation spectroscopy, which is a powerful method to study the charge carrier dynamics in RRAMs. For hafnium oxide-based devices, the electronic noise exhibits clear signatures of trap-assisted tunneling processes, whereas for yttrium oxide-based samples our results suggest a different charge transport mechanism to be predominant.

DS 14.45 Tue 17:00 Poster E

**Highly conducting thin films of PdCoO<sub>2</sub> prepared by MAD technique** — OLEG SHAPOVAL<sup>1</sup>, VLADIMIR RODDATIS<sup>2</sup>, SVEN ESSER<sup>3</sup>, THOMAS ZIMMERMANN<sup>3</sup>, PHILIPP GEGENWART<sup>3</sup>, and ●VASILY MOSHNYAGA<sup>1</sup> — <sup>1</sup>Erstes Physikalisches Institut, Georg-August-Universität Göttingen, Germany — <sup>2</sup>Institut für Materialphysik, Georg-August-Universität Göttingen, Germany — <sup>3</sup>Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, Germany

Pd-based delafossite PdCoO<sub>2</sub> (PCO) with 2D conducting layers and extremely large mean free path of electrons is of great interest for applications in thermal transport or as conducting electrodes. However, the information on the growth of PCO films is scarce. We report the structure and electric properties of PCO thin films grown by metalorganic aerosol deposition (MAD) technique on hexagonal substrates, i.e. Al<sub>2</sub>O<sub>3</sub>(0001), YSZ(111), as well as on Ca<sub>3</sub>Co<sub>4</sub>O<sub>9</sub>

buffered SrTiO<sub>3</sub>(100). Under optimized processing conditions, i.e. growth rate, deposition temperature, post-annealing, a 20 nm thick PCO(001)/YSZ(111) film shows room temperature resistivity 5\*10<sup>-6</sup> Ohmcm and residual resistance ratio, RRR(5K)=3. Low temperature magnetotransport (Hall effect and Shubnikov-de Haas oscillations) will allow us to disentangle between intrinsic and extrinsic parameters and further improve the quality of PCO films. Financial support from DFG through SFB 1073 (TPA02), MO2255-4 and TRR 80 (TP G3) is acknowledged.

DS 14.46 Tue 17:00 Poster E

**Pathways of polymer degradation of PCPDTBT and PDTSTzTz** — ●ANDREAS FRUEH<sup>1</sup>, ULF DETTINGER<sup>1</sup>, HEIKO PEISERT<sup>1</sup>, HANS-JOACHIM EGELHAAF<sup>2</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>Universität Tübingen, IPTC, Auf der Morgenstelle 18 D-72076 Tübingen, Germany — <sup>2</sup>ZAE Bayern, Auf AEG, Bau 16, 1. OG, Fürther Str. 250, D-90429 Nürnberg

The photodegradation kinetics of two prototypical low-bandgap polymers (PCPDTBT and PDTSTzTz) in thin films upon illumination with light with wavelenghts between 365 and 700 nm have been studied using UV/vis and fluorescence spectroscopy. For both polymers, two different degradation behaviors were found: There is a non-linear initial reaction kinetic and a more linear behavior in later stages of the photo oxidation. In dependence on the illumination wavelength, thereaction rate may depend on the energy of incident photons or on the number of absorbed photons giving valuable information on the most probable degradation pathway. In particular for PCPDTBT, the initial reaction rate depends on absorbance pointing to the involvement of singlet oxygen in the polymer degradation. Photoluminescence spectroscopy supports this hypothesis. In contrast, in later stages a radical mechanism is proposed, which was concluded from a clear increase of the reaction rate at higher photon energies in UV region.

DS 14.47 Tue 17:00 Poster E

**Study of Resistive Switching on La<sub>0.3</sub>Ca<sub>0.7</sub>MnO<sub>3</sub>/YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-δ</sub> Bilayers Deposited by Sputtering DC** — JOHN BETANCOURT<sup>1,2</sup>, JHON E. ORDOÑEZ<sup>1</sup>, CARLOS W. SANCHEZ<sup>1</sup>, WILSON LOPERA<sup>1</sup>, ●KATHERINE GROSS<sup>1</sup>, and MARIA E. GÓMEZ<sup>1,2</sup> — <sup>1</sup>Thin films group, Universidad del Valle, Cali, Colombia — <sup>2</sup>Centro de Excelencia en Nuevos Materiales, CENM

Devices based on phenomenon of resistive random access memory (RRAM) have been studied on different transition metal oxides. In this materials the favorable properties as low power consumption, simplicity, long retention time and even multilevel switching are very important. We have deposited La<sub>0.3</sub>Ca<sub>0.7</sub>MnO<sub>3</sub> (LCMO) films on YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-δ</sub> (YBCO)/ SrTiO<sub>3</sub> (STO) to study the resistive switching on complex oxide. In this case, LCMO (t= 60, 30 and 15 nm) was used like insulator material in contact with a fixed YBCO layer (t= 60 nm) as a bottom electrode. From XRD we found that the LCMO and YBCO layers growth textured aligned with substrate. The electrical properties with temperature using Ag like top electrode indicated the insulator and metal behavior of LCMO and YBCO respectively. The I-V curves allow us investigate the hysteretic response and the presence of two resistive states at room temperature and associated with electrical transport mechanisms like space charge limited conduction (SCLC). Finally, the resistance switching with applied voltage tests were performed indicating a relation between the thicknesses of the LCMO layer with the HRS/LRS ratio.

DS 14.48 Tue 17:00 Poster E

**Investigation of Hydrogen Gas Sorption in Thin Metal Films Using a Quartz Crystal Micro Balance** — ●SONJA SCHNEIDEWIND<sup>1</sup>, JULIAN BLASCHTSCHAK<sup>1</sup>, MAX AKER<sup>1</sup>, ANDREAS FLEISCHMANN<sup>2</sup>, LOREDANA GASTALDO<sup>2</sup>, ANDREAS REIFENBERGER<sup>2</sup>, and MAGNUS SCHLÖSSER<sup>1</sup> — <sup>1</sup>ITEP, KIT, Karlsruhe, Germany — <sup>2</sup>Kirchhoff-Institut für Physik, Heidelberg, Germany

Certain metals have the ability to solve hydrogen in their lattice structure and to subsequently form metal hydrides. Out of these materials, titanium has one of the lowest dissociation pressure which allows a quasi-irreversible hydrogen capture. However, the titanium surface tends to form an oxide layer at contact with air which acts as effective permeation barrier. The oxidation can be prevented by sputtering a thin palladium film on top allowing the hydrogen permeation through the Pd layer into the Ti getter. This technique can be used to build effective passive hydrogen pumps or by employing the radioactive isotopologue, tritium, one can build dedicated radioisotope heat sources, e.g. for calibration purposes.

In order to study kinetics, materials and loading parameters, we perform sorption experiments by using a high-resolution quartz crystal micro balance with deuterium at the ng scale. As an additional testing method, AFM and XRD are used to get information about the film structure and to verify the absorbed gas amount. Finally, the findings will be applied to a dedicated loading of identical metal films with tritium gas which will then be validated by Beta-Induced X-Ray Spectroscopy.

DS 14.49 Tue 17:00 Poster E

**Indium tin oxide (ITO) direct wafer bonding** — ●MICHAEL HÖNLE<sup>1</sup>, KURT HINGERL<sup>2</sup>, and THORSTEN WAGNER<sup>2</sup> — <sup>1</sup>OSRAM Opto Semiconductors GmbH, Leibnizstraße 4, Regensburg, 93055, Germany — <sup>2</sup>Johannes Kepler University Linz, Altenberger Straße 69, 4040 Linz, Austria

Direct wafer bonding allows combination of separately grown and prepared Si and III-V devices and, moreover, high bonding toughness can be achieved at temperatures as low as room temperature. In order to facilitate good electrical interconnection and little absorption, the intermediate bonding layer ideally should offer high electrical conductivity and high transparency. Indium tin oxide (ITO) is a material which offers both of these properties. In this work we demonstrate the feasibility of a defect free ITO-ITO direct wafer bond of non-patterned Si wafers and characterize the bond interface qualitatively and quantitatively. Moreover, to create insight into the bonding mechanism of an ITO-ITO direct wafer bond, high resolution transmission electron microscopy (HR-TEM) was employed. To show the possible application of ITO-ITO direct wafer bonding with III-V materials, we transferred epitaxially grown GaN layers to Si wafers and display that the obtained bonded wafers are robust enough for further front of line processing. In order to optimize the bonding process a good understanding of the material properties is needed, therefore ITO layers were analyzed using surface analytical methods before and after direct wafer bonding.

DS 14.50 Tue 17:00 Poster E

**Spin-orbit torques in epitaxially grown two-dimensional transition metal dichalcogenides** — ●AMILCAR BEDOYA-PINTO, AVANINDRA PANDEYA, KAI CHANG, ILYA KOSTANOVSKIY, PETER WERNER, and STUART PARKIN — NISE department, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany

Transition metal dichalcogenides (TMDCs), layered materials which have captured great attention due to their tunable electronic properties, are commonly fabricated via exfoliation of bulk crystals. Although there has been progress in fabricating devices out of exfoliated heterostructures, there are applications -such as spin transfer torques- that rely on atomically clean interfaces for an optimal performance. Our approach is to grow high-quality NbSe<sub>2</sub> layers on Al<sub>2</sub>O<sub>3</sub> (0001) by molecular beam epitaxy (MBE), gaining thereby a precise control of the layer thickness, electronic properties (doping) and improving the quality of the interfaces involved in spin transfer and spin-to-charge conversion. We use spin-torque ferromagnetic resonance (ST-FMR) of a NbSe<sub>2</sub>/NiFe/MgO device structure to quantify the spin-orbit torques (SOTs) produced by the TMDC thin films. First results show a strong symmetric component of the ferromagnetic resonance lineshape, as well as a scaling of the resonance linewidth with external DC bias, both signatures of sizable spin-orbit torques induced by the NbSe<sub>2</sub> layer. This underlines the relevance of in-situ grown TMDC/ferromagnet heterostructures towards highly efficient spin-orbitronic devices.

DS 14.51 Tue 17:00 Poster E

**Metal ions at metal/polymer interfaces** — ●MARIA SONNENBERG, RENÉ GUSTUS, and WOLFGANG MAUS-FRIEDRICH — Technische Universität Clausthal, Clausthaler Zentrum für Materialtechnik, Leibnizstraße 9, 38678 Clausthal-Zellerfeld, Germany

Understanding the interaction between thin polymer films and metal surfaces is necessary for the plastics processing industry. During the processing of plastic, polymer is melted in the extruder unit. Often thin polymer layers are formed on the surface of the extruder, which leads to peeling off of partly solidified polymer into the melt. These polymer particles will not melt again and generate weak points within the product. Basic understanding of the underlying mechanisms is important in order to avoid steel/polymer interaction. For this purpose thin layers of polycarbonate were prepared on a silicon wafer. Iron was evaporated onto the polymer surfaces under ultra-high vacuum conditions. Afterwards the samples were heated up to 200°C. The interfaces after metal evaporation and after heating were examined by

electron spectroscopy (XPS). Experiments show that the diffusion of iron atoms in the polymer melt occurs. The interaction of polycarbonate with iron atoms was investigated. XPS results indicate the formation of a carbonyl-iron bond and an interaction of iron atoms with the aromatic rings.

DS 14.52 Tue 17:00 Poster E

**Reactive Metal-Organic Interfaces Studied with HAXPES: Modify Reaction Depth and Interphase Formation** — ●STEFAN RENATO KACHEL, MARTIN SCHMID, BENEDIKT P. KLEIN, NICOLAS BOCK, and J. MICHAEL GOTTFRIED — Fachbereich Chemie, Philipps-Universität Marburg, Germany

Interfaces between organic semiconductors and metallic layers are ubiquitous in organic electronic devices and can significantly influence device functionality. The vapor deposition of a metal onto an organic layer is often followed by a diffusion of the metal atoms into the organic layers. These metal atoms can react with the organic molecules forming a reacted interphase instead of an abrupt interface. A versatile technique for the quantitative characterization of these interphase layers is the hard X-ray photoelectron spectroscopy (HAXPES), which allows for non-destructive chemical depth profiling and chemical analysis across the interphase region. Here we studied two different systems, the reactive calcium on  $\alpha$ -sexithiophene (6T) and less reactive cobalt on 2H-tetraphenylporphyrin (2HTPP) system. In order to gain control over the thickness of the interphase layer, we varied process parameters such as sample temperature and metal atom flux during interphase preparation. We found that the temperature of the organic film during metal deposition was the only parameter that significantly influenced the formation of the interphase layer by nearly a factor of 2 independent of the system. Furthermore we observed a higher reaction depth and a complex diffusion mechanism for the Ca/6T system.

DS 14.53 Tue 17:00 Poster E

**Finding and understanding surface structures with SAMPLE** — ●LUKAS HÖRMANN, ANDREAS JEINDL, ALEXANDER T. EGGER, and OLIVER T. HOFMANN — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

Even if the physical properties of an organic semiconductor are ever so promising in the bulk phase, they may drastically change upon adsorption on the surface. Specifically, surfaces can induce the formation of polymorphs with worse, or under the right conditions, also greatly improved properties. Normally, the exponential growth of possible polymorphs with system size prohibits rigorous computational studies, that could explore the full configurational and thermodynamic search space. Thus, we use SAMPLE [1,2], which employs machine learning to suitably fit a physical energy model and therewith efficiently calculate the adsorption energies of an exhaustive set of coarse grained polymorphs.

We showcase the capabilities of this approach for monolayers of molecules with very different interactions on coinage metals. With SAMPLE we not only find the best polymorphs, but also defects and other local minima. Ab-initio thermodynamics allows us to also consider temperature effects and create phase diagrams. Our unique combination of a physically inspired energy model and statistical learning enables us to gain insight into the molecular interactions on the surface. This allows us to not only tell which polymorph forms, but also which interactions are the reasons for the formation of specific structures.

[1] Hörmann et al., arXiv:1811.11702

[2] Scherbela et al., Phys. Rev. Materials 2, 043803

DS 14.54 Tue 17:00 Poster E

**Simulating Charge Transport Through Metal-Organic Semiconductor Interfaces: Bulk or Contact Limited?** — ●MARKUS KRAMMER<sup>1</sup>, PHILIPP BREITEGGER<sup>2</sup>, CHRIS GROVES<sup>3</sup>, and KARIN ZOJER<sup>1</sup> — <sup>1</sup>Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — <sup>2</sup>Institute of Electronic Sensor System, Graz University of Technology, Austria — <sup>3</sup>Department of Engineering, Durham University, United Kingdom

The performance of organic electronic devices crucially relies on an efficient charge injection. This efficiency is governed by a complex interplay of experimentally tunable properties like level alignment and disorder. The impact of this interplay on the bulk current is only poorly understood from a theoretical point of view. To overcome this lack of knowledge, we utilize mesoscopic simulations to predict the current density across the contact interface. In these simulations, charges are viewed to migrate through disordered organic semiconductors due to hopping between localised states. Parameters like injection barrier, en-

ergetic disorder, electric field, Coulomb interactions and temperature can be directly considered. This intuitive method holds the promise to understand the effects and interactions that govern the interplay between interfacial and bulk properties. We analyse the current density for instructive combinations of interface and bulk properties. This analysis yields two distinct regimes, a bulk limited regime and a contact limited regime. The evolution of the current density with respect to injection barrier, energetic disorder and electric field strength is investigated and the origin of bulk vs. contact limitation is analysed.

DS 14.55 Tue 17:00 Poster E

**Bisquinolylamide Metal Complexes for OFET** — ●PASCAL SCHWEITZER<sup>1</sup>, GEORG ALBRECHT<sup>1</sup>, CLEMENS GEIS<sup>1</sup>, HARALD LOCKE<sup>2</sup>, PETER R. SCHREINER<sup>2</sup>, and DERCK SCHLETTWEIN<sup>1</sup> — <sup>1</sup>Justus-Liebig-Universität Gießen, Institut für Angewandte Physik — <sup>2</sup>Justus-Liebig-Universität Gießen, Institut für Organische Chemie

Metal-organic complexes with two pincer-type bisquinolylamide ligands give the possibility to introduce a doubly charged metal ion M(II) center in an octahedral coordination sphere. Such coordination geometry is not commonly found in organic semiconducting complexes. Metals like Zn, Cr, Mn, Fe, Co were used in this present approach. The resulting cross-shaped complexes lead to stacking of the ligands' electronic systems in two directions of the solid, indicated by XRD measurements on single crystals. Organic field-effect transistors (OFET) prepared on microstructured interdigitated gold electrode arrays on  $SiO_2$  were used to investigate the charge-carrier mobility and electrical conductivity of these new molecular complexes. Potentiometry by atomic force microscopy in high vacuum was used to yield contact resistances between gold and the semiconductor materials in steady-state. In-situ measurements during film growth gave insight into layer and contact formation. Injection barriers between gold and the semiconductors were calculated from Kelvin probe force microscopy and data from cyclic voltammetry.

DS 14.56 Tue 17:00 Poster E

**Laterally structured dielectrics by area-selective atomic-layer-deposition** — ●DANIEL ANDERS, PHILIP KLEMENT, FABIAN MICHEL, JÖRG SCHÖRMANN, and SANGAM CHATTERJEE — Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus-Liebig-University Giessen, D-35392 Giessen, Germany

Industrial semiconductor manufacturing combines lithography, etching, and deposition processes to create (opto-) electronic devices. The quest for miniaturization of those devices has led to complex fabrication processes with multiple patterning and etching steps to achieve area-select deposition. However, for more advanced technology a tool must deposit different combinations of materials area-selectively. Atomic-layer-deposition (ALD) is a technique for depositing high-quality, ultrathin films of dielectrics with the potential of area-selective deposition that could reduce the number of manufacturing steps and allow for advanced structures. Here, we demonstrate the successful direct patterned deposition of  $TiO_2$  on  $SiO_2$  creating smooth surfaces of alternating dielectrics. A combination of electron beam lithography using a PMMA mask, ion beam etching, plasma treatment and ALD enables a patterned deposition. Several process parameters were varied, and their effect on the resulting structure was investigated by atomic force microscopy, scanning electron microscopy, and X-ray photoelectron spectroscopy. We find that a number of factors must be considered in design, patterning, and deposition to achieve reproducible results. Our work enables the realization of lateral heterostructures as central building blocks for advanced technology applications.

DS 14.57 Tue 17:00 Poster E

**Study of the in-plane lattice constant of phase change materials during deposition** — ●HETAL VAISHNAV<sup>1</sup>, MARVIN KAMINSKI<sup>1</sup>, MARC POHLMANN<sup>1</sup>, and MATTHIAS WUTTIG<sup>1,2</sup> — <sup>1</sup>I. Institute of Physics, Physics of New Materials, RWTH Aachen University, 52056 Aachen, Germany — <sup>2</sup>JARA-Insitut Energy-efficient information technology (PGI-10), FZ Jülich, 52428 Jülich, Germany

Phase change materials (PCMs) are higher order chalcogenides which can be rapidly switched between the amorphous and crystalline state upon heating. The unique properties of the crystalline phase of these chalcogenides have recently been attributed to a novel bonding mechanism which we have coined metavalent bonding (MVB). In this bonding mechanism the electrons are on the verge of delocalization. This immediately raises the question how these materials behave in reduced dimensions such as thin films, where electron delocalization is impeded. To answer this question, thin films of different chalcogenides have been

grown by molecular beam epitaxy (MBE). In the literature, two unexpected observations have been reported for GeTe thin films. For certain substrates, an increased in-plane lattice constant was observed for thin films, which reached the bulk value for thicker films. For other substrates, a transition from an amorphous to a crystalline state has been observed at a thickness of a few bilayers. These findings cannot be directly explained by strain effects or pseudomorphic growth. Hence, in this work, further investigations for different materials like SnTe and Sb<sub>2</sub>Te<sub>3</sub> will be presented and compared to GeTe thin films.

DS 14.58 Tue 17:00 Poster E

**Herstellung von Schichten aus  $MoN_x$  mittels hoch-ionisierender PVD-Verfahren** — MARTIN BALZER<sup>1</sup>, MARTIN KOMMER<sup>1</sup>, ●SABINE STÜCK<sup>2</sup>, MARTIN FENKER<sup>1</sup> und FRANK SCHMIDL<sup>2</sup> — <sup>1</sup>Forschungsinstitut Edelmetalle+Metallchemie, Katharinenstraße 17, 73525 Schwäbisch Gmünd — <sup>2</sup>Friedrich-Schiller Universität Jena, Physikalisch-Astronomische Fakultät, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena

Schichten aus Übergangsmetallnitriden finden aufgrund ihrer extremen Härte, hohen Schmelzpunkte und chemischer Stabilität vorallem Anwendung als Verschleißschuttschichten. Hier gewinnen Molybdänitride ( $MoN_x$ ) aufgrund ihrer überlegenen mechanischen Eigenschaften zunehmend an Interesse. Unter den Übergangsmetallnitriden weisen die Molybdänitride deutlich erhöhte Härtewerte und eine sich selbst ausbildende schmierende Phase (Magnéli-Phase) bei erhöhten Temperaturen auf. Diese Eigenschaften machen das Material interessant für tribologische Anwendungen.

Wir haben Schichten aus Molybdänitrid mit unterschiedlicher Kristallstruktur und Zusammensetzung hergestellt. Besonders von Interesse ist die Herstellung des hexagonalen  $\delta$ - $MoN$ , da diese Phase nicht mit allen PVD-Verfahren hergestellt werden kann. Wir verwenden die hoch-ionisierenden PVD-Verfahren HiPIMS (High Power Impulse Magnetron Sputtering) und PLD (Pulsed Laser Deposition). Die beiden Verfahren werden hier dargestellt, sowie der beobachtete Einfluss der Prozessparameter auf die Schichtbildung erörtert. Die Möglichkeiten und Grenzen der beiden Verfahren sollen hier aufgezeigt werden.

DS 14.59 Tue 17:00 Poster E

**Controlling the B-site Ordering by a Layer-by-Layer MAD growth** — ●PHILIPP KSOLL<sup>1</sup>, CHRISTOPH MEYER<sup>1</sup>, VLADIMIER RODDATIS<sup>2</sup>, and VASILY MOSHNEGA<sup>1</sup> — <sup>1</sup>Erstes Physikalisches Institut, Georg-August-Universität Göttingen — <sup>2</sup>Institut für Materialphysik, Georg-August-Universität Göttingen

Physical properties of double perovskite (DP) with general formula  $A_2BB'O_6$  ( $A$ =rare earth or alkaline earth metals;  $B/B'$  = Co/Mn, Ni/Mn, Fe/Mo) depend strongly on the degree of B-site ordering. To optimize and control the structure, magnetism and electrical properties we further developed the metalorganic aerosol deposition (MAD) technique to grow DP films in a layer-by-layer (LL) mode under a precise control of chemical composition by in situ optical ellipsometry and oxygen atmosphere during the deposition process. Epitaxial superlattices  $(ABO_3)_n/(AB'O_3)_n$  ( $A$  = La, Sr;  $B$  = Ni, Mn, Co, Fe, Mo) with  $n$  decreasing down to 1 unit cell to obtain  $A_2BB'O_6$  have been grown on  $SrTiO_3$  and  $Al_2O_3$  substrates. The films were characterized by global (X-ray diffraction, SQUID, Raman spectroscopy) and local (AFM, TEM) techniques to maintain a full control of the individual layer thickness and to elucidate its influence on the physical properties. Further on, a half-metallic ferromagnetic  $Sr_2FeMoO_6$  films with transition temperatures well above room temperature,  $T_c \sim 450$  K, have been prepared. Financial support by the DFG via project Mo2255-4 is acknowledged.

DS 14.60 Tue 17:00 Poster E

**Evaluation of sputter-damage of zinc-doped indium oxide deposition on Perovskite layers by different deposition techniques** — ●MARLENE HÄRTEL<sup>1,2</sup>, EIKE KÖHNEN<sup>2</sup>, RUSLAN MUJDINOV<sup>1</sup>, STEVE ALBRECHT<sup>2</sup>, and BERND SZYSZKA<sup>1</sup> — <sup>1</sup>Technische Universität Technologie für Dünnschicht-Bauelemente, Berlin, Deutschland — <sup>2</sup>Helmholtz-Zentrum Institut für Silizium Photovoltaik, Berlin, Deutschland

To deposit high quality transparent conductive oxides (TCOs), a lot of energy as well as high temperatures are commonly used. To be able to employ so called TCOs in monolithic Silicon / Perovskite tandem solar cell application, where the Perovskite is targeted to function as a top cell absorber, quite some challenges need to be overcome. The illumination of the bottom silicon cell happens through the top cell, therefore the front contact must be highly transparent and suf-

ficiently conductive to prevent parasitic absorption and to transport charge carriers. However, deposition conditions of high-quality TCOs are damaging for Perovskite top-cells. Therefore, methods to quantify sputter-damage are investigated. This work aims to compare different

deposition techniques in terms of applicability, and different methods to detect sputter-damage and its causes, when depositing amorphous zinc-doped indium oxide.

## DS 15: Focus Session: Direct-Write Nanofabrication and Applications I (Electron Beam Induced Processing) (joint session DS/TT)

### Part I: Advances in Focused Particle Beam Processing & New Approaches

Focused electron beam induced deposition (FEBID) and focused electron beam induced etching (FEBIE) are direct-write approaches for the fabrication of 2D- and 3D-nanostructures made from different materials, such as superconductors, magnetic materials, alloys and intermetallic compounds, as well as meta-materials in which suitable materials combinations result in a desired functionality for various application fields (strain / magnetic / dielectric sensing, multi-functional scanning probe sensors, 3D plasmonic structures, 3D magnetic structures etc).

The Focus Session aims at providing a concentrated presentation of various new developments of the most versatile direct-write techniques for functional nanostructures to a broader audience within the condensed matter community.

#### Organizers:

- Michael Huth, Physikalisches Institut, Goethe-Universität, Frankfurt, Germany
- Harald Plank, FELMI-ZFE, TU Graz, Austria

Time: Wednesday 9:30–12:30

Location: H32

#### Invited Talk

DS 15.1 Wed 9:30 H32

**3D-Nanoprinting with Focused Electron Beams. Advances and Applications** — •ROBERT WINKLER<sup>1</sup>, JASON D FOWLKES<sup>2,3,4</sup>, JÜRGEN SATTELKOW<sup>1</sup>, PHILIP D RACK<sup>2,3,4</sup>, and HARALD PLANK<sup>1,5</sup> — <sup>1</sup>Christian Doppler Laboratory - DEFINE, Institute of Electron Microscopy, Graz University of Technology, 8010 Graz, Austria — <sup>2</sup>Bredesen Center for Interdisciplinary Research, The University of Tennessee, Knoxville, 37996, USA — <sup>3</sup>Nanofabrication Research Laboratory, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, 37831, USA — <sup>4</sup>Materials Science and Engineering Department, The University of Tennessee, Knoxville, 37996, USA — <sup>5</sup>Graz Centre for Electron Microscopy, 8010 Graz, Austria

While 3D printing of objects down to the micrometer scale is well established, techniques for controlled additive manufacturing at the nanoscale are only few. Based on the progress in recent years, Focused Electron Beam Induced Deposition (FEBID) has evolved into a 3D nano-printing technology, allowing mask-less direct-write fabrication of complex 3D nano-architectures on almost any substrate. The growing availability of different precursor types expand the functionalities of those FEBID structures from electrically over magnetically towards optically active purposes, enabling applications, which have been very challenging in the past. Here, we introduce the technology and sketch possibilities and limitations for a comprehensive FEBID portfolio picture. We focus on recent advances in accuracy and predictability based on local heating effects and finally present selected applications of such 3D-nanoprinted structures in research and industry.

DS 15.2 Wed 10:00 H32

**Modeling FEBID frequency maps: Lateral deposit resolution and surface diffusion** — JAKUB JURCZYK<sup>1,2</sup>, CZESLAW KAPUSTA<sup>2</sup>, and •IVO UTKE<sup>1</sup> — <sup>1</sup>Empa, Swiss Federal Laboratories for Materials Science and Technology, Feuerwerkstrasse 39, CH-3602 Thun, Switzerland — <sup>2</sup>AGH University of Science and Technology Krakow, Al. Mickiewicza 30, 30-059 Kraków, Poland

Focused electron beam induced deposition (FEBID) is governed by four main processes: adsorption, desorption, surface diffusion and dissociation of precursor molecules on the sample surface [1],[2]. All of them influence growth rate, lateral resolution and shape of deposited structures; hence we can distinguish four different deposition regimes: reaction-rate limited, mass transport limited, diffusion enhanced and the combination of the two latter [3]. In their recent work, Sanz-Hernandez et al. [4] visualized these regimes based on characteristic

frequencies for every process, creating frequency maps for the growth rates and coverage [4]. In this contribution we expand this approach to include the lateral deposit resolution and the influence of surface diffusion into the frequency maps. Results of simulations will be discussed in the context of their physical basis and future designed experiments. [1] I. Utke et al., J. Vac. Sci. Technol. B, 26, (2008), 1197-1276; [2] M. Toth et al. Beilstein J. Nanotech., 6, (2015), 1518\*1540[3]; A. Szkudlarek et al., Appl. Phys. A, 117, (2014), 1715\*1726;[4] D. Sanz-Hernandez et al., Beilstein J. Nanotechnol., 8, (2017), 2151\*2161

DS 15.3 Wed 10:15 H32

**On the reduction of proximity effects by exploring (metal-) organic materials as substrates/resists for gas-assisted electron beam lithography** — CHRISATIAN PREISCHL, ELIF BILGILISOY, FLORIAN VOLLNHALS, and •HUBERTUS MARBACH — Physikalisches Chemie II, FAU Erlangen-Nürnberg

We investigated organic and metal-organic materials as substrates/resists in different Focused Electron Beam Induced Processing (FEBIP) techniques. Here, FEBIP methods rely on the local decomposition of the volatile precursors Fe(CO)<sub>5</sub> and Co(CO)<sub>3</sub>NO, by the direct impact of the focused electron beam (Electron Beam Induced Deposition, EBID) or through the interaction of the precursor with pre-irradiated/activated surface areas (Electron Beam Induced Surface Activation, EBISA).<sup>1–3</sup> The investigated materials range from porphyrin layers<sup>1,2</sup> over surface anchored metal-organic frameworks (SURMOFs)<sup>3</sup> to self-assembled monolayers (SAMs).<sup>4</sup> Application of our surface science approach, i.e. working in an ultra-high vacuum environment, allows to obtain chemically well-defined deposits. A major advantage of the used materials are reduced electron proximity effects, i.e. reduced electron scattering and quenching of secondary electrons within the latter materials.<sup>1–3</sup> An illustrative example is the fabrication of test structures with Fe(CO)<sub>5</sub> on a SURMOF with an average line width value below 10 nm.<sup>3</sup>

[1] Marbach, H., Appl. Phys. A, 117 (2014) 987-995. [2] Drost, M., et al., Small methods, 1(2017)1700095. [3] Drost, M., et al., ACS Nano. 12 (2018) 3825 . [4] Turchanin, A., et al., Adv. Mater. 28 (2016) 6075.

DS 15.4 Wed 10:30 H32

**FEBIP on Self-Assembled-Monolayers and Carbon Nanomembranes** — •CHRISTIAN PREISCHL<sup>1</sup>, ELIF BILGILISOY<sup>1</sup>, FLORIAN VOLLNHALS<sup>1</sup>, LE HOANG LINH<sup>2</sup>, SASCHA KOCH<sup>2</sup>, ARMIN GÖLZHÄUSER<sup>2</sup>, and HUBERTUS MARBACH<sup>1</sup> — <sup>1</sup>Physik. Chemie II,



FAU Erlangen-Nürnberg, GER — <sup>2</sup>PSS, Bielefeld University, GER

In our approach, we investigate two different FEBIP methods in UHV on Self-Assembled-Monolayers (SAM) and on nanometer thick Carbon Nanomembranes (CNM). These thin CNM sheets can be produced out of SAMs by electron-induced crosslinking.<sup>[1]</sup> The two FEBIP methods of choice are EBID<sup>[2]</sup> and Electron-Beam-Induced-Surface-Activation (EBISA). In EBISA, the surface is locally activated by an electron beam and the subsequently dosed precursor is catalytically decomposed at the activated sites and forms a deposit.<sup>[3]</sup> These two approaches were explored on 1,1',4',1''-terphenyl-4-thiol (TPT) and the corresponding cross-linked CNM with Fe(CO)<sub>5</sub> and Co(CO)<sub>3</sub>NO. Whereas EBID works with both precursors on both substrates, EBISA can only be driven successfully on the non cross-linked TPT with Fe(CO)<sub>5</sub>. Regarding this result, we observe a chemical selectivity in EBISA between the two precursors, which was already reported in previous studies on different substrates.<sup>[4]</sup> Furthermore upon crosslinking, TPT loses its catalytic activity towards the EBISA process.

<sup>[1]</sup> A. Turchanin, A. Götzhäuser, Adv. Mater. 28 (2016), 6075 <sup>[2]</sup> W. van Dorp, C.W. Hagen, J. Appl. Phys. 104 (2008), 081301 <sup>[3]</sup> H. Marbach, Appl. Phys. A 117 (2014), 987 <sup>[4]</sup> Drost et al., Small Methods 1 (2017), 1700095; M. Drost et al., ACS Nano. 12 (2018), 3825

DS 15.5 Wed 10:45 H32

**Fabrication of Photonic and Optomechanics Devices in hBN by Electron Beam Induced Etching** — ●JOHANNES FROECH<sup>1</sup>, SE-JEONG KIM<sup>1</sup>, PRASOON SHANDILYA<sup>2</sup>, BISHNUPADA BEHERA<sup>2</sup>, CHRIS HEALY<sup>2</sup>, JAMES BISHOP<sup>1</sup>, MATTHEW MITCHELL<sup>2</sup>, DAVID LAKE<sup>2</sup>, PAUL BARCLAY<sup>2</sup>, IGOR AHARONOVICH<sup>1</sup>, and MILOS TOT<sup>1</sup> — <sup>1</sup>University of Technology Sydney, Ultimo, NSW, 2007, Australia — <sup>2</sup>University of Calgary, Calgary, AB, T2N 1N4, Canada

Exceptional efforts have been undertaken in recent years to identify suitable platforms for solid state quantum photonic technologies. Several schemes exploit materials that typically host on-demand single photon emitters and can be easily processed in a robust and reliable manner to yield functional nanostructures. A potential material for applications in this field is hexagonal Boron Nitride (hBN), based on the discovery of room-temperature, stable, ultra-bright quantum emitters. However, until recently, fabrication of complex hBN geometries was not viable. Here, we demonstrate new processing approaches for the fabrication of complex photonic and optomechanics nanostructures in suspended hBN and hBN/ Si hybrid systems using the technique of Electron Beam Induced Etching (EBIE). It is minimally invasive and allows for post fabrication editing to tune optical properties. In combined systems, the etching technique is highly selective and allows for precise and maskless fabrication. Overall, our methodology and results set the foundation for cavity quantum electrodynamics experiments and further work in integrated optomechanics systems to be performed utilizing hBN quantum emitters.

DS 15.6 Wed 11:00 H32

**Energy from Green House Gas Stored in Nanogranular Material** — ●HANS KOOPS — HaWilKo GmbH, Ober-Ramstadt, Germany

Light energy from the sky having Ultra-Violet to 10 μm wavelengths is stored as Bosons in nano-granular material. The upper atmosphere of the earth contains layers of green-house material and this emits infrared radiation with 380 W/ m<sup>2</sup>, as measured by NASA in 2009. Nanogranular compound material, Platinum nanocrystals in Fullerene crystals layers, can absorb the IR-radiation and stores it in electron-hole-Bosons with parallel spin. There the electrons can tunnel to the close by conductor, which carries a potential higher than the Boson-layers. Experiments at KNMF in KIT delivered from a Pt/C ribbon of 150 nm thickness and 1 μm width a 4 V a current of 0,6 A without melting the nano-granular Pt/C ribbon. The stored charge can be moved using a field gradient, which shifts the Bosons to the end of the material. There the electrons can tunnel to the close by conductor, which carries a potential higher than the Boson-layers. Experiments at KNMF in KIT delivered from a Pt/C ribbon of 150 nm thickness and 1 μm width a 4 V a current of 0,6 A without melting the nano-granular Pt/C ribbon.

15 min. break.

Invited Talk

DS 15.7 Wed 11:30 H32

**Resist-free fabrication of graphene devices using focused ion**

**beam patterning and direct-write ALD** — ●AGEETH BOL — Eindhoven University of Technology, Eindhoven, the Netherlands

Graphene has long been proposed as ideal candidates to replace silicon in future nanoelectronic devices and has therefore attracted considerable attention from the scientific community. Regardless, graphene struggles to leave the lab as many challenges for large-scale integration still exist. This presentation addresses one of these challenges: the resist-free fabrication of graphene devices. For the fabrication of graphene devices, graphene sheets must be patterned into individual devices, and then contacted to form electrical connections. The conventional approach involves lithography using resist films. To avoid contamination by resist residues as much as possible, a direct patterning and contacting approach was developed. We showed that a focused ion beam (FIB) is able to directly etch graphene from a substrate. By optimizing the pressure as well as reducing the amount of ions used, ion scattering could be minimized, making FIB patterning a feasible alternative to conventional lithography. Next, the FIB-patterned graphene was used to fabricate and characterize electrical devices. For the first time, Pt contacts were deposited by using a combination of electron-beam induced deposition and area-selective Pt which further avoids the use of resist films. The ALD-contacted devices show remarkable improvements compared to conventionally deposited Pt contacts.

DS 15.8 Wed 12:00 H32

**Atomic layer deposition on electron beam written nanostructures** — CASPAR HAVERKAMP<sup>1</sup>, HANNO KRÖNCKE<sup>1</sup>, PATRYK KUSCH<sup>2</sup>, FELIX OERTEL<sup>1</sup>, CATHERINE DUBOURDIEU<sup>1,3</sup>, STEPHANIE REICH<sup>2</sup>, and ●KATJA HÖFLICH<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin — <sup>2</sup>Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin — <sup>3</sup>Freie Universität Berlin, Institut für Chemie und Biochemie, Takustr. 3, 14195 Berlin

The uniform coverage of complex three-dimensional structures is highly beneficial for the process of direct electron beam writing. Thereby, crucial issues in thermal and chemical stability of electron beam written structures can be successfully addressed, while in other cases the desired material response may be realized. Atomic layer deposition (ALD) is a self-limited deposition technique, that allows to deposit conformal ultrathin films on surfaces. The deposition consists of an iterative growth sequence of four steps. First, precursor molecules bind to the surface forming a monolayer. Then, excess precursor molecules and volatile byproducts are purged from the reactor. In a third step, the co-reactant is introduced to react with the chemisorbed precursor molecules. Finally, all volatile products are purged again. While mostly known for the deposition of oxides, other materials and especially metals are available for ALD as well. Therewith, atomic layer deposition constitutes an ideal counterpart to trigger various applications of direct electron beam writing. Examples are demonstrated for plasmonic antennas of different types, optimized for chiroptical interaction, tip-enhanced Raman scattering or nonlinear interactions.

DS 15.9 Wed 12:15 H32

**Towards all-metallic nano-structures using FEBID and ALD** — ●PETER GRUSZKA and MICHAEL HUTH — Goethe Universität, Frankfurt am Main, Deutschland

In recent years, conventional methods of nano-structuring are slowly reaching their lower limits. A novel bottom-up and maskless approach emerged<sup>[1]</sup>, which combines focused electron beam induced deposition (FEBID) and area-selective atomic layer deposition (AS-ALD). FEBID is a serial, bottom-up and direct-write technique yielding structures with superior lateral resolution (< 10 nm), but with poor material quality. In contrast, ALD and especially AS-ALD are parallel bottom-up approaches with exceptional thickness control in the sub-nm regime resulting in high purity films.

We successfully performed the AS-ALD process in our custom ALD micro-reactor on ultra-thin platinum seed layers prepared in a Nova 600 Dual Beam scanning electron microscope by FEBID. The seed layers were purified with a technique developed by Sachser et al.<sup>[2]</sup>. Additionally, we monitored the AS-ALD process via in-situ conductance measurements which enabled us to tune the resistance to a desired value. Low-temperature measurements on standard four-probe structure show metallic behaviour with an RRR of about 2.6 and a Debye temperature of about 230K. First results on high-resolution nanostructure fabrication by FEBID/AS-ALD and their low-temperature transport characteristics are presented.

<sup>[1]</sup> Mackus, et al., J. Appl. Phys 107 (2010), 116102

<sup>[2]</sup> Sachser, et al., ACS Appl. Mater. Interfaces 6 (2014), 15868

## DS 16: Organic Thin Films, Organic-Inorganic Interfaces

Time: Wednesday 9:30–12:30

Location: H39

DS 16.1 Wed 9:30 H39

**Visualising the Vertical Energetic Landscape in Organic Photovoltaics** — •VINCENT LAMI<sup>1</sup>, ANDREAS WEU<sup>1</sup>, JIANGBIN ZHANG<sup>2</sup>, YONGSHENG CHEN<sup>3</sup>, ZHUPING FEI<sup>4</sup>, MARTIN HEENEY<sup>4</sup>, RICHARD FRIEND<sup>2</sup>, and YANA VAYNZOF<sup>1</sup> — <sup>1</sup>KIP/CAM, Heidelberg University, GER — <sup>2</sup>Cavendish Laboratory, University of Cambridge, UK — <sup>3</sup>Nankai University, Tianjin, China — <sup>4</sup>Chemistry & CPE, Imperial College London, UK

Energy level diagrams in organic photovoltaic (OPV) devices play a crucial role in interpretation of device physics, since they determine elementary processes such as charge generation, transport or extraction. Despite the importance of these diagrams, they are currently often constructed by combining energetic values of the individual device components, without taking into account interfacial effects, such as band bending or dipole formation. Herein, we demonstrate that combining ultra-violet photoemission spectroscopy (UPS) with gas cluster ion beam sputtering allows for a damage-free depth profiling and hence, an accurate determination of the vertical energetic landscape of active layers. First, we utilize a model photovoltaic system, then we demonstrate our method on other high efficiency fullerene and non-fullerene systems. We are not only able to accurately measure the highest occupied molecular orbital (HOMO) offset of the contributing materials and to quantify energy losses, but also to obtain compositional information with a very high vertical depth resolution. Finally, as UPS depth profiling can be performed at any point in device lifetime, it offers valuable information after device operation or degradation.

DS 16.2 Wed 9:45 H39

**Titanylphthalocyanine Films on Ag(111): an Epitaxial Metal/Organic Hetero-System with Exceptional Smooth Surface** — •MICHAEL KOTHE, FELIX WIDDASCHECK, and GREGOR WITTE — Philipps-Universität, Marburg, Germany

The chemical and thermal robustness of titanyl-phthalocyanine (TiOPc) in combination with its high optical absorption favours its application as photoconductor or chromophore for light-harvesting in organic photovoltaic applications. Beside such device application there is a large interest in the controlled fabrication of smooth molecular spacer layers of controlled thickness in order to prepare molecular heterostructures. While many pi-conjugated materials form highly ordered mono- and bilayer films on metallic (single crystalline) substrates, the films exhibit a notable roughness upon increasing film thickness. Here, we demonstrate that TiOPc forms extremely smooth films on Ag(111), not only in the mono- and bilayer regime but also for films exceeding a thickness of 10nm. Combining various techniques including atomic force and scanning tunnelling microscopy (AFM, STM), with X-ray photoelectron spectroscopy (XPS), near-edge X-ray absorption fine structure spectroscopy (NEXAFS) and X-ray diffraction (XRD), we show that for substrate temperatures below 450 K TiOPc forms molecularly smooth films with a small overall film roughness. The analysis shows that the films are stabilized by molecular bilayers of alternately (up and down) oriented titanyl. Finally, we show that even the thick films are epitaxially oriented with respect to the azimuth direction of the Ag(111) surface.

DS 16.3 Wed 10:00 H39

**Vacuum-deposited organic monolayers for work function modification of noble metal electrodes** — •FELIX WIDDASCHECK, ALRUN ALINE HAUKE, and GREGOR WITTE — Molekulare Festkörperphysik, Philipps-Universität Marburg, D-35032 Marburg, Germany

The energy level alignment between organic semiconductors and the respective (metal) electrodes in organic electronic devices is of key importance for efficient charge carrier injection. For many years, researchers have attempted to control this energy level alignment by means of functional self-assembled monolayers (SAMs) or the insertion of thin injection layers (made e.g. of doped organic semiconductors or pure dopants). The present work demonstrates an alternative approach, namely the use of phthalocyanine monolayers as contact primers which are deposited onto noble metal electrodes by means of vacuum deposition. We show that polar as well as non-polar phthalocyanines modify the work functions of clean Au(111) and Ag(111) surfaces as a function of their coverage and thus enable quantitative control of the metal work functions. This behavior is successfully replicated for polycrys-

talline metal surfaces and it is found that full monolayers can even withstand air exposure when protected by sacrificial multilayers which are afterwards removed by thermal desorption.

DS 16.4 Wed 10:15 H39

**Thermal emission from a hybrid plasmonic structure in the strong coupling regime** — •HALA MEMMI, OLIVER BENSON, SERGEY SADOFEV, and SASCHA KALUSNIAK — Institut für Physik, Humboldt Universität zu Berlin, Berlin, Germany

We report on thermal emission from an organic/inorganic plasmonic hybrid structure where a carbonyl stretching vibration is strongly coupled with a surface plasmon polariton. The structure consists of a polyvinyl-methyl-ketone layer deposited on top of a silver layer. Emission measurements in Kretschmann-Raether configuration using a calcium fluoride hemicylindrical prism as decoupling medium were conducted at 140°C and collected in transverse magnetic polarization. Two clear maxima corresponding to upper and lower polariton branch were observed in the emission spectra. They also reproduce the anti-crossing behavior in the dispersion relation as revealed from Attenuated-total-reflection measurements. The intensity of the emission maxima as a function of the varying temperature confirms the different nature of the branches.

DS 16.5 Wed 10:30 H39

**Reaction of Calcium with Tetraphenylporphyrin Thin Films: Reaction Energies and Reaction Depths** — •MAIK SCHÖNIGER, STEFAN RENATO KACHEL, CLAUDIO K. KRUG, TABEA KOEHLER, MARTIN SCHMID, and J. MICHAEL GOTTFRIED — Philipps-Universität Marburg, Fachbereich Chemie, Hans-Meerwein-Str. 4, 35032 Marburg

We have investigated the interface reaction of vapour-deposited calcium (Ca) with tetraphenylporphyrin (2HTPP) thin films (20-30 nm) by means of Hard X-Ray Photoemission Spectroscopy (HAXPES) and Nanojoule Adsorption Calorimetry (NAC). The importance of low work-function materials and organic semiconductors is obvious as they are commonly used in organic electronics. However, their interfacial interactions are poorly understood. Clarifying diffusion and reaction processes occurring during metal deposition onto the organic material is crucial for a deeper understanding of the performance of such systems. The Ca/2HTPP system is a model system that allows us to study the energetics of a typical interface reaction and to establish concentration depth profiles of the resulting interphase layer, which here consists of the reaction product CaTPP. Using HAXPES, we measured depth profiles of the interface region for different preparation conditions of the interface. Parameters such as temperature or flux of the Ca atoms were varied. As complementary data, we will report enthalpies of adsorption and reaction, measured using NAC coupled with a pulsed Ca atomic beam source. The apparatus allows the direct measurement of these quantities, which cannot be obtained by temperature-programmed desorption or similar frequently used methods.

DS 16.6 Wed 10:45 H39

**Measuring and Modelling Electric Potential Distributions at Organic Semiconductor Interfaces** — •MARKUS FRERICKS<sup>1,2</sup>, CHRISTOF PFLUMM<sup>3</sup>, WOLFRAM JAEGERMANN<sup>1,2</sup>, and ERIC MANKEL<sup>1,2</sup> — <sup>1</sup>Technische Universität Darmstadt, Darmstadt — <sup>2</sup>InnovationLab, Heidelberg — <sup>3</sup>Merck KGaA, Darmstadt

Photoelectron spectroscopy (PES) is an important characterization method in the field of semiconductor physics. Consecutive deposition of thin layers of an adsorbate on a substrate monitored by PES allows for an analysis of the electronic structure at semiconductor interfaces. For organic semiconductors (OSCs), several publications, e.g. [1], indicate that the key to understand contact formation and doping mechanisms lies in the disorder of organic molecules and its influence on the density of states (DOS). Supporting this idea, we developed a model based on the ones presented by Salzmann et. al. and Lange et. al. [1,2] to numerically calculate the potential distribution at OSC interfaces. Combining these calculations with the approach of Ohashi et. al. [3] to simulate PES data, we derived an algorithm to fit the results of above-mentioned type of interface experiment. By this means, we obtained a tool that supports the importance of the DOS and allows for further investigations on its influence and behavior at contacts. After

presenting the procedure, we will demonstrate its applicability on the results of interface experiments with differently doped hole transport materials.

[1] Salzmann et. al., *Acc. Chem. Res.* 49 (2016) [2] Lange et. al., *PRL* 106 (2011) [3] Ohashi et. al., *Appl. Phys. Lett.* 101 (2012)

### 15 min. break.

DS 16.7 Wed 11:15 H39

**Semi-transparent organic detectors for standing wave sensing applications** — ●VLADISLAV JOVANOVIĆ<sup>1</sup>, PATRICE DONFACK<sup>1</sup>, ARNE MÜLLER<sup>1</sup>, ARNULF MATERNY<sup>1</sup>, DIETMAR KNIPP<sup>2</sup>, and VEIT WAGNER<sup>1</sup> — <sup>1</sup>Jacobs University Bremen, 28759 Bremen, Germany — <sup>2</sup>Stanford University, Stanford, CA 94305, USA

Organic semiconductor materials are widely used for the development and realization of optoelectronic devices because of their compatibility with solution processing fabrication and printing techniques. Currently, light emitting diodes and solar cells are the most developed areas of application of organic materials. The huge potential of organic materials is still not fully explored in other application areas among which optical sensing and spectrometers could be very promising. In this investigation, a fast and compact standing wave spectrometer based on semi-transparent organic photodetectors is developed [1]. The semi-transparent organic detectors are realized using polymer-fullerene material systems and solution-based fabrication. The fabricated semi-transparent detectors exhibit an overall transmittance of about 20% in the visible range of the electromagnetic spectrum. The realization of a standing wave spectrometers is achieved by combining fabricated semi-transparent organic detectors with a movable mirror controlled by a piezo micro-actuator. The unique advantages of standing wave sensing devices based on organic materials as well as the required material properties are presented and discussed.

[1] V. Jovanov, P. Donfack, A. Müller, A. Materny, D. Knipp, and V. Wagner, *J. Mater. Chem. C* 6, 11457-11464 (2018).

DS 16.8 Wed 11:30 H39

**Pentacene and Perfluoropentacene Bilayers – Well-Defined Interfaces vs. Molecular Intermixture** — ●PIERRE DOMBROWSKI, TOBIAS BREUER, STEFAN RENATO KACHEL, J. MICHAEL GOTTFRIED, and GREGOR WITTE — Philipps-Universität Marburg, Germany

Precisely studying organic donor/acceptor systems is crucial for the improved understanding and design of organic optoelectronic devices. Heterostructures of p-type organic semiconductors (OSCs) and fluorinated n-type OSCs are particularly attractive donor/acceptor systems as they tend to form H-F bonds that favor the formation of intermixed supramolecular assemblies. Within these, pentacene (PEN) and perfluoropentacene (PFP) are an interesting model system due to their structural compatibility. The present study combines near-edge X-ray absorption fine structure (NEXAFS), temperature programmed desorption (TPD) and scanning tunneling microscopy (STM) measurements to characterize the intermixture of PEN and PFP on molybdenum disulfide as well as the Ag(111) and Au(111) surfaces. NEXAFS spectra of PEN and PFP bilayers show that it is possible to prepare nicely ordered bilayers without mutual intermixing. Only upon annealing, molecular intermixture is activated. TPD measurements reveal an attractive intermolecular interaction in the heterostructure, in contrast to repulsive interaction in the unitary phases, and suggest the formation of a thermally stabilized 1:1 intermixture, in line with previous TPD results [1]. STM images directly show intermixed phases that support the model of a stabilization by H-F bonds.

[1] T. Breuer and G. Witte, *J. Chem. Phys.* (2013), 138, 114901

DS 16.9 Wed 11:45 H39

**Low-Dimensional Hybrid Interfaces Between Acenes and TMDCs: Pentacene and Perfluoropentacene on MoS<sub>2</sub>** — ●STEFAN RENATO KACHEL, PIERRE DOMBROWSKI, TOBIAS BREUER, GREGOR WITTE, and J. MICHAEL GOTTFRIED — Philipps-Universität Marburg, Germany

Pentacene (PEN) is a widely investigated organic semiconductor used

for fabrication of thin film transistors. Upon fluorination, the electronic configuration of perfluoropentacene (PFP) undergoes drastic changes that influence its adsorption and growth behavior. The differences of PEN and PFP have been studied on bulk as well as on 2D layered MoS<sub>2</sub> by multiple techniques such as near-edge X-ray absorption fine structure (NEXAFS), X-ray photoelectron spectroscopy (XPS), temperature-programmed desorption (TPD) and optical spectroscopy. In NEXAFS, we found flat-laying monolayers of PEN and PFP on both bulk and 2D layers MoS<sub>2</sub>. TPD shows a distinct monolayer peak characterized by a typical peak broadening and a peak maximum shift to lower temperatures as often found for organic adsorbates. Moreover, PFP submonolayers desorb at 30 K higher temperatures than PEN giving evidence for a higher binding energy to the substrate. The multilayer desorption is in agreement with other studies. Gentle heating allows the reliable desorption of the multilayers while leaving a well-defined monolayer behind, both on bulk as well as 2D-MoS<sub>2</sub>. This preparation gives rise to further spectroscopic methods allowing the examination of the electronic properties of a perfectly defined interface between precisely one OSC layer and a 2D-TMDC substrate.

DS 16.10 Wed 12:00 H39

**Multi-analytical investigation of tetrapodal self-assembled monolayers on gold: Formation and Functionality** — ●VALENTINA ROHNACHER<sup>1,2</sup>, FRANK SIMON BENNECKENDORF<sup>2,3</sup>, MAYBRIT MÜNCH<sup>2,4</sup>, SEBASTIAN BECK<sup>1,2</sup>, and ANNEMARIE PUCCI<sup>1,2</sup> — <sup>1</sup>Kirchhoff Institute for Physics, Uni Heidelberg — <sup>2</sup>Innovationlab, Heidelberg — <sup>3</sup>Institute of Organic Chemistry, Uni Heidelberg — <sup>4</sup>Surface Science Division, TU Darmstadt

Self-assembled monolayer (SAMs) have proven to form stable and well-defined layers on various electrode materials increasing the interfacial compatibility in organic electronic devices.[1,2] A novel tetrapodal SAM molecule with four thiol-anchor groups was synthesized which enables fourfold binding to the gold substrate, enforcing a perpendicular orientation of the molecular dipole relative to the metal surface. We perform infrared reflection-absorption spectroscopy (IRRAS) measurements on tetrapodal diazaitycene molecules on evaporated gold substrates to probe the orientation and quality of the SAMs. In comparison with contact angle measurement and photoelectron spectroscopy, a better understanding about the SAM formation and electrode modification was achieved.

[1] Jesper et al. *Langmuir* 2015, 31, 37, 10303-10309

[2] Benneckendorf et al. *J. Phys. Chem. Lett.* 2018, 9, 13, 3731-3737

DS 16.11 Wed 12:15 H39

**Switching the surface electronic properties of polar ZnO crystals with photochromic pyridyl-dihydropyrene molecular layers** — ●QIANKUN WANG<sup>1</sup>, GIOVANNI LIGORIO<sup>1</sup>, RAPHAEL SCHLESINGER<sup>1</sup>, VALENTIN DIEZ-CABANES<sup>2</sup>, DAVID CORNIL<sup>2</sup>, YVES GARMSHAUSEN<sup>1</sup>, STEFAN HECHT<sup>1</sup>, JÉRÔME CORNIL<sup>2</sup>, EMIL J. W. LIST-KRATOCHVIL<sup>1</sup>, and NORBERT KOCH<sup>1</sup> — <sup>1</sup>Humboldt-Universität zu Berlin — <sup>2</sup>University of Mons

Remote control of the electronic energy levels by external stimuli such as light will enable optoelectronic devices with improved or additional functionalities. Here, we demonstrate that the electronic properties of ZnO interfaced with molecular negative T-type photoswitches, i.e., pyridyl-dihydropyrene (Py-DHP), can indeed be photomodulated. Using photoemission spectroscopy and density functional theory (DFT) modelling, we show that the photochromic ring closure/opening process results in reversible shift of the frontier occupied molecular level by 0.7 eV with respect to the Fermi level. Notably, in both molecular configurations, the energy level alignment at the ZnO/Py-DHP interface is governed by a Fermi level pinning of the lowest unoccupied molecular level. Moreover, upon switching, we observe an increase in the ionization energy for Py-DHP multilayers compared to that of a monolayer. We attribute this to a different preferred molecular orientation in monolayer versus multilayer films. Our results show that dynamic tuning of the interface energy level alignment at inorganic/organic junctions by external stimuli is indeed possible and will aid the development of photoprogrammable opto-electronic devices.

## DS 17: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge V (joint session O/ CPP/ DS/ TT)

Time: Wednesday 10:30–13:15

Location: H9

**Topical Talk**

DS 17.1 Wed 10:30 H9

**Theoretical Investigations of Electrochemical CO<sub>2</sub> Reduction** — ●KAREN CHAN — Department of Physics, Technical University of Denmark

The electroreduction of CO<sub>2</sub> has the potential to store energy from intermittent renewable sources and to produce carbon-neutral fuels and chemicals; In this talk, I will discuss new developments in modeling the electrochemical interface. I will then present the application of these models of the interface to CO<sub>2</sub> reduction: the determination of reaction pathways and kinetics on transition metals, field and solvation effects, pH effects on C<sub>2</sub> product selectivity, and implications for catalysis design.

**Topical Talk**

DS 17.2 Wed 11:00 H9

**First-principles approach to model electrochemical reactions at the solid-liquid interface** — ●MIRA TODOROVA, SUDARSAN SURENDRALAL, and JÖRG NEUGEBAUER — MPI für Eisenforschung, Düsseldorf

Processes at solid-liquid interfaces are at the heart of many present day technological challenges related to the improvement of battery materials, electro-catalysis, fuel cells, corrosion and others. Describing and quantifying the underlying fundamental mechanisms is equally challenging for experimental and theoretical techniques.

Utilizing concepts from semiconductor physics, we have developed a novel potentiostat design, which enables us to perform *ab initio* calculations under controlled bias conditions. Easily applied in standard density functional theory codes, it controls the electrode potential of the system by tuning the excess charge of the working electrode and allows us to obtain direct insight into key mechanisms of electrocatalysis and corrosion. As a prototype example, we consider one of the most corrosive systems under wet conditions - Mg. Using the new approach we solve a 150-year-old problem, which links H-evolution under anodic conditions to Mg dissolution [1].

[1] S. Surendralal, M. Todorova, M.W. Finnis and J. Neugebauer, *Phys. Rev. Lett.* 120, 246801 (2018).

DS 17.3 Wed 11:30 H9

**Towards out of the box implicit solvation at liquid-liquid interfaces** — ●JAKOB FILSER<sup>1</sup>, MARKUS SINSTEIN<sup>1</sup>, CHRISTOPH SCHEURER<sup>1</sup>, SEBASTIAN MATERA<sup>2</sup>, KARSTEN REUTER<sup>1</sup>, and HARALD OBERHOFER<sup>1</sup> — <sup>1</sup>Technische Universität München — <sup>2</sup>Freie Universität Berlin

Implicit solvation models are widely used to incorporate solvent effects in electronic structure theory. Treating the solvent as a structureless dielectric continuum, they lift the necessity to explicitly sample solvent degrees of freedom. However, even state of the art models currently cannot treat solvation at technically highly important dielectric interfaces, e.g. between two immiscible liquids.

As a remedy, we modify the multipole expansion (MPE) model to also account for liquid-liquid interfaces, specifically focusing on the electrostatics of mutually interacting dielectric regions. Non-electrostatic free energy contributions thereby are treated with a simple linear model, fitted to experimental free energies of solvation in the two liquids. We demonstrate the efficacy of this approach for small molecules at a water-1-octanol interface, which show the correct qualitative behaviour with respect to orientation and position at the interface.

Future, quantitative applications of our new implicit solvation interface methods are clearly possible but will necessitate both improvements to the non-electrostatic free energy terms and a more exhaustive parameterization effort for a wide range of solvents.

DS 17.4 Wed 11:45 H9

**Continuum models of the electrochemical diffuse layer in electronic-structure calculations** — ●FRANCESCO NATTINO<sup>1</sup>, OLIVIERO ANDREUSSI<sup>2</sup>, and NICOLA MARZARI<sup>1</sup> — <sup>1</sup>Theory and Simulations of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — <sup>2</sup>Department of Physics, University of North Texas, Denton, TX 76207, USA

The electrical diffuse layer is a structure that spontaneously forms at essentially any solvated interface, such that its presence in electrochemistry is ubiquitous. While first-principles methods are desirable to describe any process occurring at the surface, fully-atomistic models of electrolyte solutions suffer from computational limitations. In this context, continuum models represent a practical tool to bypass these difficulties and to account for the presence of the diffuse layer at electrified interfaces. However, despite the increasing popularity of continuum models in the field of materials science, even relatively simple observables such as the differential capacitance (DC) of single-crystal electrode surfaces remain challenging to model quantitatively. I will present and discuss the performance of a hierarchy of continuum diffuse-layer models that we have implemented and coupled to an atomistic first-principles description of a charged metal surface. In particular, I will compare computed DC values for the prototypical Ag(100) surface in an aqueous solution to experimental data, and validate in this way the accuracy of the models considered.

DS 17.5 Wed 12:00 H9

***Ab initio* molecular dynamics of Pt(111)/H<sub>2</sub>O interfaces in an electrolytic cell setup** — ●SUDARSAN SURENDRALAL, MIRA TODOROVA, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany.

Recently, we developed a novel scheme to perform density functional theory (DFT) simulations of electrochemical interfaces under conditions of constant applied voltage utilizing charge transfer from a semiconductor counter electrode [1]. We use a fractionally doped Ne counter electrode because of its inertness, wide band gap, and low deformation potential. Our DFT based molecular dynamics calculations of the Pt(111)/H<sub>2</sub>O interface in this setup reveals that we are able to accurately reproduce macroscopic observables like the potential of zero charge (PZC). We discuss the work function drop at the interface at the PZC, due to the charge polarization by the non-dissociative chemisorption of water molecules at the Pt surface. Possible pitfalls due to the choice of the DFT exchange-correlation functional, non-converged computational parameters and confinement effects due to the presence of the counter electrode will also be discussed.

[1] S. Surendralal, M. Todorova, M. W. Finnis, and J. Neugebauer, *Phys. Rev. Lett.* 120, 246801 (2018).

DS 17.6 Wed 12:15 H9

**Swipe left for water molecules? - Implicit vs explicit descriptions of liquid water at interfaces.** — ●NICOLAS HÖRMANN<sup>1</sup>, OLIVIERO ANDREUSSI<sup>2</sup>, and NICOLA MARZARI<sup>1</sup> — <sup>1</sup>Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), EPFL, CH-1015 Lausanne, Switzerland — <sup>2</sup>Department of Physics, University of North Texas, Denton, TX 76207, USA

We present a study of relevant electrochemical interfaces, such as semiconductor-water and metal-water interfaces based on periodic density functional theory (DFT) calculations with the interface modelled with different degrees of complexity. Water at metallic surfaces is modelled within the self-consistent continuum solvation scheme (SCCS) [1] with explicit application of a potential which allows the comparison of pH dependent properties with experimental results [2,3]. In the case of semiconductors, different amounts of interfacial water are substituted with implicit solvent and observables such as the measured band alignment are obtained from thermal averaging over molecular dynamics snapshots. We find that it is necessary and sufficient to include strongly bound interfacial water molecules (dissociated or not) explicitly and replace the rest with an implicit model, in order to obtain consistent results with all-explicit simulations [4]. Based on these result we simulate the surface Pourbaix diagrams of the most stable surfaces of GaAs, GaN, GaP, CdS and anatase and rutile TiO<sub>2</sub>.

[1] *J. Chem. Phys.* **136**, 064102 (2012); [2] *Nat Commun.* **9**, 3117 (2018). [2,3] NH (2018) submitted

DS 17.7 Wed 12:30 H9

**Transition metal oxide nanoparticles as efficient catalysts for proton exchange membrane electrolyzers: morphology, activity and stability** — ●DANIEL OPALKA, YONGHYUK LEE, JAKOB TIM-

MERMANN, CHRISTOPH SCHEURER, and KARSTEN REUTER — Technische Universität München

Transition metal oxides such as RuO<sub>2</sub> and IrO<sub>2</sub> are currently the best known electrocatalysts for the oxygen evolution reaction from liquid water in proton exchange membrane (PEM) electrolyzers. However, dynamic load operation of PEM cells induces transformations of the catalyst morphology leading to metal dissolution and catalyst degradation. We present a computational model to predict the morphology, activity and stability from *ab initio* electronic structure theory and fundamental thermodynamic principles. Based on this model, we have explored novel strategies to reduce material expenses and improve catalyst stability while preserving high catalytic activity via nanoparticles with a core-shell design. From an analysis of different surface coverages with oxygen, hydroxyl and hydroxo species, voltage-dependent phase diagrams for catalyst surfaces are presented which correlate with characteristic features observed in cyclovoltammetric measurements. Results from atomistic models of selected nanoparticles on the basis of Wulff's Theorem show negligible size effects, but a strong influence of the facet terminations on the surface relaxation.

DS 17.8 Wed 12:45 H9

**Modelling the fingerprint of chemical reactions on catalytic surfaces in core-electron binding energies** — ●JOHANNES LISCHNER and JUHAN MATTHIAS KAHK — Imperial College London

Core-electron X-ray photoemission spectroscopy is a powerful experimental technique to gain information about chemical reactions on catalytic surfaces. Interpreting experimental spectra, however, is often challenging and theoretical modelling of core-electron binding energies is required to meaningfully assign peaks to adsorbate species. In this talk, I will present a novel first-principles modelling strategy to calculate core-electron binding energies of molecules on metallic surfaces. Specifically, we combine plane-wave/pseudopotential DFT calculations

## DS 18: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge VI (joint session O/DS/ CPP/TT)

Time: Wednesday 15:00–17:45

Location: H9

DS 18.1 Wed 15:00 H9

**First-principles quantum transport simulations including strong correlation effects** — ●ANDREA DROGHETTI<sup>1</sup>, WILHELM APPELT<sup>2</sup>, LIVIU CHIONCEL<sup>2</sup>, MILOS RADONJIC<sup>3</sup>, ENRIQUE MUÑOZ<sup>4</sup>, STEFAN KIRCHNER<sup>5</sup>, DAVID JACOB<sup>1</sup>, DIETER VOLLHARDT<sup>2</sup>, ANGEL RUBIO<sup>6</sup>, and IVAN RUNGER<sup>7</sup> — <sup>1</sup>University of the Basque Country (Spain) — <sup>2</sup>University of Augsburg (Germany) — <sup>3</sup>University of Belgrade (Serbia) — <sup>4</sup>Pontificia Universidad Católica de Chile — <sup>5</sup>Zhejiang University (China) — <sup>6</sup>Max Planck Institute for the Structure and Dynamics of Matter (Germany) — <sup>7</sup>National Physical Laboratory (UK)

When magnetic molecules are brought into contact with metals the electron-electron interaction leads to the appearance of the correlated Kondo state. In this talk we will present the results of first-principles calculations for the electronic structure and the linear-response conductance of radical molecules adsorbed on metallic surfaces in the Kondo regime [Phys. Rev. B 95, 085131 (2017), Nanoscale 10, 17738 (2018)]. In particular we will outline the methodological approach as implemented in the Smeagol electron transport code and we will benchmark the results against experiments. The method relies in the first place on the combination of Density Functional Theory with the Green's functions technique. We will explain how a molecular device is projected onto an effective Anderson impurity problem, which is then solved either by continuum time quantum Monte Carlo or numerical renormalization group. Finally, we will describe some work-in-progress aimed at computing transport properties beyond linear-response.

DS 18.2 Wed 15:15 H9

**Density functional theory for transport through correlated systems** — ●STEFAN KURTH — Univ. of the Basque Country UPV/EHU, San Sebastian, Spain — IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — Donostia International Physics Center DIPC, San Sebastian, Spain

A recently proposed density functional formalism to describe electronic transport through correlated systems in the steady state uses both the density on the junction and the steady current as basic variables. The

of surface slab models for geometry optimizations with all-electron Delta-SCF calculations on cluster models for determining accurate core-electron binding energies. This approach is computationally efficient and yields good agreement with experimental measurements for a wide range of adsorbates on copper(111) surfaces.

DS 17.9 Wed 13:00 H9

**What Makes a Successful Photoanode? - The Role of the Semiconductor-Catalyst Interface** — ●FRANZISKA SIMONE HEGNER<sup>1</sup>, BENJAMIN MOSS<sup>2</sup>, JAMES DURRANT<sup>2</sup>, SIXTO GIMENEZ<sup>3</sup>, JOSÉ-RAMÓN GALÁN-MASCARÓS<sup>1</sup>, and NÚRIA LÓPEZ<sup>1</sup> — <sup>1</sup>Institute of Chemical Research of Catalonia (ICIQ) — <sup>2</sup>Imperial College London — <sup>3</sup>Institute of Advanced Materials, Castellón

A large scale implementations of artificial photosynthesis is still limited by the low efficiencies of the employed photoelectrochemical systems. A common strategy to improve performance is to deposit a co-catalyst on the light-harvesting photoanode. However, the role of the catalyst is controversial; is it acting as a true catalyst, i.e. transferring charges, or is it merely influencing the electronic structure of the semiconductor?[1]

The semiconductor-catalyst interface is key to catalytic performance, but its accurate description is limited since linear scaling relationships no longer apply. Herein the function of the co-catalyst (cobalt hexacyanoferrate) is discussed on two photoanode interfaces, Fe<sub>2</sub>O<sub>3</sub> and BiVO<sub>4</sub>. Density Functional Theory and time-resolved spectroscopy were used to shed light on the underlying charge-transfer processes. Taking into account the advantages and disadvantages of all applied techniques, a relationship between electronic structure alignment, interface morphology, and photocatalytic efficiency is proposed.[2]

[1] D. R. Gamelin, Nat. Chem., 4 (2012), 965-967. [2] F. S. Hegner, D. Cardena-Moscoros, S. Gimenez, N. López, J. R. Galán-Mascarós. ChemSusChem, 10 (2017) 4552-4560.

corresponding Kohn-Sham system features two exchange-correlation (xc) potentials, a local xc potential and an xc contribution to the bias, which are universal functionals of the basic variables.

A recent parametrization of the xc potentials for the single-impurity Anderson model correctly incorporates both the Kondo and Coulomb blockade regimes. It allows for calculation of currents and differential conductances at arbitrary bias and temperature at negligible numerical cost but with the accuracy of sophisticated renormalization group methods. A time-local version of this functional is used to study the Anderson model under the influence of both DC and AC biases. We observe interaction-induced shifts of the photon-assisted conductance peaks, suppression of the Kondo plateau at zero temperature and lifting of Coulomb blockade at finite temperature.

DS 18.3 Wed 15:30 H9

**Exact factorization of the many-electron wave function** — ●CAMILLA PELLEGRINI<sup>1</sup>, ANTONIO SANNA<sup>1</sup>, and EBERHARD K. U. GROSS<sup>1,2</sup> — <sup>1</sup>Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany — <sup>2</sup>Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

The exact factorization approach [1], originally developed for a system of electrons and nuclei, is extended to a system of electrons only. This allows for a two-particle Schrödinger equation, which uniquely defines the exact effective interaction between two electrons in the medium. This interaction differs from the effective interaction,  $W$ , used in many-body Green's function techniques. In particular, it is spin-dependent. We illustrate the formalism for the simplest case of exchange interactions only.

[1] A. Abedi, N.T. Maitra, E.K.U. Gross, PRL 105, 123002 (2010).

DS 18.4 Wed 15:45 H9

**Many-body spectral functions from steady state density functional theory** — ●DAVID JACOB<sup>1,2</sup> and STEFAN KURTH<sup>1,2,3</sup> — <sup>1</sup>Dpto. de Física de Materiales, Universidad del País Vasco UPV/EHU, San Sebastián, Spain — <sup>2</sup>IKERBASQUE, Basque Foundation for Science,

Bilbao, Spain — <sup>3</sup>DIPC, San Sebastián, Spain

We present a scheme to extract the true many-body spectral function of an interacting many-electron system from an equilibrium density functional theory (DFT) calculation [1]. To this end we devise an ideal STM-like setup and employ the recently proposed steady-state DFT formalism (i-DFT) which allows to calculate the steady current through a nanoscopic region coupled to two biased electrodes [2]. In our setup one of the electrodes serves as a probe ("STM tip"). In the ideal STM limit of vanishing coupling to the tip, the system to be probed is in quasi-equilibrium with the "substrate" and the normalized differential conductance yields the exact equilibrium many-body spectral function. Moreover, from the i-DFT equations we derive an exact relationship which expresses the interacting spectral function in terms of the Kohn-Sham one. Making use of i-DFT xc functionals that capture Coulomb blockade as well as Kondo physics, the method yields spectral functions for Anderson impurity models in good agreement with NRG calculations. It is thus possible to calculate spectral functions of interacting many-electron systems at the cost of an equilibrium DFT calculation.

**References:** [1] D. Jacob and S. Kurth, *Nano Lett.* **18**, 2086 (2018) [2] G. Stefanucci and S. Kurth, *Nano Lett.* **15**, 8020 (2015)

DS 18.5 Wed 16:00 H9

**Magnetic phase transitions induced by pressure and magnetic field: the case of antiferromagnetic USb<sub>2</sub>** — ●LEONID SANDRATSKII — Max Planck Institute of Microstructure Physics, Halle, Germany

Fascinating phenomena observed under applied pressure and magnetic field are currently attracting much research attention. Recent experiments have shown that application of the pressure or magnetic field to the USb<sub>2</sub> compound induce the transformations of the ground-state antiferromagnetic (AFM) up-down-down-up structure to, respectively, ferromagnetic (FM) or ferrimagnetic configurations. Remarkably, the magnetic critical temperature of the FM state, induced by pressure, is more than two times smaller than the Neel temperature of the ground state. We performed density-functional theory (DFT) and DFT+U studies to reveal the origin of the unusual magnetic ground-state of the system and the driving mechanisms of the phase transitions. We investigate both the magnetic anisotropy properties and the parameters of the interatomic exchange interactions. To study pressure-induced effects we carry out calculations for reduced volume and demonstrate that the AFM-FM phase transformation indeed takes place but depends crucially on the peculiar features of the magnetic anisotropy. We also explain why the magnetic field that couples directly to the magnetic moments of atoms leads to the phase transition to the ferrimagnetic state whereas the pressure that does not couple directly to magnetic moments results in the FM structure.

DS 18.6 Wed 16:15 H9

**Charge localization at a weakly coupled molecule-metal system studied by linear expansion  $\Delta$ -self-consistent field density-functional theory ( $\Delta$ SCF-DFT)** — ●HADI H. AREFI<sup>1,2</sup>, DANIEL CORKEN<sup>3</sup>, REINHARD MAURER<sup>3</sup>, F. STEFAN TAUTZ<sup>1,2</sup>, and CHRISTIAN WAGNER<sup>1,2</sup> — <sup>1</sup>Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — <sup>2</sup>JARA-Fundamentals of Future Information Technology — <sup>3</sup>Department of Chemistry, University of Warwick, Coventry, United Kingdom

Predicting the charge arrangements at the interface between molecules and metals represents a formidable challenge for semi-local approximations to Density Functional Theory (DFT). This could become even more critical when molecules are only weakly coupled to the metal. Single-molecular devices based on such weak coupling have recently been created by molecular manipulation with a scanning probe microscope (SPM), where a single PTCDA (perylene-tetracarboxylic dianhydride) molecule was placed in a free-standing upright configuration either on a SPM tip [1] or on a pedestal of two adatoms on the Ag(111) surface [2]. There are indications that the mechanism stabilizing these unexpected configurations is linked to an integer charge transfer creating a singly occupied molecular orbital. We use the  $\Delta$ SCF-DFT method [3] to confine charge on the LUMO of the PTCDA and study the consequences with vdW-corrected DFT.

[1] C. Wagner et al. *Phys. Rev. Lett.* **115**, 026101 (2015) [2] T. Esat et al. *Nature* **558**, 573 (2018) [3] R. J. Maurer, K. Reuter, *JCP* **139**, 014708 (2013)

DS 18.7 Wed 16:30 H9

**Dispersion corrected density functional theory studies on**

**PVDF/hydrated aluminium nitrate composite system** — ●RANJINI SARKAR and TARUN KUNDU — Indian Institute of Technology, Kharagpur

Electro-active polymer Polyvinylidene fluoride (PVDF) based ferroelectric composites have gained significant technological importance over conventional ceramic ferroelectrics. This article provides quantum chemical description of PVDF/ hydrated aluminium nitrate salt composite system in the light of density functional theory. Four monomer units of pristine  $\alpha$  and  $\beta$ -PVDF, pure Al(NO<sub>3</sub>)<sub>3</sub>·9H<sub>2</sub>O, and PVDF/Al(NO<sub>3</sub>)<sub>3</sub>·9H<sub>2</sub>O structures are optimized using dispersion corrected exchange correlation functional B3LYP-D and 6-311+G(d,p) basis set. Similar to the experimental findings, the current theoretical investigation also suggests that hydrogen bond interaction between PVDF and the hydrated salt molecule plays the major role for the enhancement of ferroelectric properties in this composite system. Non-covalent interaction phenomenon is elucidated on the basis of natural bond orbital analysis, Bader's quantum theory of atoms in molecules and reduced density gradient analysis. Chemical Reactivity and charge transfer mechanisms are explained using atomic-dipole corrected Hirshfeld population analysis, molecular electrostatic potential plot and frontier molecular orbital analyses, respectively.

DS 18.8 Wed 16:45 H9

**Band-structure effects in vertical layered material heterostructures** — ●NICHOLAS D. M. HINE<sup>1</sup>, GABRIEL C. CONSTANTINESCU<sup>2</sup>, NELSON YEUNG<sup>1</sup>, SIOW-MEAN LOH<sup>1</sup>, JOSÉ MARÍA ESCARTÍN<sup>2</sup>, CUAUHTEMOC SALAZAR GONZALEZ<sup>1</sup>, and NEIL R. WILSON<sup>1</sup> — <sup>1</sup>Department of Physics, University of Warwick, United Kingdom — <sup>2</sup>Cavendish Laboratory, University of Cambridge, 19 JJ Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Controlling the properties of layered material heterostructures is crucial to the success of devices based on the novel capabilities of 2D materials, yet theoretical insight has been limited by the large system sizes required to study rotated, incommensurate interfaces. We use linear-scaling DFT calculations with non-local vdW functionals to explore large-scale models of heterostructures of interest for device applications. Results will be presented for heterostructures including MoS<sub>2</sub>/MoSe<sub>2</sub>, MoSe<sub>2</sub>/WSe<sub>2</sub>, and other Transition Metal Dichalcogenide pairings, TMDCs with graphene and hBN substrates, and hBN/Phosphorene. Band-structure changes caused by stacking and rotation of the layers are obtained by unfolding the supercell spectral function into the primitive cells, incorporating spin-orbit coupling. Changes in spectral weight and band-structure between the monolayers and heterostructured interfaces show how lattice mismatch (MoS<sub>2</sub>/MoSe<sub>2</sub>) or spacer layers (Phosphorene/hBN/Phosphorene) can allow the component monolayers to retain more independence in heterostructures than in homo-stacks. Finally, applying electric fields allows the behaviour of gated structures to be predicted and explained.

DS 18.9 Wed 17:00 H9

**Global Trends in Calcium-Silicate-Hydrate Phases Identified by Infrared Spectroscopy and Density Functional Theory** — ●MOHAMMADREZA IZADIFAR, FRANZ KÖNIGER, ANDREAS GERDES, CHRISTOF WÖLL, and PETER THISSEN — Karlsruhe Institute of Technology (KIT), Institute of Functional Interfaces (IFG), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Building and construction industry are at the same time the backbone and the driving force of our modern society. Nearly all our today's technical infrastructure is based on cement-based materials. Detailed, spectroscopic investigations of model reactions on well-defined mineral substrates under UHV-conditions are largely lacking, thus prohibiting a validation of theoretical methods. Eight different Calcium-Silicate-Hydrate (CSH) phases, namely Tobermorite 14Å, Tobermorite 11Å, and Tobermorite 9Å, Wollastonite, Jaffeite, Jennite,  $\gamma$ -C<sub>2</sub>S, and  $\alpha$ -C<sub>2</sub>SH, are calculated with the help of Density Functional Theory using the Vienna ab initio simulation package (VASP). First, we take care of the mechanical properties of the material. Our results revealed that Jaffeite,  $\gamma$ -C<sub>2</sub>S, and  $\alpha$ -C<sub>2</sub>SH have a linear bulk modulus due to the monomer structure of silicate tetrahedra. Tobermorite 14Å and Jaffeite have the lowest and highest bulk modulus, respectively. In the second part, the optimized geometries allow for the precise calculations vibrational eigenmodes and frequencies by the force-constant (FC) approach. The proportions of C/S and H/C are major criteria for the classification of the calculated wavenumber of  $\nu$ (Si-O) for all phases in our model system.

DS 18.10 Wed 17:15 H9

**Origin of carbon 1s binding energy shifts in amorphous carbon materials** — ●MICHAEL WALTER<sup>1,4,5</sup>, FILIPPO MANGOLINI<sup>2</sup>, ROBERT W. CARPICK<sup>3</sup>, and MICHAEL MOSELER<sup>4,5</sup> — <sup>1</sup>FIT, University of Freiburg, Germany — <sup>2</sup>University of Texas at Austin, USA — <sup>3</sup>University of Pennsylvania, USA — <sup>4</sup>Fraunhofer IWM, Freiburg, Germany — <sup>5</sup>Physikalisches Institut, Universität Freiburg, Germany

The quantitative evaluation of the carbon hybridization state by X-ray photoelectron spectroscopy (XPS) has been a surface-analysis problem for the last three decades due to the challenges associated with the unambiguous identification of the characteristic binding energy values of sp<sup>2</sup>- and sp<sup>3</sup>-bonded carbon. Here, we compute the binding energy values for model structures of various carbon allotropes, including graphite, diamond, doped-diamond, and amorphous carbon (a-C), using density functional theory (DFT). The large band-gap of diamond allows defects to pin the Fermi level, which results in large variations of the C(1s) core electron energies for sp<sup>3</sup>-bonded carbon, in agreement with the large spread of experimental C(1s) binding energy values for sp<sup>3</sup> carbon. In case of hydrogen-free a-C, the C(1s) core electron binding energy for sp<sup>3</sup> carbon atoms is approximately 1 eV higher than the binding energy for sp<sup>2</sup>-hybridized carbon. However, the introduction of hydrogen hinders the unambiguous quantification of the carbon hybridization state on the basis of C(1s) XPS alone. This work can assist surface scientists in the use of XPS for the accurate characterization of carbon-based materials.

DS 18.11 Wed 17:30 H9  
**Mechanically tuned conductivity of graphene grain boundaries from first-principles calculations** — DELWIN PERERA, ●JOCHEN ROHRER, and KARSTEN ALBE — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Nanocrystalline graphene has recently been shown to have a strong piezoresistivity and strain gauge factors that are notably higher compared to single- or microcrystalline graphene [1]. The origin of the enhanced piezoresistivity in nanocrystalline graphene is still not fully understood, but several theoretical works suggest that grain boundaries are the main cause as these can evoke transport gaps.

In our work we test this assumption with density functional theory based transport calculations of graphene bicrystals. In particular, we extend our analysis of the interplay between grain boundary structure and transport properties [2] by including mechanical strain. We compute transmission functions and current-voltage curves and compare them with tight binding calculations. Our findings suggest that the strain-induced transport gap modulation can be fully described by the response of the bulk graphene band structure towards strain.

[1] Riaz *et al.*, *Nanotechnology* **26**, 325202 (2015)

[2] Perera *et al.*, *Phys. Rev. B* **98**, 155432 (2018)

## DS 19: Focus Session: Direct-Write Nanofabrication and Applications II (Electron Beam Induced Processing) (joint session DS/TT)

Part II: New Approaches & Chemistry

### Organizers:

- Michael Huth, Physikalisches Institut, Goethe-Universität, Frankfurt, Germany
  - Harald Plank, FELMI-ZFE, TU Graz, Austria
- (Synopsis provided with part I of this session)

Time: Wednesday 15:00–18:00

Location: H32

**Invited Talk** DS 19.1 Wed 15:00 H32  
**Fabrication of functional nanostructures by electron and ion beams** — ●MILOŠ TOŤH — University of Technology Sydney, Australia

Focused electron and ion beams can be used to restructure/mill materials and initiate surface reactions supplied by gas-phase precursor molecules. The chemical reactions give rise to processes that fall into two broad categories: direct-write lithography and emergent phenomena. The latter include topographic surface patterns defined by the crystal symmetry of the sample and chemical structure of a precursor gas, and self-assembly of complex 3D nanostructures. Here I will review the underlying mechanisms, and applications of the techniques to materials used in optoelectronics, plasmonics and quantum photonics. Specific applications include the fabrication and iterative editing/tuning of plasmonic nanostructures and dielectric optical cavities, site-selective electron beam induced fluorination of surfaces, fabrication of isolated colour centres that act as on-demand single-photon-emitters in 2D hBN, and dynamic SEM studies of the degradation of phosphorene in which an electron beam is used to simultaneously initiate chemical reactions and to image propagating reaction fronts. These applications demonstrate the benefits and shortcomings of ion beam and electron beam techniques in terms resolution, throughput and damage imparted to functional materials by beams comprised of electrons, and Ga, Xe, O and He ions.

DS 19.2 Wed 15:30 H32

**Avoiding amorphization in silicon nano structures** — ●GREGOR HLAWACEK<sup>1</sup>, XIAOMO XU<sup>1,2</sup>, HANS-JÜRGEN ENGELMANN<sup>1</sup>, KARL-HEINZ HEINIG<sup>1</sup>, WOLFGANG MÖLLER<sup>1</sup>, AHMED GHARBI<sup>3</sup>, RALUCA TIRON<sup>3</sup>, LOTHAR BISCHOFF<sup>1</sup>, THOMAS PRÜFER<sup>1</sup>, RENE HÜBNER<sup>1</sup>, STEFAN FACSKO<sup>1</sup>, and JOHANNES VON BORANY<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — <sup>2</sup>Faculty of Physics, Technische Universität Dresden, Dresden, Germany — <sup>3</sup>CEA-Leti, Grenoble, France

The usage of ion beam irradiation on vertical nanopillar structures is

a prerequisite for fabricating a vertical GAA-SET device. After room temperature irradiation ( $2 \times 10^{16}$  ions/cm<sup>2</sup>) of nanopillars (with a diameter of 35 nm-50 nm and a height of 70 nm) with either 50 keV broad beam Si<sup>+</sup> or 25 keV focused Ne<sup>+</sup> from a helium ion microscope (HIM), strong plastic deformation has been observed which hinders further device integration. This differs from predictions made by Monte-Carlo based simulations using the program TRI3DYN. To avoid this, ion irradiation at elevated temperatures (up to 672 K) has been performed and no plastic deformation was observed under these conditions. Additionally a pillar diameter reduction by 50% can be achieved in this way without changing the shape of the pillar.

This work is supported by the European Union's H-2020 research project *IONS4SET* under Grant Agreement No. 688072.

DS 19.3 Wed 15:45 H32

**Non-classical Liquid Metal Ion Sources for advanced FIB nano-patterning** — ●PAUL MAZAROV<sup>1</sup>, LOTHAR BISCHOFF<sup>2</sup>, WOLFGANG PILZ<sup>2</sup>, NICO KLINGNER<sup>2</sup>, ACHIM NADZEYKA<sup>1</sup>, JORG STODOLKA<sup>1</sup>, and JACQUES GIERAK<sup>3</sup> — <sup>1</sup>Raith GmbH, Konrad-Adenauer-Allee 8, 44263 Dortmund, Germany — <sup>2</sup>Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, 01328 Dresden, Germany — <sup>3</sup>LPN-CNRS, Route de Nozay, 91460 Marcoussis, France

Focused Ion Beam (FIB) processing has been developed into a well-established and still promising technique for direct patterning and proto-typing on the nm scale. Exploring the Liquid Metal Alloy Ion Sources (LMAIS) potential represents a promising alternative to expand the global FIB application fields. Especially, ion beam nanofabrication as direct, resistless and three-dimensional patterning enables a simultaneous in-situ process control by cross-sectioning and inspection. Thanks to this, nearly half of the elements of the periodic table are made available in the FIB technology as a result of continuous research in this area during the last forty years. Recent developments could make these sources to an alternative technology feasible for nano-patterning challenges. In this contribution the operation principle, the preparation and testing process as well as prospective domains for

modern FIB applications will be presented. As an example we will introduce a Ga<sub>35</sub>Bi<sub>60</sub>Li<sub>5</sub> LMAIS in detail. It enables high resolution imaging with light Li ions and sample modification with Ga or heavy polyatomic Bi clusters, all coming from one ion source.

DS 19.4 Wed 16:00 H32

**Opening the Door to New Beam Induced Processing Applications: A Compact and Flexible Gas Injection System** — ●ANDREW JONATHAN SMITH, KLAUS SCHOCK, ANDREAS RUMMEL, and STEPHAN KLEINDIEK — Kleindiek Nanotechnik, Aspenhastr. 25, 72770 Reutlingen, Deutschland

A flexible GIS module that can be filled with precursor material by the user is introduced. This module is comprised of a small temperature controlled reservoir, a nozzle, and a motor that actuates a valve. Using a micromanipulator, it is possible to position the GIS nozzle precisely while being able to move it far away from the sample so that it is not an obstacle during other processing/imaging steps.

The reservoir can be loaded with solid or liquid precursor materials. It is also possible to feed gaseous precursors from a source outside of the microscope's vacuum chamber. The gas is then introduced using a precisely controllable needle valve.

This approach allows for a high degree of flexibility in choosing precursor materials. Switching precursors is as simple as exchanging the plug-in module on the MM3A-EM micromanipulator. Also, utilizing multiple GI-Systems for specialized tasks is made easy and cost effective.

Having a compact and flexible GIS that can be loaded with virtually any precursor material provides a multitude of possibilities for exploring novel solutions to existing problems as well as new applications for beam induced deposition processes.

DS 19.5 Wed 16:15 H32

**FXBID - an X-ray based sibling to FEBIP** — ●ANDREAS SPÄTH<sup>1</sup>, KIM THOMANN<sup>1</sup>, FLORIAN VOLLNHALS<sup>1</sup>, JÖRG RAABE<sup>2</sup>, KEVIN C. PRINCE<sup>3</sup>, ROBERT RICHTER<sup>3</sup>, WOLFGANG HIERINGER<sup>4</sup>, HUBERTUS MARBACH<sup>1</sup>, and RAINER H. FINK<sup>1</sup> — <sup>1</sup>Physikalische Chemie II, FAU Erlangen-Nürnberg, Germany — <sup>2</sup>Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland — <sup>3</sup>Elettra Sincrotrone, Basovizza, Italy — <sup>4</sup>Theoretische Chemie, FAU Erlangen-Nürnberg, Germany

Focused X-ray beam induced deposition (FXBID) is a novel technique for the additive fabrication of metallic nanostructures by illuminating metal organic precursor molecules with focused soft X-rays in a Fresnel zone plate based scanning transmission X-ray microscope (STXM)[1,2]. An advantage of the technique is the possibility to optimize precursor fragmentation by proper selection of the incident photon energy. For a better understanding of basic X-ray induced fragmentation processes, we have performed photon energy dependent mass spectrometry and secondary electron spectroscopy studies for several metal organic precursors[3]. The results are correlated with TD-DFT calculations of the molecular orbitals relevant for soft X-ray absorption and have been transferred to advanced deposition experiments. We have started to explore the capabilities of in-situ cleaning procedures (reactive gases, annealing, etc.) to enhance the chemical purity of FXBID deposits. The project is funded by DFG grant SP 1775/1-1.

[1] A. Späth et al., RSC Advances, 2016, 6, 98344.

[2] F. Tu et al., J. Vac. Sci. Technol. B, 2017, 35(3), 031601.

[3] A. Späth et al., Microsc. Microanal. 2018, 24(S2), 114.

## 15 min. break

### Invited Talk

DS 19.6 Wed 16:45 H32

**Fundamentals of low-energy electron induced dissociation of focused electron beam induced deposition precursors** — ●ODDUR INGÓLFSSON — Science Institute and the Department of Chemistry, University of Iceland, Dunhagi 3, 107 Reykjavík, Iceland.

When high-energy electron beams imping on a solid surface, as is the case in FEBID, backscattered and secondary electrons (SEs) are abundant. The energy distribution of the SEs typically peaks well below 10 eV, has a significant contribution close to 0 eV and a tail to higher energies. In this energy range, electron induced bond ruptures through Dissociative Ionization, Dissociative Electron Attachment and Neutral and Dipolar Dissociation can be very efficient. These processes have different energy dependence and the nature and thus the reactivity of the fragments formed is also distinctly different. The cross sections for these processes and the branching ratios for different dissociation paths depend critically on the respective molecular composition. This, in turn opens opportunities to tailor the sensitivity of potential

FEBID precursors towards preferred paths to achieve better deposition efficiency and better composition control. In this contribution fundamental aspect of electron induced dissociation processes are discussed in context to their role in FEBID. Acknowledgement; This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 722149.

DS 19.7 Wed 17:15 H32

**Which molecular structures in metal organic compounds are favourable for electron-induced decomposition?** — KAI AHLENHOFF and ●PETRA SWIDEREK — University of Bremen, Institute for Applied and Physical Chemistry, Bremen, Germany

Electron beam induced processing calls for precursor molecules or materials that can be converted to a deposit with well-defined final composition. An approach to this problem is to use ligands which fragment to non-reactive and volatile products leaving behind only the desired material. This concept can guide the design of precursor materials. We have started to investigate this hypothesis by comparing the electron-induced decomposition of surface-grown copper-containing coordination materials that are constructed using different organic counterions, namely, copper(II)oxalate, copper(II)squarate, and HKUST-1 [1]. As a second class of compounds, silver carboxylates with different organic side chain have been considered. Using these examples, we discuss in this contribution a new concept for precursor design. [1] K. Ahlenhoff et al., Phys. Chem. Chem. Phys., submitted.

DS 19.8 Wed 17:30 H32

**Cisplatin as potential Pt FEBID precursor: NH<sub>3</sub> ligands enhance the electron-induced removal of chlorine** — ●MARKUS ROHDENBURG<sup>1</sup>, KAI AHLENHOFF<sup>1</sup>, SASCHA KOCH<sup>2</sup>, ARMIN GÖLZHÄUSER<sup>2</sup>, and PETRA SWIDEREK<sup>1</sup> — <sup>1</sup>Institute for Applied and Physical Chemistry, University of Bremen, Leobener Str. 5, 28359 Bremen, Germany — <sup>2</sup>Department of Physics, University of Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

As recently shown, electron beam exposure to crystals of cisplatin (cis-Pt(NH<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>) leads to a violent reaction. The crystal literally boils with a deposit of pure Pt remaining behind [1]. We have proposed that this reaction is driven by the electron-induced fragmentation of the NH<sub>3</sub> ligands which supplies hydrogen that converts chlorine ligands into HCl. In contrast, the structurally similar cis-Pt(CO)<sub>2</sub>Cl<sub>2</sub> rapidly loses CO upon irradiation but yields deposits with high chlorine contents that can only be removed by extensive electron exposure [2]. We therefore present new results that confirm the formation of HCl by use of electron-stimulated desorption (ESD) experiments. Furthermore, XPS data reveals that electron irradiation removes N and Cl from cisplatin on a similar time scale. The exposure required for quantitative removal of Cl is much smaller in the case of cisplatin than for cis-Pt(CO)<sub>2</sub>Cl<sub>2</sub> underlining the favourable effect of the NH<sub>3</sub> ligands.

[1] J. Warneke et al., J. Phys. Chem. C 120 (2016) 4112.

[2] J.A. Spencer et al., J. Am. Chem. Soc. 138 (2016) 9172.

DS 19.9 Wed 17:45 H32

**Amidinate and carboxylate coordination compounds for focused electron beam induced deposition (FEBID)** — KATARZYNA MADAJSKA and ●IWONA SZYMAŃSKA — Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland

Focused electron beam induced deposition (FEBID) is said to play a fundamental role for making sophisticated 2D and 3D nanostructures with an ultimate resolution of less than 1 nm. It is frequently so-called \*3D nanoprinting\*. [1] The choice of the precursor is crucial for the success of FEBID: its chemical nature and dissociation behavior determine the composition of the deposit. [2]

Research was focused on the copper(II), silver(I) and rhodium(III) complexes with an amidinate and/or carboxylate ligands, which seems to be promising for a FEBID process. Mass spectrometry (EI MS) exhibited in the gas phase following ions: [C<sub>x</sub>(NH<sub>2</sub>(NH=)CR<sub>1</sub>)<sub>y</sub>(O<sub>2</sub>CR<sub>2</sub>)<sub>z</sub>]<sup>+</sup>, [Ag<sub>x</sub>(NH(NH=)CR<sub>1</sub>)<sub>y</sub>(O<sub>2</sub>CR<sub>2</sub>)<sub>z</sub>]<sup>+</sup>, [Ag<sub>z</sub>(NH(NH=)CR<sub>1</sub>)<sub>y</sub>]<sup>+</sup>, [Re<sub>2</sub>Cl<sub>x</sub>(NH(NH=)CR<sub>1</sub>)<sub>y</sub>], where R<sub>1</sub>, R<sub>2</sub> = perfluorinated aliphatic groups. Sublimation experiments and temperature-variable infrared spectroscopy were carried out to determine compounds volatility and decomposition mechanisms.

References [1] D. Belić, M. M. Shawrav, E. Bertagnolli, H. D. Wanzenboeck, Beilstein J. Nanotechnol. 8 (2017) 2530\*2543. [2] I. Utke, P. Hoffmann, J. Melngailis, J. Vac. Sci. Technol. B, 26 (2008) 1197\*1276.



## DS 20: Annual General Meeting of the Thin Films Division

Time: Wednesday 18:30–19:30

Location: H39

Duration 60 min.

## DS 21: Focus Session: Growth, Properties and Application of Epitaxial Graphene (joint session DS/O/HL)

Graphene is the only 2D material, which up to now can be grown almost defect-free on large scales. The application of epitaxial concepts has turned out as a breakthrough in graphene research, because it provides control over the interface and surface structure of epitaxial graphene (EG) layers with atom-scale precision and in an efficient and technologically compatible way. A wide variety of physical phenomena have been observed in graphene-based structures, including topologically protected states, high charge carrier mobility, electron correlation or superconductivity. This versatility makes EG an ideal platform for the integration of graphene-based structures into electronic applications.

This Focus Session aims at fostering the cooperation between groups working in the field of the synthesis, characterization and integration of systems based on large, structurally well-ordered graphene layers. For this purpose it collects state-of-the-art contributions to all involved aspects of EG research, from the growth, functionalization and characterization to the integration of EG-based materials.

**Organizers:**

- Sibylle Gemming, Institut für Physik, TU Chemnitz, D-09107 Chemnitz
- Christoph Tegenkamp, Institut für Physik, TU Chemnitz, D-09107 Chemnitz

Time: Thursday 9:30–12:45

Location: H32

**Invited Talk** DS 21.1 Thu 9:30 H32  
**Epitaxial graphene on SiC(0001) studied by electron spectroscopy and microscopy** — •FLORIAN SPECK — Professur für Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany

The growth of epitaxial graphene (EG) on silicon carbide (SiC) by sublimation of silicon in an inert atmosphere has received considerable attention due to its scalability up to wafer size, and over the past years, the homogeneity of the graphene films could be significantly enhanced by a polymer assisted growth process [1]. Intricate transfer procedures can be dispensed with when semi-insulating SiC substrates are used, facilitating the use of EG in electronics. Yet, interfaces to other materials and the presence of a substrate can affect the graphene layers, e.g. with respect to their structural and electronic properties. As will be shown in this talk, EG grown on SiC(0001) constitutes an intriguing model system to study such interactions due to diverse possibilities of manipulating its properties for instance by intercalation of different elements at the interface to the substrate. To this end, we employ mainly surface science methods such as electron spectroscopies, low-energy electron diffraction and microscopy. Discussed topics include doping of EG induced by hexagonal SiC polytypes, interface modification by means of intercalation, dislocations in EG and investigations of graphene prepared by polymer assisted growth.

[1] M. Kruskopf et al., 2D Mater. **3**, 041002 (2016).

DS 21.2 Thu 10:00 H32  
**Uniform large-scale quasi-freestanding monolayer and bilayer graphene on SiC** — DAVOOD MOMENI PAKDEHI<sup>1</sup>, •KLAUS PIERZ<sup>1</sup>, STEFAN WUNDRACK<sup>1</sup>, JOHANNES APROJANZ<sup>2</sup>, T.T. NHUNG NGUYEN<sup>3</sup>, THORSTEN DZIOMBA<sup>1</sup>, FRANK HOHLS<sup>1</sup>, ANDREY BAKIN<sup>4,5</sup>, RAINER STOSCH<sup>1</sup>, CHRISTOPH TEGENKAMP<sup>2,3</sup>, FRANZ J. AHLERS<sup>1</sup>, and HANS. W. SCHUMACHER<sup>1</sup> — <sup>1</sup>Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig — <sup>2</sup>Institut für Festkörperphysik, LU Hannover, Appelstraße 2, 30167 Hannover — <sup>3</sup>Institut für Physik, TU Chemnitz, Reichenhainer Straße 70, 09126 Chemnitz — <sup>4</sup>Institut für Halbleitertechnik, TU Braunschweig, 38106 Braunschweig, — <sup>5</sup>Laboratory of Emerging Nanometrology, TU Braunschweig, 38106 Braunschweig

Epitaxial graphene growth is often accompanied by step bunching of the underlying SiC substrate and graphene bilayer formation which can deteriorate the quality of graphene-based devices, e.g., the resistance quantization of the quantum Hall effect. We show AFM, STM, Raman and electronic transport data which indicate that improved buffer layer growth is the key to obtain homogenous large-area mono-

layer graphene. Particularly, the substantial impact of the so-far less regarded Ar flow rate on the graphene quality is investigated in this study and explained by a quasi-equilibrium model at the growing surface. The quality of our ultra-smooth graphene layers is proven by the high uniformity of quasi-freestanding graphene sheets obtained by hydrogen intercalation which is underlined by the very small resistance anisotropy of such samples on  $\mu\text{m}$  and  $\text{mm}$  scales.

DS 21.3 Thu 10:15 H32  
**Influence of minivalleys and Berry curvature on electrostatically induced nanostructures in gapped bilayer graphene** — •ANGELIKA KNOTHE and VLADIMIR FAL'KO — National Graphene Institute, University of Manchester, United Kingdom

We theoretically investigate the properties electrostatically confined nanostructures in gapped bilayer graphene (BLG). We show how the spectrum of subbands in a quantum wire in gapped BLG, and the energy levels in a quantum dot, manifest the minivalley structure and Berry curvature via the associated magnetic moment of the states in the low-energy bands. These features determine the degeneracies of the low-energy minibands / -levels and their valley splitting, which develops linearly in a weak magnetic field. In a quantum point contact, magneto-conductance reflects such degeneracies in the heights of the first conductance steps which develop upon the increase of the channel doping:  $8e^2/h$  steps in a wide channel in BLG with a large gap,  $4e^2/h$  steps in narrow channels, all splitting into a staircase of  $2e^2/h$  steps upon lifting valley degeneracy by a magnetic field  $B$ . For quantum dots, we investigate how optical selection rules are influenced by the minivalleys and the orbital magnetic moment, as well as by shapes of the confinement.

References: A. Knothe and V. Fal'ko, Phys. Rev. B **98**, 155435 (2018); H. Overweg, A. Knothe, V. I. Fal'ko, K. Ensslin, T. Ihn, et al., arXiv:1809.01920; R. Kraft, I.V. Krainov, V. Gall, A.P. Dmitriev, R. Krupke, I.V. Gornyi, R. Danneau, arXiv:1809.02458

DS 21.4 Thu 10:30 H32  
**Tuning the doping level of graphene near the Van Hove singularity via ytterbium intercalation** — •HRAG KARAKACHIAN, PHILIPP ROSENZWEIG, STEFAN LINK, KATHRIN MÜLLER, and ULRICH STARKE — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

At extremely high doping levels, when pushing the Fermi level to the vicinity of graphene's Van Hove singularity (VHs), exotic electronic ground states are expected to occur driven by many-body interactions. These competing electronic phases such as chiral superconductivity,

charge or spin density waves, find their stability based on the amount of doping induced in the graphene layer [1]. In this work, we present a method for effectively tuning graphene's doping level near its VHS. Epitaxially grown graphene on SiC(0001) is decoupled from the SiC substrate and strongly *n*-doped up to its VHS via ytterbium intercalation. By annealing the graphene/Yb system at different temperatures, a topological transition at the Fermi level is observed and a continuous shift in Dirac point energy is measured, indicating a change in carrier density. The Yb atoms go through different order patterns at different heating stages, and their concentration is modified as a function of temperature. These variations significantly affect the amount of charge transferred to the graphene layer and allow the systematic control of graphene's doping level near its VHS. Thus, the Yb intercalation technique can provide a reliable way of accessing and switching between different possible ordered electronic ground states in graphene.

[1] A.M. Black-Schaffer et al., J. Phys. CM **26**, 423201 (2014).

DS 21.5 Thu 10:45 H32

**Substrate induced nanoscale resistance variation in epitaxial graphene** — ●ANNA SINTERHAUF<sup>1</sup>, GEORG A. TRAEGER<sup>1</sup>, DAVOOD MOMENI PAKDEHI<sup>2</sup>, PHILIP SCHÄDLICH<sup>3</sup>, FLORIAN SPECK<sup>3</sup>, PHILIP WILLKE<sup>4,5</sup>, THOMAS SEYLLER<sup>3</sup>, CHRISTOPH TEGENKAMP<sup>3</sup>, KLAUS PIERZ<sup>2</sup>, HANS WERNER SCHUMACHER<sup>2</sup>, and MARTIN WENDEROTH<sup>1</sup> — <sup>1</sup>IV. Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany — <sup>2</sup>Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — <sup>3</sup>Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany — <sup>4</sup>Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — <sup>5</sup>Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea

Electron transport in graphene is often crucially influenced by the underlying substrate which induces scattering mechanisms on a local scale. Using scanning tunneling potentiometry we investigate the transport properties of graphene on 6H-silicon carbide (0001) grown by polymer-assisted sublimation growth (PASG) down to the nanometer scale. We find a significant variation in the sheet resistance of up to 195% on neighboring terraces directly related to the stacking of the 6H-SiC substrate. Thus, our data clearly shows the strong influence of the substrate below the graphene layer on its local transport properties. In addition, we performed temperature dependent measurements to gain insight into the dominant scattering mechanism. This work is financially supported by the DFG through the SFB1073.

15 min. break.

Invited Talk

DS 21.6 Thu 11:15 H32

**Patternable non-polar epigraphene for nanoelectronics and Dirac point physics** — VLADIMIR PRUDKOVSKIY<sup>1,3</sup>, YIRAN HU<sup>1</sup>, HUE HU<sup>1</sup>, LEI MA<sup>2</sup>, CLAIRE BERGER<sup>1,3</sup>, and ●WALT DE HEER<sup>1,2</sup> — <sup>1</sup>Georgia Institute of Technology, Atlanta USA — <sup>2</sup>TICNN, Tianjin China — <sup>3</sup>Neel Institute, CNRS, Grenoble, France

Recently reported measurements of epitaxial graphene nanoribbons grown on sidewalls etched in the 0001 face of h-SiC, Nature, 506, 349, (2014) indicate that both spin and valley degeneracies are lifted, resulting in the observed 10 micron scale, temperature independent, single channel transport. These highly unusual properties were further investigated in SiC wafers that were cut at an angle to the 0001 face were prepared at the Tianjin International Center for Nanoparticles and Nanostructures. The wafers were graphitized and 10 micron scale top gated Hall bar structures were patterned using standard lithography methods. Magnetotransport measurements revealed striking transport properties. Single channel ballistic transport is observed even at the Dirac point. Moreover, an anomalous quantum Hall plateau is observed. Its anomalous value is caused by a quantized current that does not have a Hall effect, and that is in parallel with an equal current that does have a Hall effect. These properties are likely to be caused by edge currents, with energies that are pinned at the Dirac point. The ballistic transport is essentially temperature independent and consistent with that observed in sidewall ribbons. These results indicate that nonpolar epigraphene is a promising candidate for epigraphene nanoelectronics and important for Dirac point physics.

DS 21.7 Thu 11:45 H32

**Epitaxial growth of ferromagnetic semiconducting CrBr<sub>3</sub>**

**monolayer** — ●WEIJIONG CHEN<sup>1</sup>, ZEYUAN SUN<sup>1</sup>, LEHUA GU<sup>1</sup>, SHIWEI WU<sup>1,2</sup>, and CHUNLEI GAO<sup>1,2</sup> — <sup>1</sup>State Key Laboratory of Surface Physics, Key Laboratory of Micro and Nano Photonic Structures (MOE), Department of Physics, and Institute for Nanoelectronic Devices and Quantum Computing, Fudan University, Shanghai 200433, China — <sup>2</sup>Collaborative Innovation Center of Advanced Microstructures, Nanjing 210093, China

Recent discovery of two-dimensional (2D) ferromagnetic semiconducting materials greatly expands the family of 2D materials and invokes tremendous interests in novel magnetic related applications in 2D limit. Similar to most 2D materials, ferromagnetic 2D semiconductor is also firstly found in the mechanically exfoliated micrometer sized flakes, which hinders its further application. Here, we report the successful growth of ferromagnetic semiconducting monolayer CrBr<sub>3</sub> by compound source molecular beam epitaxy (CS-MBE). CrBr<sub>3</sub> compounds are directly evaporated onto the Highly Oriented Pyrolytic Graphite (HOPG) substrate and form CrBr<sub>3</sub> thin films with a precise thickness control. The atomic, electronic and magnetic properties were characterized by in-situ spin-polarized scanning tunneling microscopy. This growth method can be applied to other layered transition metal trihalides (LTMTs) as well, which provides a simple way of growing LTMTs for exploring their electronic and magnetic properties to the monolayer limit.

DS 21.8 Thu 12:00 H32

**Tuning the electronic properties of PbPb molecules by epitaxial graphene** — ●T.T.NHUNG NGUYEN<sup>1</sup>, U. GERSTMANN<sup>2</sup>, T.N.HA NGUYEN<sup>1</sup>, and C. TEGENKAMP<sup>1,3</sup> — <sup>1</sup>TU Chemnitz, Germany — <sup>2</sup>Universität Paderborn, Germany — <sup>3</sup>Leibniz Universität Hannover, Germany

Functionalization of graphene aimed for its application in nanoelectronics is an important step. Among a variety of surface tailoring methods, molecular self-assembly gives rise to precisely control their interface by choosing appropriate molecules, e.g. non-planar lead-phthalocyanine (PbPc). By means of scanning tunneling microscopy and density functional theory (DFT) we studied in detail the adsorption of PbPc on graphene/SiC(0001). Thereby, we used as template both n-doped monolayer (MLG) and neutral quasi-free monolayer graphene (QFML). On both surfaces PbPc forms almost identical monolayer structures, in agreement with DFT. Upon adsorption of the molecules, where the central atom points away from the surface, the benzene rings undergo pronounced distortions, where adjacent rings rotate and bend in opposite directions giving rise to a chiral single domain structure. Despite the same adsorption geometry, the molecular states of PbPc on these two surfaces are strongly shifted with respect to each other. First DFT results show that the negatively charged MLG is responsible for this effect.

Invited Talk

DS 21.9 Thu 12:15 H32

**Intrinsic stacking domains in graphene on silicon carbide: A pathway for intercalation** — TOBIAS A DE JONG<sup>1</sup>, EUGENE E KRASOVSKIY<sup>2</sup>, CHRISTIAN OTT<sup>3</sup>, RUDOLF M TROMP<sup>4,1</sup>, SENSE JAN VAN DER MOLEN<sup>1</sup>, and ●JOHANNES JOBST<sup>1</sup> — <sup>1</sup>Leiden Institute of Physics, Leiden, The Netherlands — <sup>2</sup>Universidad del País Vasco, San Sebastián/Donostia, Spain — <sup>3</sup>Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Erlangen, Germany — <sup>4</sup>IBM T. J. Watson Research Center, Yorktown Heights, USA

Graphene on silicon carbide (SiC) bears great potential for future graphene electronic applications because it is available on the wafer scale and its properties can be custom tailored by inserting various atoms into the graphene/SiC interface. It remains unclear, however, how atoms can cross the impermeable graphene layer during this widely used intercalation process. Here we demonstrate that in contrast to the current consensus, graphene layers grown in argon atmosphere on SiC are not homogeneous, but instead are composed of domains of different crystallographic stacking as they have been observed in other systems. We show that these domains are the AB and AC versions of Bernal stacking, that they are intrinsically formed during growth and that dislocations between domains dominate the (de)intercalation dynamics of hydrogen. Tailoring the resulting dislocation networks, e.g., through substrate engineering, will increase the control over the intercalation process and could open a playground for topological and correlated electron phenomena on the wafer scale.

## DS 22: Thin Film Applications

Time: Thursday 9:30–12:15

Location: H39

DS 22.1 Thu 9:30 H39

**Spin-to-charge conversion using NbSe<sub>2</sub> thin films grown by MBE** — ●AVANINDRA KUMAR PANDEYA, AMILCAR BEDOYA PINTO, KAI CHANG, ILYA KOSTANOVSKIY, EDOUARD LESNE, and STUART PARKIN — Max Planck Institute of Microstructure Physics

Transition metal dichalcogenides (TMDCs) are commonly fabricated via exfoliation of high-quality bulk crystals. Although there has been tremendous progress in fabricating devices out of exfoliated heterostructures, there are other effects, such as spin transfer, that need atomically clean interfaces for an optimum harvesting. We grow high-quality NbSe<sub>2</sub> layers on Al<sub>2</sub>O<sub>3</sub> (0001) by molecular beam epitaxy (MBE), in order to gain a precise control of the layer thickness, electronic properties (doping) and improve the quality of the interfaces involved in spin transfer and spin-to-charge conversion experiments. In this work, we use spin-torque ferromagnetic resonance (ST-FMR) to explore the spin-orbit torques (SOTs) produced by the TMDC. In order to maximize the SOT transfer, we rely on the growth of a single-crystalline NbSe<sub>2</sub> layer and a Permalloy (Ni<sub>80</sub>Fe<sub>20</sub>) layer in ultra-high vacuum conditions. Preliminary ST-FMR results at room temperature show a strong symmetric component on the lineshape of the voltage detected across the ferromagnetic resonance, as well as a change of the resonance linewidth by applying an external DC bias through the bilayer, both signatures of sizable spin-orbit torques induced by the NbSe<sub>2</sub> layer via spin-hall effect. This underlines the relevance of in-situ TMDC/ferromagnet heterostructures towards highly efficient spin-orbitronic devices.

DS 22.2 Thu 9:45 H39

**Electrical and optical characterization of the correlated metals AMoO<sub>3</sub> (A = Ca, Sr, Ba)** — ●MAHDAD MOHAMMADI, ALDIN RADETINAC, ILIYA RADULOV, LEOPOLD DIOP, PHILIPP KOMISSINSKIY, and LAMBERT ALFF — Institute of Materials Science, Technische Universität Darmstadt, Darmstadt

Transparent conducting materials (TCMs) are facing a steadily increasing demand for a variety of applications such as capacitive touchscreens, LCDs, solar cells and LEDs. In the majority of devices, ITO, a doped wide-gap semiconductor, is used due to the very good transparency in the visible light spectrum. Recently, correlated metals have gained attention as an alternative material class for application as TCMs. One prominent representative of this material class is the perovskite compound SrMoO<sub>3</sub> [1]. In this work, the influence of the A-site cation on the electrical and optical properties has been investigated by substituting Sr with Ca and Ba. The compounds were epitaxially grown using pulsed-laser deposition and characterized via XRD, XPS, UPS, Hall transport measurements and UV/VIS spectrophotometry. Due to the high conductivity of the molybdates, very thin films in the range of 10-30 nm are sufficient to achieve application relevant sheet resistances below 50 Ω/□. This leads to similar transparencies in the visible light spectrum at comparable sheet resistances compared to ITO. Among the three investigated compounds, BaMoO<sub>3</sub> showed the highest transparency with resistivities around 30 μΩcm.

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

DS 22.3 Thu 10:00 H39

**Enhancing Performance of Sputter Deposited Photocatalytic Thin Films** — SALIH VEZIROGLU, MUHAMMAD ZUBAIR GHORI, BODO HENKEL, ALEXANDER VAHL, OLEKSANDR POLONSKYI, THOMAS STRUNSKUS, ●ORAL CENK AKTAS, and FRANZ FAUPEL — Institute for Materials Science, Multicomponent Materials, Faculty of Engineering, Christian-Albrechts-University of Kiel, Kaiserstraße 2, Kiel 24143, Germany

Semiconductor oxides such as TiO<sub>2</sub>, ZnO, etc. have been used in various photocatalytic processes including environmental remediation, energy harvesting, anti-bacterial and self-cleaning applications. Several methods including decorating metallic nanoparticles on such oxides and/or adding a second oxide (mixed oxide) have been developed to enhance the photocatalytic performance of such oxides. Most of these preparation methods are mainly based on wet-chemical techniques (solution-based). In comparison, physical vapour deposition methods offer solvent-free synthesis, high purity and precise control of amount of the added second phase (metallic nanoparticle or oxide). In this current work we present various approaches to enhance the per-

formance of sputter deposited photocatalytic thin films. First a novel approach, which leads to increasing the effective surface area of sputter deposited photocatalytic thin films by inducing controlled nanocrack networks, will be presented. Then the use of cluster source to decorate photocatalytic thin films with metallic nanoparticles will be discussed. The plasmon induced photocatalysis will be covered briefly. Additionally, some case studies on photocatalytic mixed oxide thin films will be shown.

DS 22.4 Thu 10:15 H39

**Novel deposition approach of MoS<sub>2</sub> thin films for hydrogen evaluation reaction** — ●TALHA NISAR, TORSTEN BALSTER, FRANCIS OLIVER VINAY GOMES, and VEIT WAGNER — Jacobs University Bremen gGmbH, Campus Ring 1, 28759, Bremen

Electrolytic hydrogen evolution reaction is a promising way to store solar energy. It requires suitable materials as a catalyst to lower overpotential and minimize energy consumption. MoS<sub>2</sub> has been demonstrated to be a very promising candidate for hydrogen evolution reaction. In this work, MoS<sub>2</sub> films are deposited by spin coating using a Molybdenum (V) chloride precursor solution on Au and ITO substrates. The thickness of the deposited films is linearly dependent on the concentration of precursor. After spin-coating the thin layers are converted to MoS<sub>2</sub> by post annealing at temperature above 450°C with an additional sulfur source. The thickness of the films ranges from 2nm to 50nm. Raman measurements show E<sub>2g</sub> and A<sub>1g</sub> modes of MoS<sub>2</sub>. The modes have reduced FWHM for higher annealing temperatures, confirming the formation of high quality crystals. This interpretation is supported by XPS, UV-Vis, AFM and XRD measurements. Finally hydrogen evolution activity is determined in dependence of the thickness.

DS 22.5 Thu 10:30 H39

**Noise properties of oxygen engineered HfO<sub>2-x</sub> based Resistive Random Access Memory devices** — ●ESZTER PIROS<sup>1</sup>, MARTIN LONSKY<sup>2</sup>, STEFAN PETZOLD<sup>1</sup>, ERIC JALAGUIER<sup>3</sup>, EMMANUEL NOLOT<sup>3</sup>, CHRISTELLE CHARPIN<sup>3</sup>, JENS MÜLLER<sup>2</sup>, and LAMBERT ALFF<sup>1</sup> — <sup>1</sup>Institute of Materials Science, Advanced Thin Film Technology, Technische Universität Darmstadt, Darmstadt, Germany — <sup>2</sup>Institute of Physics, Goethe-University Frankfurt, Frankfurt am Main, Germany — <sup>3</sup>CEA, LETI, Grenoble, France

Resistive Random Access Memory (RRAM) is one of the most promising candidates amongst emerging non-volatile memories because of their fast read/write speed, high endurance, and good retention properties. One of the biggest challenges, however, is to improve device reliability and variability, highlighting the necessity of a comprehensive physical picture on the resistive switching mechanism. Therefore, we comparatively investigated the noise properties of oxygen engineered stoichiometric and highly oxygen deficient hafnia [1], by electrical fluctuation spectroscopy to explore the physical nature of conduction in the high and low resistive state, finding a strong dependence on stoichiometry, voltage bias amplitude, and DC cycling. The investigations were carried out in both the time- and frequency domain. The observation of multilevel- and anomalous random telegraph noise and corresponding Lorentzian spectra are also discussed.

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

15 min. break.

DS 22.6 Thu 11:00 H39

**High resolution fast X-ray reflectivity data acquisition** — ●MILENA LIPPMANN, ANITA EHNE, and OLIVER SEECK — DESY, Hamburg

A new method for fast x-ray reflectivity data acquisition is presented. The method is based on a fast rotating, slightly tilted sample reflecting to a stationary mounted position sensitive detector and it allows for measurements of reflectivity curves in a quarter of a second. The resolution in q-space mainly depends on the beam properties and the pixel size of the detector. Maximum qz-value of 1 Å<sup>-1</sup> can be achieved. The time-temperature depending structure changes of poly(N-isopropylacrylamide) (PNIPAM) thin films were investigated in situ by applying the fast-reflectivity setup.

DS 22.7 Thu 11:15 H39

**Integration of electro-optical devices in LiNbO<sub>3</sub>** — ●FELIX VOM BRUCH, PATRICK BARTKOWIAK, SEBASTIAN LENGELING, RAIMUND RICKEN, VICTOR QUIRING, HARALD HERRMANN, and CHRISTINE SILBERHORN — Universität Paderborn, Warburger Str. 100, 33098 Paderborn

The interest in quantum technology increases steadily within the last years. Many concepts are based on the utilisation of light and its quantum properties for encoding and transferring information. Comparable to integrated electronic devices, integrated electro-optical elements enable one to scale complex laboratory setups down to convenient and handy dimensions. Furthermore, this approach is suitable for an effective reduction of the expense for setups and experiments.

From many numerous telecom applications it is well known that ferroelectric LiNbO<sub>3</sub> provides an excellent platform for devices, such as frequency converters, phase and polarization modulators. For this purpose, the non-linear electro-optic properties of this material can be used to tailor conversion processes and modulators. Functionalities and characteristics of the latter parts are mainly governed by the design of electrodes used. However, scaling and integration of devices for quantum-optic applications remains challenging in terms of performance and robustness. For enhancing these features, studies on different concepts and architectures become inevitable. Here the influence of different thin layer systems, used as electrodes for modulators, is examined in terms of e.g. excess loss, switching speed and long-term stability.

DS 22.8 Thu 11:30 H39

**Microfabricated switchable THz flat lenses made out of VO<sub>2</sub> thin films** — ●FLORIAN KÜHL<sup>1</sup>, ANGELIKA POLITY<sup>1</sup>, YAN ZHANG<sup>2</sup>, and PETER J. KLAR<sup>1</sup> — <sup>1</sup>Institute of Experimental Physics I and Center for Materials Research (ZfM/LaMa), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, DE-35392 Giessen, Germany — <sup>2</sup>Beijing Key Lab for Metamaterials and Devices, Capital Normal University, Beijing, China

Terahertz radiation and its various applications have gained a lot of interest in the last few years and, thus, the importance of switchable THz devices has increased. Thermochromic VO<sub>2</sub> shows a semiconductor to metal transition and hence is a suitable material for designing thermally switchable structures.

We present microfabricated resonator structures in rf-magnetron sputtered VO<sub>2</sub> thin films. It is necessary to choose the type of substrate and to optimize the properties of the buffer layer and the thin film. The resonator structures were transferred into the thin films via photolithography and ion-beam etching. Measurements on unstructured thin films of VO<sub>2</sub> show the typical switching behaviour in the infrared region and typical switching temperatures for thin films of about 55 °C. The switching behaviour of structured thin films was investigated with terahertz time-domain spectroscopy (THz-TDS) at low and high temperatures to demonstrate the two desired operating modes of

the designed structures. While no effect on incoming radiation could be observed at low temperatures, a focussing behaviour was detected at higher temperatures when the VO<sub>2</sub> micro resonators become metallic.

DS 22.9 Thu 11:45 H39

**Investigations of the physical properties of lithium-based solid electrolyte thin films in the system Li-P-S-O-N** — ●FABIAN MICHEL<sup>1,3</sup>, MARTIN BECKER<sup>1,3</sup>, JÜRGEN JANEK<sup>2,3</sup>, and ANGELIKA POLITY<sup>1,3</sup> — <sup>1</sup>I. Institute of Experimental Physics, JLU Gießen, 35392 Gießen — <sup>2</sup>Institute of Physical Chemistry, JLU Gießen, 35392 Gießen — <sup>3</sup>Center for Material Research (ZfM/LaMa, JLU Gießen, 35392 Gießen

Using the technique of x-ray photoelectron spectroscopy (XPS) the composition of the radio-frequency sputtered lithium-based solid electrolyte thin films was determined. Additional electrochemical impedance spectroscopy (EIS) was performed to gain knowledge about the electrochemical properties especially the ionic conductivity of such films. An optimization of the physical properties, which are important for a battery (ionic conductivity) or electrochromic applications (transmission), was attained by changing the deposition parameters. During this optimization process a maximum in ionic conductivity of about 15.8 μS/cm was found referring to the different composition (sulfur content) and process parameters (ratio between argon and nitrogen flux). Compared with earlier findings of related investigations one can monitor the improvements made.

DS 22.10 Thu 12:00 H39

**Highly rectifying contacts on Ga<sub>2</sub>O<sub>3</sub>, In<sub>2</sub>O<sub>3</sub> and (In,Ga)<sub>2</sub>O<sub>3</sub> thin films** — ●DANIEL SPLITH — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Leipzig, Germany

Oxide semiconductors like gallium oxide or indium oxide are promising materials for a new generation of transparent electronic devices. Additionally, alloying both materials allows band-gap engineering, enabling e.g. the fabrication of wave-length selective photodetectors. In order to realize devices like diodes, field-effect transistors and photodetectors, the fabrication of rectifying contacts is essential. Further, such contacts also enable the investigation of the materials by means of space charge region based methods like thermal admittance spectroscopy.

In this contribution the properties of Schottky contacts and pn-heterojunctions on heteroepitaxial Ga<sub>2</sub>O<sub>3</sub> and In<sub>2</sub>O<sub>3</sub> thin films grown by pulsed laser deposition are discussed. Additionally, the properties of such rectifying contacts on (In,Ga)<sub>2</sub>O<sub>3</sub> thin films having a lateral composition gradient are presented. In order to improve the rectification of the contacts, different vertical layouts were investigated. Further, a comprehensive model, taking into account thermionic emission, thermionic field emission and charging currents as well as non-idealities like barrier height inhomogeneities, current spreading and variations of the net-doping density in growth direction, was employed in order to understand the measured characteristics.

## DS 23: Direct-Write Nanofabrication and Applications III (Electron Beam Induced Processing) (joint session DS/TT)

Part III: Material Properties &amp; Applications

### Organizers:

- Michael Huth, Physikalisches Institut, Goethe-Universität, Frankfurt, Germany
- Harald Plank, FELMI-ZFE, TU Graz, Austria  
(Synopsis provided with part I of this session)

Time: Thursday 15:00–17:45

Location: H32

### Invited Talk

DS 23.1 Thu 15:00 H32

**Artificial nano-granular heterostructures: fundamentals and applications** — ●OLEG UDALOV<sup>1,2</sup> and IGOR BELOBORODOV<sup>1</sup> — <sup>1</sup>California State University, Northridge, USA — <sup>2</sup>Institute for Physics of Microstructures RAS, Nizhny Novgorod, Russia

Granular composites are a large class of artificial materials in which nanograins are embedded into a hosting matrix. Combining different types of grains and matrix one can obtain composites with desirable functionalities. Fabrication of granular materials is scalable and is

much cheaper than, for example, the thin film preparation techniques. Such an advantage makes these materials very attractive for various applications, including medical, photonic, radiofrequency, mechanical, etc. Properties of granular materials are defined by the interplay of disorder, dimensionality, surface and size effects, superconductivity, magnetic interactions, strain, the Coulomb blockade, etc. Therefore, studying of these materials is a complicated challenge promising unexpected novel properties. Nanograins ensembles are often used as a prototype of systems with competitive interactions and strong many-body effects. This makes granular materials of a great fundamental

interest. In this talk we will focus on recent developments in solid granular materials. First, we discuss different types of granular media and their applications. In particular, we will consider granular metals, ferromagnets, superconductors and semiconductors. Next, we will discuss granular multiferroics where two order parameters are combined: 1) magnetization and 2) polarization. We will consider theoretical and experimental works on magneto-electric coupling in these materials.

DS 23.2 Thu 15:30 H32

**Ac conductivity of nano-granular metals prepared via FEBID** — ●MARC HANEFELD<sup>1</sup>, MICHAEL HUTH<sup>1</sup>, JOSHUA GIES<sup>2</sup>, and MARTIN KIND<sup>2</sup> — <sup>1</sup>Physikalisches Institut, Goethe Universität, Max-von-Laue-Str. 1 — <sup>2</sup>Institut für Anorg. und Analyt. Chemie, Goethe Universität, Max-von-Laue-Str. 7, 60438 Frankfurt a. M., Germany

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

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

We present recent results on the ac conductance response of nano-granular Pt(C)-FEBID deposits and show the capabilities of FEBID to create an ideal model environment for an in depth analysis of the ac conduction characteristics of granular metals. Possible applications of these results in dielectric sensors combining nano-granular Pt(C) with metal-organic frameworks will be discussed.

[1] Huth, et al., *Microelect. Eng.* 2017. doi:10.1016/j.mee.2017.10.012.

[2] Bakkali, et al., *Sci. Rep.* 2016;6:29676. doi:10.1038/srep29676.

DS 23.3 Thu 15:45 H32

**Post-growth electron beam irradiation of co-deposited PtC-FeCo FEBID nanostructures** — ●ROLAND SACHSER and MICHAEL HUTH — Physikalisches Institut, Goethe-University, Frankfurt am Main, Germany

FEBID using the precursor  $(CH_3)_3CH_3C_5H_4Pt$  leads to low conductive, nanogranular samples. The resistivity is determined by the coupling of Pt nanocrystals by the carbonaceous matrix. This matrix, and thus the conductivity, can be strongly influenced by post-growth electron beam irradiation. On the other hand, deposits prepared employing the precursor  $HFeCo_3(CO)_{12}$  feature high metal contents and metallic resistivity behavior. These samples are ferromagnetic but the tunability of their transport properties by post-growth treatments is limited. By co-deposition using both precursors under well-controlled mixing ratios it is possible to obtain a highly tunable granular ferromagnet. Granular ferromagnetic systems are known to show an enhanced anomalous Hall effect, which can also be observed in our deposits that are treated by post-growth electron beam irradiation under in situ conductance monitoring. The conductance can be tuned over a wide range, which is also prominently reflected in the magneto-transport properties that can be directly monitored in situ in the low field regime at room temperature. Complementary low temperature magneto-transport measurements reveal the optimal post-growth irradiation dose to obtain the largest anomalous Hall effect.

DS 23.4 Thu 16:00 H32

**Micro-Hall Magnetometry of FEBID-fabricated 3D magnetic nano-architectures** — ●JENS MÜLLER<sup>1</sup>, MOHANAD AL MAMOORI<sup>1</sup>, LUKAS KELLER<sup>1</sup>, MICHAEL HUTH<sup>1</sup>, and CHRISTIAN SCHRÖDER<sup>2</sup> — <sup>1</sup>Institute of Physics, Goethe University Frankfurt — <sup>2</sup>Institute for Applied Materials Research, Bielefeld University of Applied Sciences

Whereas most of the previous studies of nanoscale magnetic structures – owing to the fabrication by means of lithographic processes – have focused on one- or two-dimensional (1D/2D) nanomagnets, thanks to advances in fabrication and sensing techniques it is now possible to investigate free-standing magnetic 3D structures individually, in small arrays, or in complex connected lattice architectures. Here we report on the combination of focused electron beam induced deposition (FEBID) and micro-Hall magnetometry, as fabrication and high-resolution sensing tools, respectively. Free-form structures with minimal feature size of a few tens of nm of the metallic ferromagnets Fe, Co and Fe-Co are deposited directly on a semiconductor Hall sensor which serves as the

substrate and allows to detect the magnetic stray field as a function of the external magnetic field and temperature. In the talk, we will discuss the measured and simulated magnetization reversal of small arrays of Fe-Co nanotrees and -cubes [1,2]. Furthermore, we will give an outlook on future possibilities of fabricating magnetic structures with geometrical frustration (towards 3D artificial spin ice) and studying dynamical processes by means of magnetic flux noise spectroscopy.

[1] L. Keller et al., *Sci. Rep.* **8**, 6160 (2018).

[2] M. Al Mamoori et al., *Materials* **11**, 289 (2018).

15 min. break

**Invited Talk** DS 23.5 Thu 16:30 H32  
**3D nanomagnetism and superconductivity: Current status and potential for future work** — ●OLEKSANDR DOBROVOLSKIY and MICHAEL HUTH — Goethe University, Frankfurt am Main

Extending 2D structures into the third dimension has become a general trend in various areas, including photonics, plasmonics and magnetics. This approach provides a means to modify conventional and to launch novel functionalities by tailoring vector potentials inducing anisotropic and chiral effects. Recently, there has been significant progress in the fabrication of free-standing ferromagnetic and superconducting nanostructures by focused particle direct-write techniques which is in part reviewed in [1]. In this respect, 3D shell structures such as framed tubes, spheres, Swiss rolls and helices are especially interesting as they offer unprecedented prospects for nanomagnetism and superconductivity because of topology and geometry-controlled effects. Namely, in magnetism, curvilinear geometry brings about two exchange driven interactions - effective anisotropy and antisymmetric vector exchange, i.e. an effective Dzyaloshinskii-Moriya interaction. In addition, another magneto-chiral contribution emerges due to the dipole-dipole interaction. In the case of superconducting nanostructures, the combination of low-dimensionality with a curvilinear geometry allows in principle for the observation of topology-driven effects, such as unconventional phase slips, reversible and irreversible switching, fractional flux-flow instabilities, and the Berezinskii-Kosterlitz-Thouless transition. [1] M. Huth, F. Porrati, O. V. Dobrovolskiy, FEBID meets materials science, *Microelectron. Engineering*, 185-186, 9-28 (2018).

DS 23.6 Thu 17:00 H32

**3D Nano-Printing via FEBID: Complex 3D Nano-Structures** — ●LUKAS KELLER and MICHAEL HUTH — Institute of Physics, Goethe University, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

[3]: <https://youtu.be/v8s24WvGj9E>

Fabrication of three-dimensional (3D) nano-architectures by focused electron beam induced deposition (FEBID) has matured to a level that highly complex and functional deposits are becoming available for nanomagnetics [1] and plasmonics. The main issue of generating a desired 3D nano-structure is to navigate the electron beam in the x-y-plane.

Here we present our pattern file generator program [2]. It considers several issues caused by limited precursor replenishment dynamics, which is important for the successful fabrication of 3D nano-structures. The target geometry can be defined by hand or using powerful 3D software tools like "blender" [3]. Several examples of 3D nano- and micro-structures using different precursors are presented.

[1]: *Scientific Reports* **8**, 6160 (2018)

[2]: *Beilstein J. Nanotechnol.*, **9**, 2581-2598 (2018)

[3]: <https://youtu.be/v8s24WvGj9E>

DS 23.7 Thu 17:15 H32

**Crystalline NbC superconducting nanowires by direct-writing** — ●FABRIZIO PORRATI<sup>1</sup>, SVEN BARTH<sup>2</sup>, ROLAND SACHSER<sup>1</sup>, OLEKSANDR DOBROVOLSKIY<sup>1</sup>, ANJA SEYBERT<sup>3</sup>, ACHILLEAS FRANGAKIS<sup>3</sup>, and MICHAEL HUTH<sup>1</sup> — <sup>1</sup>Goethe-University, Institut of Physics, Frankfurt a. M. — <sup>2</sup>TU Wien, Institute of Materials Chemistry — <sup>3</sup>Goethe-University, Buchmann Institute

We present a comparative study of planar nanowires and 3D free-standing nanowires grown by focused electron- / ion (Ga<sup>+</sup>)-beam induced deposition (FEBID/FIBID) using the novel precursor Nb(NMe<sub>2</sub>)<sub>3</sub>(N-*t*-Bu). FEBID planar nanowires contain 67at%Nb, 22at%N and 11at%Nb; FIBID planar nanowires 42.9at%Nb, 12.9at%N, 15.5at%Ga and 28.7at%Nb. TEM analysis shows that FEBID samples are amorphous, while FIBID samples are made of fcc NbC polycrystals, with grains of 15-20nm diameter and lattice constant 4.47Å. The

RT electrical resistivity is  $\approx 10^4 \mu\Omega\text{cm}$  and  $550 \mu\Omega\text{cm}$  for FEBID and FIBID samples. Conductivity vs. temperature measurements show that the FEBID nanowires are insulating, following a variable-range-hopping behavior. FIBID nanowires, with  $\text{RRR}=0.87$ , become superconducting at  $T_C=5.0$  K.  $T_C$  can be slightly tuned either by an electron irradiation treatment ( $T_C=5.4$ , for  $20\text{nC}/\text{m}^2$ ) or by changing the width of the nanowires ( $T_C=4.3\text{--}6.4$ , for  $w=50\text{--}1000$  nm). 3D free-standing nanowires were grown by FIBID. TEM experiments confirm a fcc NbC microstructure. The electrical measurements of these nanowires, with  $\text{RRR}=1.02$ , show a superconducting transition with  $T_C=11$  K, a value close to the value of bulk NbC.

DS 23.8 Thu 17:30 H32

**Effective protection of few-layer black phosphorus from reactive species generated by in-situ focused electron beam irradiation.** — ●LOBO CHARLENE and ELBADAWI CHRISTOPHER — School of Mathematical and Physical Sciences, University of Technology Sydney, Ultimo NSW 2007

Recent studies have shown that exposure of few-layer black phospho-

rus (FLBP) to reactive oxygen species (ROS) via photoactivated oxidation induces an immediate and permanent reduction in the electron and hole mobility of FLBP. Electron-beam irradiation in H<sub>2</sub>O vapour is known to generate ROS (such as \*O<sub>2</sub>-, \*OH and OH-) that are responsible for the degradation of FLBP in ambient environment, but FLBP stability has not been assessed during prolonged exposure to other gaseous environments.

Here, we study the stability of FLBP in H<sub>2</sub>O, O<sub>2</sub>, NF<sub>3</sub> and NH<sub>3</sub> environments using environmental scanning electron microscopy (ESEM) and in situ electrical conductance measurements. The electron beam is used both for ESEM imaging, and also to generate reactive species such as \*O, \*OH, \*F and \*H that can drive spatially-localized chemical reactions at the sample surface. Using this approach, we demonstrate two promising methods of protecting FLBP and other moisture-sensitive two-dimensional materials from degradation by ROS. Encapsulation of FLBP with ionic liquids dramatically slows the rate of degradation in ROS environments. FLBP degradation can also be prevented by maintaining the temperature in the range  $\sim 125\text{--}300$  °C during ROS exposure, without requiring any protective coating.

## DS 24: Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...) Part I

Time: Thursday 15:00–18:15

Location: H39

DS 24.1 Thu 15:00 H39

**Magnetic skyrmions in FeGd multilayer thin films** — ●ZAHRA INANLOO MARANLOO<sup>1</sup>, MICHAEL HEIGL<sup>2</sup>, HENRIK GABOLD<sup>1</sup>, GEORG BENKA<sup>1</sup>, MANFRED ALBRECHT<sup>2</sup>, and PETER BÖNI<sup>1</sup> — <sup>1</sup>Physics Department E21, Technical University of Munich, 85748 Garching, Germany — <sup>2</sup>Experimental Physics IV, Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

Magnetic skyrmions are topological magnetic entities that are observed in an increasing number of bulk and thin film systems[1]. Fe/Gd multilayers, in which Fe and Gd are antiferromagnetically coupled, are of high interest because they can form skyrmions at room temperature[2].

In this project, the magnetic structure of multilayers  $[\text{Fe}(0.34\text{nm})/\text{Gd}(d)]_{80}$  with  $d=0.35$  nm,  $0.40$  nm,  $0.45$  nm have been investigated. The magnetic properties have been tuned by varying the thickness of the Gd layers in order to study how the expected skyrmion phase will be affected and changed. The structure and morphology were studied by X-ray reflectivity measurements. We will show measurements of magnetic hysteresis loops and topological Hall effect that can be used to identify the shift of the skyrmion phase with respect to the temperature and magnetic field. Finally, the process of the magnetic domain evolution at zero and different in-plane and out-of-plane applied magnetic fields will be discussed on the basis of results using magnetic force microscopy.

Reference

[1]W. Jiang, et. al., Physics Reports 704(2017).

[2]S. A. Montoya, et. al., Phys. Rev. B 95, 024415(2017).

DS 24.2 Thu 15:15 H39

**Synthesis and characterization of Graphene/Neutral red dye composite** — ●DMITRII POTOROCHIN<sup>1,2,3</sup>, SERGUEI MOLODTSOV<sup>2,3,4</sup>, PAVEL BRUNKOV<sup>2,5</sup>, MARINA BAIDAKOVA<sup>2,5</sup>, MAXIM RABCHINSKII<sup>5</sup>, NIKOLAI ULIN<sup>5</sup>, DMITRY MARCHENKO<sup>6</sup>, ALEXANDER CHAIKA<sup>7</sup>, OLGA MOLODTSOVA<sup>1,2</sup>, and VICTOR ARISTOV<sup>1,7</sup> — <sup>1</sup>DESY, Hamburg, Germany — <sup>2</sup>ITMO University, Saint Petersburg, Russian Federation — <sup>3</sup>TU Bergakademie Freiberg, Freiberg, Germany — <sup>4</sup>European XFEL, Schenefeld, Germany — <sup>5</sup>Ioffe Institute RAS, Saint Petersburg, Russian Federation — <sup>6</sup>Helmholtz-Zentrum Berlin, Berlin, Germany — <sup>7</sup>ISSP RAS, Chernogolovka, Russian Federation

Graphene/Neutral red dye composite has been synthesized by covalent binding of dye molecules to the basal plane of graphene through diazonium chemistry approach. Resulting nanosystem was studied by synchrotron-based high-resolution X-ray photoelectron spectroscopy (HR-XPS), photoemission electron microscopy (PEEM), and scanning tunneling microscopy (STM). Obtained data verifies high stability of the nanostructure even after exposure of the samples into ultrasonic bath and annealing in ultrahigh vacuum conditions. This work was supported by RAS, RFBR (Grant Nos. 17-02-01139, 17-02-01291) and Minobrnauki of Russia (Project 3.3161.2017/4.6).

DS 24.3 Thu 15:30 H39

**Mono- and few-layer MoS<sub>2</sub> films on muscovite mica substrates** — ●JONATHAN ROMMELFANGEN, EVANDRO LANZONI, DANIEL SIOPA, PHILLIP DALE, MICHELE MELCHIORRE, and ALEX REDINGER — Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg

In this contribution, we discuss the growth of MoS<sub>2</sub> films on muscovite mica substrates. This substrate is used to ensure a van der Waals epitaxy and furthermore ensures a flat and well-defined surface to characterize the films via atomic force microscopy (AFM). The MoS<sub>2</sub> films are synthesized via DC sputtering of metallic Molybdenum on  $2.5 \times 2.5$  cm<sup>2</sup> mica sheets, followed by a sulfurization in a tubular furnace. The sulfurization has been carried out at different temperatures and dwell times in order to find the optimum growth temperature. The thickness of the Mo layer has been varied in order to study the growth mode in detail. Raman measurements performed with different excitation wavelengths (325 nm, 442 nm, 532 nm) corroborate a transition from monolayer/bilayer MoS<sub>2</sub> to bulk-like MoS<sub>2</sub> as a function of the Mo precursor thickness, independent of the sulfurization temperature. For all temperatures used in this study (500°C–700°C) we observe a transition from a 2D to a 3D island growth mode. Based on our AFM measurements we propose a growth mechanism and discuss the results in the context of the observed Raman shifts. The AFM and Raman measurements will be supplemented with Photoluminescence measurements.

DS 24.4 Thu 15:45 H39

**X-ray absorption spectroscopy studies on transition metal dichalcogenide heterostructures** — ●FLORIAN RASCH<sup>1</sup>, DANIELLE HAMANN<sup>2</sup>, GAVIN MITCHSON<sup>2</sup>, DAVID JOHNSON<sup>2</sup>, JAVIER HERRERO<sup>3</sup>, MANUEL VALVIDARES<sup>3</sup>, MANUEL RICHTER<sup>1</sup>, BERND BÜCHNER<sup>1,4</sup>, and JORGE HAMANN-BORRERO<sup>1,4</sup> — <sup>1</sup>Leibniz Institute for Solid state and Materials Research Dresden, Dresden, Germany — <sup>2</sup>Department of Chemistry and Materials Science, University of Oregon, Eugene, Oregon, United States — <sup>3</sup>ALBA Synchrotron Light Source, Cerdanyola del Valles, Spain — <sup>4</sup>Department of Physics, TU Dresden, Dresden, Germany

Over the last years transition metal dichalcogenides (TMDs) provided a vast playground for the exploration of emergent physics in the crossover from 3D bulk to 2D monolayer. A novel way to investigate this crossover is given by TMD heterostructures with chemical formula  $(\text{MX})_n/(\text{TX})_m$  with metal M, chalcogen X and transition metal T, where  $n$  and  $m$  denote the number of consecutive layers. The compositions M, T and dimensionalities  $n$ ,  $m$  can be precisely controlled, allowing for systematic studies of the materials electronic properties as a function of those parameters. We have performed X-ray absorption spectroscopy measurements at the Nb L<sub>2,3</sub> edges on  $(\text{MSe})_1/(\text{NbSe}_2)_1$  ( $M = \text{Bi, Sn, Pb}$ ) and observed pronounced differences in the spectral lineshape as compared to the XAS of bulk NbSe<sub>2</sub> as well as systematic

changes within the heterostructures. We will discuss details of these changes in the electronic structure based on our XAS measurements in combination with density functional theory (DFT) calculations.

DS 24.5 Thu 16:00 H39

**K and Ba implantation in FeSb<sub>3</sub> thin films** — ●FELIX TIMMERMANN, MARC LINDORF, and MANFRED ALBRECHT — Universität Augsburg, Universitätsstraße 1, 86135 Augsburg, Germany

Increasing interest in the development of alternative energy sources led to an extended research in the field of thermoelectricity. For a good efficiency of thermoelectric generators, materials with special transport properties are needed. The goal is to find compounds with a large Seebeck coefficient  $\alpha$ , high electrical conductivity  $\sigma$ , and low thermal conductivity  $\kappa$ . Skutterudites, such as FeSb<sub>3</sub>, are materials that meet those criteria well. The insertion of filler atoms like K or Ba in the metastable FeSb<sub>3</sub> leads to stabilization of this phase and has the potential to improve the thermoelectric properties further [1].

In this work, as a preface to prepare polycrystalline skutterudite thin films, amorphous Fe-Sb films were deposited on SiO<sub>2</sub>(100nm)/Si(100) and glass substrates by molecular beam deposition. After ion implantation with K and Ba, the films were annealed while measuring the electrical conductivity and Seebeck coefficient. The composition and film thickness before and after implantation were compared by Rutherford Backscattering Spectrometry (RBS) and Energy Dispersive X-Ray spectrometry (EDX). Structural characterization by X-Ray Diffraction (XRD) and Transmission Electron Microscopy (TEM) gives insight to the formation of the desired skutterudite and secondary phases.

[1] N. Stetson et al., J. of Solid State Chem. 91, 140-147 (1991)

DS 24.6 Thu 16:15 H39

**Deposition of thin films of lithium nickel cobalt manganese oxide (NCM) cathode materials by using the sol-gel spin coating approach** — ●HENDRIK HEMMELMANN<sup>1</sup> and MATTHIAS T. ELM<sup>1,2,3</sup> — <sup>1</sup>Center for Materials Research, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen — <sup>2</sup>1. Physical Institute, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen — <sup>3</sup>Physical Chemical Institute, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 17, 35392 Gießen

Thin films are ideal model systems to study the interface properties of a materials system. To investigate the interfaces properties of the electrolyte-electrode interface of Lithium-ion batteries lithium nickel cobalt manganese oxide (NCM) layered cathode thin films were prepared using a sol-gel approach followed by a spin coating process. By varying the spin coating process parameters homogenous films with a smooth surface were obtained. The as prepared films were structurally and electrochemically characterized using GIXRD, high resolution electron microscopy (HREM), energy dispersive X-ray spectroscopy (EDX) and cyclic voltammetry (CV). Furthermore, atomic layer deposition (ALD) was used to deposit Al<sub>2</sub>O<sub>3</sub> and CeO<sub>2</sub> coatings of a few nanometres on the cathode materials to study the effect of a protective coating on the structural stability and electrochemical performance of the cathode material.

15 min. break.

DS 24.7 Thu 16:45 H39

**Spectroscopic Investigation of Disorder in Spinel Ferrite Thin Films** — ●VITALY ZVIAGIN<sup>1</sup>, PAULA HUTH<sup>2</sup>, CHRIS STURM<sup>1</sup>, JÖRG LENZNER<sup>1</sup>, ANNETTE SETZER<sup>1</sup>, REINHARD DENECKE<sup>2</sup>, PABLO ESQUINAZI<sup>1</sup>, MARIUS GRUNDMANN<sup>1</sup>, and RÜDIGER SCHMIDT-GRUND<sup>1</sup> — <sup>1</sup>Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstr. 5, Leipzig — <sup>2</sup>Universität Leipzig, Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Linnéstr. 2, Leipzig

Zn<sub>x</sub>Fe<sub>3-x</sub>O<sub>4</sub> (0 ≤ x ≤ 1.26) and ZnFe<sub>2</sub>O<sub>4</sub> (ZFO) thin films were fabricated on TiN/(100)MgO and (100) SrTiO<sub>3</sub> substrates by pulsed laser deposition. The bulk and surface cation distribution, determined from analysis of the spectroscopic ellipsometry as well as Fe 3p and 2p XPS core level spectra, is compared as a function of Zn (x) concentration. Antiphase boundary defect and nanocrystalline formation are related to the ferrimagnetic and superparamagnetic behavior of x = 0 and 1.26 films, respectively. The net magnetic response is related to the tetrahedral occupation by Fe<sup>3+</sup> in the ZFO film and is correlated to the increase of O<sup>2-</sup> 2p-Fe<sup>3+</sup> 3d electronic transition amplitude in the dielectric function (DF) spectra with the decrease in substrate temperature.[1] ZFO films, grown at low and high oxygen pressure, were annealed at temperatures 250 - 375 °C in oxygen and argon atmo-

spheres, respectively. The defect type and concentration was found to decrease as the cations are redistributed with the increase in annealing temperature in both environments, evident from the strength of DF electronic transitions as well as net magnetic moment.

[1] V. Zviagin et al., Appl. Phys. Lett. 108, 13 (2016)

DS 24.8 Thu 17:00 H39

**Controlling defect distribution and intrinsic domain structure in ultrathin ferroelectric films** — ●CHRISTIAN WEYMANN<sup>1</sup>, CÉLINE LICHTENSTEIGER<sup>1</sup>, STÉPHANIE FERNANDEZ-PEÑA<sup>1</sup>, LIV DEDON<sup>2</sup>, LANE MARTIN<sup>2</sup>, AARON NADEN<sup>3</sup>, AMIT KUMAR<sup>3</sup>, JEAN-MARC TRISCONE<sup>1</sup>, and PATRYCJA PARUCH<sup>1</sup> — <sup>1</sup>DQMP, University of Geneva — <sup>2</sup>MSE, UC Berkeley — <sup>3</sup>SMP, QU Belfast

Domains significantly affect the properties of ultrathin ferroelectric films. Controlling the domain structure is thus crucial for applications, and of great fundamental interest. It results from the interplay of the depolarizing field, destabilizing the uniform polarization configuration, and of any built-in field favoring one polarization direction. The former must be compensated by screening to maintain a uniform polarization configuration. The latter results from an asymmetry in this screening or from internal sources, such as charged defect dipoles.

We show that we can manipulate both these fields, acting on the screening of the bound charge using dielectric spacer layers, or modulating the built-in field and defect distribution through changes in the growth temperature of PbTiO<sub>3</sub> thin films, allowing full control over the intrinsic polarization state. Combining PFM mapping of the domain structure, RBS to quantify differences in defect density and distribution, and XRD measurements of the strain profile in the films, we propose a defect-dipole gradient mechanism to explain the observed results, in agreement with Ginzburg-Landau-Devonshire modeling. We also take advantage of this unique control over the domain structure to investigate the microstructure of the domains themselves.

DS 24.9 Thu 17:15 H39

**GeTe(111) ferroelectric and (GeMn)Te multiferroic Rashba semiconductor: a novel paradigm for spintronic applications** — ●JURAJ KREMPASKY<sup>1</sup>, HUGO DIL<sup>2</sup>, GUNTHER SPRINGHOLZ<sup>3</sup>, JAN MINAR<sup>4</sup>, and MATTHIAS MUNTWILER<sup>1</sup> — <sup>1</sup>Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — <sup>2</sup>Institute of Physics, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland — <sup>3</sup>Institut für Halbleiter- und Festkörperphysik, Johannes Kepler Universität, A-4040 Linz, Austria — <sup>4</sup>New Technologies-Research Center University of West Bohemia, Pilsen, Czech Republic

The control of the electron spin in functional materials by an external electric field is a key issue for spintronic devices. Because the spin is not directly influenced by a realistic electric field, the coupling has to be indirect and thus especially ferroelectric and multiferroic materials bear large promise. In this respect a novel class of multiferroic materials based on ferroelectric GeTe(111) enabled to combine ferroelectric order with Rashba type switching of spin textures. The system thus constitutes an intriguing route for non-volatile and static electrical control of the spin degrees of freedom. Based on photoemission studies in spin and momentum-resolved ways, combined with x-ray photoelectron-diffraction experiments, we found that besides ferroelastic and depolarization effects, a depth of six atomic layers below the GeTe surface significantly deviates from the expected truncated bulk structure. In this context the limitations of the electric control of the Rashba states are discussed.

DS 24.10 Thu 17:30 H39

**Reference-free quantification of thin layered alloys with synchrotron radiation based experiments** — ●ANDRÉ WÄHLISCH, CORNELIA STREECK, and BURKHARD BECKHOFF — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany

X-ray fluorescence analysis is a nondestructive technique to investigate a wide range of different materials. Quantitative results of unknown samples are typically obtained by utilizing well known reference samples. Alloyed multilayers with layer thicknesses in the order of one micrometer were analyzed in the present work. Since for this type of material appropriate reference materials are often not available, a reference-free approach based upon SI traceability is employed by the Physikalisch-Technische Bundesanstalt (PTB), the national metrology institute of Germany. The PTB operates fully characterized beamlines at the electron storage ring BESSY II in Berlin. The radiometrically calibrated instrumentation and the reference-free fundamental parameter approach using monochromatized synchrotron radiation allow for a direct quantification of the mass deposition of individual layers in

the multilayers and a reliable uncertainty budget can be calculated.

DS 24.11 Thu 17:45 H39

**Epitaxial Mn<sub>5</sub>Ge<sub>3</sub> (100) layer on Ge (100) substrates obtained by flash lamp annealing** — ●YUFANG XIE<sup>1</sup>, YE YUAN<sup>2</sup>, MAO WANG<sup>1</sup>, CHI XU<sup>1</sup>, RENE HUEBNER<sup>1</sup>, JOERG GRENZER<sup>1</sup>, YUJIA ZENG<sup>3</sup>, MANFRED HELM<sup>1</sup>, SHENGQIANG ZHOU<sup>1</sup>, and SLAWOMIR PRUCNAL<sup>1</sup> — <sup>1</sup>Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — <sup>2</sup>Physical Science and Engineering Division, King Abdullah University of Science and Technology, 23955-6900 Thuwal, Saudi Arabia — <sup>3</sup>Shenzhen Key Laboratory of Laser Engineering, College of Optoelectronic Engineering, Shenzhen University, 518060 Shenzhen, China

Mn<sub>5</sub>Ge<sub>3</sub> thin films have been demonstrated as promising spin-injector materials for germanium-based spintronic devices. So far, Mn<sub>5</sub>Ge<sub>3</sub> has been grown epitaxially only on Ge (111) substrates. In this letter, we present the growth of epitaxial Mn<sub>5</sub>Ge<sub>3</sub> films on Ge (100) substrates. The Mn<sub>5</sub>Ge<sub>3</sub> film is synthesized via sub-second solid-state reaction between Mn and Ge upon flash lamp annealing for 20 ms at the ambient pressure. The single crystalline Mn<sub>5</sub>Ge<sub>3</sub> is ferromagnetic with a Curie temperature of 283 K. Both the c-axis of hexagonal Mn<sub>5</sub>Ge<sub>3</sub> and the magnetic easy axis are parallel to the Ge (100) surface. The millisecond-range flash epitaxy provides a new avenue for the fabrication of Ge-based spin-injectors fully compatible with CMOS technology.

DS 24.12 Thu 18:00 H39

**Chemical order in Heusler thin films determined by X-ray diffraction** — ●DOMINIK KRIEGNER<sup>1</sup>, ANASTASIOS MARKOU<sup>1</sup>, PETER SWEKIS<sup>1</sup>, JOERG GRENZER<sup>2</sup>, and CLAUDIA FELSER<sup>1</sup> — <sup>1</sup>Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — <sup>2</sup>Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany

The chemical order of Heusler materials largely determines their physical properties [1]. For bulk materials powder diffraction with X-rays and neutrons are established tools to determine the chemical order and potential disorder between various lattice sites in Heusler compounds. On the other hand for epitaxial thin films due to the low sample volume and more complicated measurement geometries for the diffraction experiments the established models for polycrystals do only apply with modifications. Using a coplanar diffraction geometry we show how experimental data have to be collected and how corrections (for the diffraction geometry) have to be applied that common polycrystal models can be used to determine the chemical order of cubic Co<sub>2</sub>MnGa [2] and tetragonal MnPtSn compounds thin film [3].

[1] C. Felser, A. Hirohata (Eds.) *Heusler Alloys, Properties, Growth, Applications*; Springer Series in Materials Science [2] H. Reichlova, et al. *Appl. Phys. Lett.* 113, 212405 (2018) [3] P. Swekis, et al. submitted

## DS 25: Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...) Part II

Time: Friday 9:30–12:45

Location: H32

DS 25.1 Fri 9:30 H32

**Reducing residual stress and dislocation density in AlN films grown on SiC by MOCVD for UV-C LED applications** — ●CHRISTIAN J. ZOLLNER<sup>1</sup>, ABDULLAH ALMOGBEL<sup>1</sup>, BURHAN SAIF ADDIN<sup>1</sup>, MICHAEL IZA<sup>1</sup>, STEVEN P. DENBAARS<sup>1,2</sup>, JAMES S. SPECK<sup>1</sup>, and SHUJI NAKAMURA<sup>1,2</sup> — <sup>1</sup>Materials Department, UC Santa Barbara, CA, USA — <sup>2</sup>Department of Electrical and Computer Engineering, UC Santa Barbara, CA, USA

In nitride optoelectronics, the most important figures of merit for buffer layers grown on foreign substrates are threading dislocation density (TDD) and residual stress. Residual stress can lead to polarization fields in GaN and AlN, as well as wafer bowing and film cracking. Threading dislocations are detrimental to optical emission efficiencies, laser lifetimes, and carrier mobilities, but growing low TDD nitride buffers has proven more challenging than in conventional semiconductors. I will discuss the tradeoff between low TDD and low stress in MOCVD grown AlN films, and how this tradeoff can be mitigated. As a result, TDD (measured by x-ray diffraction and TEM) has been reduced from 10<sup>10</sup> cm<sup>-2</sup> to 4 × 10<sup>8</sup> cm<sup>-2</sup>, and stress (measured with the x-ray radius of curvature method) has been reduced from nearly 2 GPa to below 500 MPa. The mechanisms of TDD and stress reduction are explored using TEM and secondary-ion mass spectroscopy, and theoretical contributions of different sources of stress are calculated and compared with experiment. Significant reductions in both TDD and stress yield higher performance in UV-C LED devices grown on improved AlN/SiC buffers.

DS 25.2 Fri 9:45 H32

**Mass separated low-energy nitrogen ion assisted thin film growth** — ●MICHAEL MENSING, PHILIPP SCHUMACHER, CHRISTOPH GRÜNER, JÜRGEN W. GERLACH, and BERND RAUSCHENBACH — Leibniz Institute of Surface Engineering (IOM), Leipzig, Germany

Ion beam or plasma assistance is consistently and increasingly utilized to enhance the capabilities of physical deposition techniques. The impact of their applications range from precise engineering of film properties to the alleviation of process constraints. Albeit the influence of the energetic particle flux has been extensively studied, the distinct contributions of individual ion species to film growth are typically not investigated due to the extensive efforts required. In this study the application of an energy and mass selected ion-beam assisted deposition (EMS-IBAD) setup is presented. It features a compact quadrupole mass filter system to separate the prominent ion species (N<sup>+</sup>, N<sub>2</sub><sup>+</sup>) involved in the growth processes of nitride thin films on the example

of GaN. The thin films are deposited on 6H-SiC(0001) by employing different nitrogen ion species and compared with regards to their topography, crystalline quality and phase composition for different ion kinetic energies and ion-to-atom arrival ratios. The chosen hyperthermal ion energy range is <200 eV. The higher energy atomic nitrogen ions could be identified to impede the formation of the metastable zinc-blende GaN phase whereas the crystalline quality deteriorates. Molecular nitrogen ions are demonstrated to efficiently dissociate for kinetic energies as low as 20 eV, providing increased growth rates while preserving the crystalline quality.

DS 25.3 Fri 10:00 H32

**Valence profiling of LaMnO<sub>3</sub>/SrTiO<sub>3</sub> by use of resonant X-ray reflectometry and crystal field theory** — ●MICHAEL DETTBARN<sup>1</sup>, VOLODYMYR B. ZABOLOTNYI<sup>1</sup>, ROBERT GREEN<sup>2</sup>, MICHAEL ZAPF<sup>1</sup>, KIRILL MILLER<sup>1</sup>, MATTHIAS SCHMITT<sup>1</sup>, ENRICO SCHIERLE<sup>3</sup>, MICHAEL SING<sup>1</sup>, RALPH CLAESSEN<sup>1</sup>, and VLADIMIR HINKOV<sup>1</sup> — <sup>1</sup>Universität Würzburg and Röntgen Center for Complex Material Systems (RCCM), Würzburg — <sup>2</sup>University of Saskatchewan, Saskatoon, Canada — <sup>3</sup>HZB, Berlin

We have measured resonant X-ray reflectivity (RXR) and X-ray absorption spectra (XAS) on a bulk stoichiometric La<sub>7/8</sub>Sr<sub>1/8</sub>MnO<sub>3</sub> sample and three thin LaMnO<sub>3</sub> films of 3, 12 and 30 u.c. thickness. The manganese in the La<sub>7/8</sub>Sr<sub>1/8</sub>MnO<sub>3</sub> sample can be modeled by a 3+ valence, whose line shape we fit theoretically by use of crystal-field theory, including a Jahn-Teller distortion.

We model the RXR spectra of the three LaMnO<sub>3</sub> films by a mixture of Mn<sup>3+</sup> and Mn<sup>2+</sup> contributions, and deduce the depth profiles of the two different valencies. We compare our results with previous microscopy studies, in which a preferred occurrence of Mn<sup>2+</sup> near the interface and surface regions was observed.

DS 25.4 Fri 10:15 H32

**HAXPES study of oxygen vacancies forming in thin film HfO<sub>2</sub>-based MIM structures** — ●THOMAS SZYJKA<sup>1</sup>, RONJA HINZ<sup>1</sup>, MAI HUSSEIN<sup>1</sup>, PAUL ROSENBERGER<sup>1</sup>, MAREK WILHELM<sup>1</sup>, TERENCE MITTMANN<sup>2</sup>, UWE SCHRÖDER<sup>2</sup>, and MARTINA MÜLLER<sup>1,3</sup> — <sup>1</sup>PGI-6, FZ Jülich GmbH, Jülich, DE — <sup>2</sup>NaMLab gGmbH, Dresden, DE — <sup>3</sup>Fakultät Physik, TU Dortmund, Dortmund, DE

Hf-based dielectrics have replaced the traditional SiO<sub>2</sub> and SiON as gate dielectric materials for conventional CMOS devices. Due to the recently discovered ferroelectric properties in strained HfO<sub>2</sub>, new applications like ferroelectric FETS are currently under development.



The ferroelectric properties are linked to the orthorhombic phase in  $\text{HfO}_2$  which can be stabilized via doping or the creation of oxygen vacancies. In this context, it is crucial to understand the processes and engineering of the interface properties of strained- $\text{HfO}_2$  and electrode materials. Different thin film metal-insulator-metal (MIM) capacitors were fabricated with doped  $\text{HfO}_2$  using different electrode materials ( $\text{TaN}$ ,  $\text{TiN}$ ,  $\text{IrO}_2$ ) leading to various forming of oxygen vacancies. In addition, films with undoped  $\text{HfO}_2$  and  $\text{TiN}$  electrodes were fabricated using either no or 2 sccm additional oxygen flow during the fabrication in order to reduce the amount of oxygen vacancies. Hard X-ray photoelectron spectroscopy (HAXPES) was performed at DESY (Hamburg) and BESSY (Berlin) to analyse the interface processes. The spectral features of the  $\text{Hf}4f$ ,  $\text{N}1s$  and  $\text{O}1s$  core levels indicate an intermixing of the layers and provide a direct relation between the growth process and the formation of oxygen vacancies.

DS 25.5 Fri 10:30 H32

**X-ray spectroscopic composition analysis of amorphous  $\text{ZnSnO}_y$  grown by magnetron sputtering** — ●AINUR ZHUSSUPBEKOVA<sup>1</sup>, AITKAZY KAISHA<sup>1</sup>, KARSTEN FLEISCHER<sup>1,2</sup>, IGOR V. SHVETS<sup>1</sup>, and DAVID CAFFREY<sup>1</sup> — <sup>1</sup>School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Dublin 2, Ireland — <sup>2</sup>School of Physics, Dublin City University, Dublin 9, Ireland

The conductivity of Amorphous Transparent Conducting Oxide (a-TCO) materials is not dependent on their long range crystallographic order, making them ideal materials for flexible electronics. A potential candidate to take a prominent place in this field is amorphous  $\text{ZnSnO}_y$  (a-ZTO) because, unlike amorphous  $\text{InGaZnO}_4$  (a-IGZO), it does not contain any non-abundant or expensive components such as indium.

In this study, X-ray Photoelectron Spectroscopy (XPS) is used to perform an extensive composition analysis of a- $\text{ZnSnO}_y$  grown by reactive and non-reactive magnetron sputtering. An identical maximum conductivity of 225 S/cm is achieved via both techniques. However, analysis of the a- $\text{ZnSnO}_y$  composition reveals that the distinct Zn/Sn ratios at which this maxima occurs varies depending on growth technique. The Zn/Sn ratios observed at each maxima have been found to correspond to theoretical unstable polymorphs of a- $\text{ZnSnO}_y$ . We confirm the existence of two corresponding distinct local bonding arrangements depending on deposition methodology via Raman spectroscopy.

DS 25.6 Fri 10:45 H32

**MBE growth of oxide thin films on silicon** — ●LUQMAN MUSTAFA — ZIK SiLi-nano, Martin-Luther-University Halle-Wittenberg, Halle, Germany

Complex oxide thin films can exhibit many different physical properties. The epitaxial growth of these films on silicon enables the integration of their properties in silicon technology for the development of novel devices and optimizing existing technologies. Lately, ferroelectric oxide thin films has gained more interest in photonic applications, for example, waveguid structures made of  $\text{BaTiO}_3$  on silicon-on-oxide (SOI) wafers were developed exhibiting strong linear electro-optical effect, with effective Pockels coefficient higher than commercial optical modulators.

The greatest challenge in the epitaxial growth of oxides on silicon is the formation of amorphous silicon oxide layer at the interface once the silicon surface is exposed to oxygen, making the intended heteroepitaxy of the film on silicon extremely difficult. Here we report on the optimized growth conditions of complex oxide thin films on SOI substrates.  $\text{BaTiO}_3$  thin films were grown using MBE technique.  $\text{BaO}$  and  $\text{SrTiO}_3$  were used as a buffer layer to reduce strain. the thin film morphology, structural, and ferroelectric properties were investigated.

15 min. break.

DS 25.7 Fri 11:15 H32

**Orbital character of the mobile and localized electron states at the LAO/STO interface** — ●ALLA CHIKINA<sup>1,2</sup>, FRANK LECHERMANN<sup>3</sup>, MARIUS-ADRIAN HUSANU<sup>1,4</sup>, MARCO CAPUTO<sup>1</sup>, CLAUDIA CANCELLIERI<sup>5</sup>, THORSTEN SCHMITT<sup>1</sup>, MILAN RADOVIC<sup>1</sup>, and VLADIMIR N. STROCOV<sup>1</sup> — <sup>1</sup>Swiss Light Source, Paul Scherrer Institute, Villigen CH-5232, Switzerland — <sup>2</sup>IFW Dresden, P.O. Box 270116, Dresden D-01171, Germany — <sup>3</sup>Institut für Theoretische Physik, Universität Hamburg, Jungiusstrasse 9, Hamburg DE-20355, Germany — <sup>4</sup>National Institute of Materials Physics, Atomistilor 405A, Magurele RO-077125, Romania — <sup>5</sup>Empa, Swiss Federal Laboratories for Materials Science & Technology, Ueberlandstrasse

129, Duebendorf CH-8600, Switzerland

Interfacing different transition-metal oxides opens a route to functionalizing their rich interplay of electron, spin, orbital, and lattice degrees of freedom for electronic and spintronic devices. Electronic and magnetic properties of a mobile two-dimensional electron system (2DES) of  $\text{SrTiO}_3$ -based interfaces are strongly influenced by oxygen vacancies, where strongly correlated localized electrons in the in-gap states (IGSS) coexist with noncorrelated delocalized 2DES. Here, we use resonant soft-X-ray photoelectron spectroscopy to probe the eg character of the IGSSs, as opposed to the  $t_{2g}$  character of the 2DES in the paradigmatic  $\text{LaAlO}_3/\text{SrTiO}_3$  interface. Supported by a self-consistent combination of density functional theory and dynamical mean field theory calculations, this experiment identifies local orbital reconstruction that goes beyond the conventional eg-vs- $t_{2g}$  band ordering.

DS 25.8 Fri 11:30 H32

**PFM and SHG study of ferroelastic twin domain crossings in  $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$**  — ●PHILIPPE TÜCKMANTEL<sup>1</sup>, GRÉGORIE TAUPIER<sup>2</sup>, KOKOU D. DORKENOO<sup>2</sup>, JOSHUA C. AGAR<sup>3</sup>, LANE W. MARTIN<sup>3</sup>, PATRYCJA PARUCH<sup>1</sup>, and SALIA CHERIFI-HERTEL<sup>2</sup> — <sup>1</sup>DQMP University of Geneva, Geneva, Switzerland — <sup>2</sup>University of Strasbourg CNRS, IPCMS, Strasbourg, France — <sup>3</sup>University of California, Berkeley, DMSE, USA

Domains walls in ferroelectrics can exhibit properties absent from their parent material, such as a higher electric conductivity, photovoltaic effect, and ferromagnetic ordering, leading to a surge in interest in potentially using these nanoscale interfaces as active device components. Both theoretical and experimental studies have recently focused on the complex structure of these domain walls, underlying the rich functional behaviour. For example, SHG experiments have confirmed the non-Ising character of  $180^\circ$  domain walls in  $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$  and  $\text{LiTaO}_3$  which locally show Néel and Bloch like polarisation, respectively. However, relatively little is known about how such domain walls respond to disorder, variations of electrostatic boundary conditions or strain, which strongly influence polarisation in bulk and thin film samples, and which could affect the emergent properties of the domain walls.

Here, we report on the interplay of disorder and electromechanical effects, using SHG and PFM to focus on the crossings of  $180^\circ$  domain walls and ferroelastic twin domain walls in  $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$  grown by PLD on a  $\text{DyScO}_3$  substrates, highlighting their complex polarisation patterns and the key role of strain.

DS 25.9 Fri 11:45 H32

**Topotactic transition mechanisms in  $\text{SrCoO}_{2.5+x}$  films** — ●PATRICK SCHÖFFMANN<sup>1</sup>, SABINE PÜTTER<sup>1</sup>, ANIRBAN SARKAR<sup>2</sup>, AMIR SYED-MOHD<sup>1</sup>, MARKUS WASCHK<sup>2</sup>, TANVI BHATNAGAR<sup>2</sup>, PAUL ZAKALEK<sup>2</sup>, and THOMAS BRÜCKEL<sup>2</sup> — <sup>1</sup>Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — <sup>2</sup>Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Jülich, Germany

Strontium cobaltite ( $\text{SrCoO}_{3-\delta}$ ) exists in two topotactic phases, depending on the oxygen content.  $\text{SrCoO}_3$  is a ferromagnetic metal ( $T_C=305\text{K}$ ) with perovskite structure while  $\text{SrCoO}_{2.5}$  is an antiferromagnetic insulator ( $T_N=570\text{K}$ ) with brownmillerite structure. Because of the multivalent Co states and high oxygen mobility it is a promising material for energy and information applications [1]. To control the oxygen content, several possibilities exist. We focus on annealing in oxidising conditions and applying variable strain with a piezoelectric substrate to the film.

We grow thin films of  $\text{SrCoO}_{2.5}$  by molecular beam epitaxy on various substrates including a piezoelectric with a conducting buffer layer.

To be able to transfer strain from the substrate to the film, a high sample quality and epitaxy is mandatory, thus we present the results of the film growth and quality, as well as first results of the magnetic characterisation by SQUID and neutron reflectometry.

[1] H. Jeen et al., Nature Materials 12, 2013

DS 25.10 Fri 12:00 H32

**Effect of Interfaces in the Oxide Transport Process in Platinum Coated Porous Frameworks of Yttria-Stabilized Zirconia (YSZ)** — ●MICHELE BASTIANELLO<sup>1</sup>, JAN-OVE SÖHNGEN<sup>1</sup>, and MATTHIAS T. ELM<sup>1,2,3</sup> — <sup>1</sup>Center for Materials Research, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen — <sup>2</sup>Institute of Experimental Physics I, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen — <sup>3</sup>Institute of Physical Chemistry, Justus-Liebig-University Gießen,

Germany, Heinrich-Buff-Ring 17, 35392 Gießen

Mixed ionic and electronic conductors (MIEC) are used for many applications, i.e. as electrolyte for oxygen separation membranes. Here we present the preparation of artificial MIECs. Different YSZ-Pt-YSZ multilayered thin films were prepared as model systems using pulsed laser deposition (PLD) together with porous YSZ thin films subsequently coated with a thin layer of metallic platinum using atomic layer deposition (ALD). The as-prepared materials were structurally characterized using grazing incidence X-ray diffraction (GIXRD) and scanning electron microscopy (SEM). The electrical transport properties were investigated performing electrochemical impedance spectroscopy (EIS) at different temperatures and oxygen partial pressures to determine the conductivity as well as the activation energy of the thin films.

DS 25.11 Fri 12:15 H32

**Structure evolution of hydrogenated TiO<sub>2</sub> by means of Perturbed Angular Correlation** — •DMITRY ZYABKIN<sup>1</sup>, JULIANA SCHELL<sup>2,3</sup>, ULRICH VETTER<sup>1</sup>, and PETER SCHAAF<sup>1</sup> — <sup>1</sup>Chair materials for Electronics, Institute of Materials Engineering and Institute of Micro- and Nanotechnologies MacroNano<sup>®</sup>, Gustav-Kirchhoff-Str. 5, 98693 Ilmenau, Germany — <sup>2</sup>European Organization for Nuclear Research (CERN), CH- 1211 Geneva, Switzerland — <sup>3</sup>Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 45141 Essen, Germany

Hydrogenated titania has been recently attracting plenty of attention due to its promising properties. Not quite long ago some results proved that H is able to create a bond with Ti via Ti-OH and stays connected up to 530-550 K when it starts to dissociate and leave, additionally V<sub>0</sub> start to rearrange. To study this phenomena we applied recent perturbed  $\gamma\gamma$ -angular correlation (PAC) studies of TiO<sub>2</sub>:H thin films using the probe <sup>111m</sup>Cd, which was implanted at the online isotope separator ISOLDE at CERN. The films were produced by reactive magnetron sputtering on Si substrates. The subsequent H<sub>2</sub> plasma

treatment was performed at various temperatures up to 663K. After implantation with 10<sup>11</sup> probe atoms the samples were transported to a PAC setup and measured in various atmospheres (O<sub>2</sub>, air and vacuum) and in a range of temperatures to follow structure refinement. In order to preserve H-bondings no after implantation annealing was done. Time-differential R(t) spectra were fitted against electric quadrupole interaction parameter sets corresponding to fractions of probes.

DS 25.12 Fri 12:30 H32

**Epitaxial growth of Ba<sub>2</sub>SiO<sub>4</sub> thin films on Si(001)** — •JULIAN KOCH and HERBERT PFNÜR — Leibniz Universität Hannover, Inst. für Festkörperphysik, Appelstr. 2, 30167 Hannover

Ba<sub>2</sub>SiO<sub>4</sub> is a very promising candidate as a high-k dielectric [1]. Previously, Ba<sub>2</sub>SiO<sub>4</sub> films were grown by diffusion of Si from the Si(001) substrate into a deposited BaO layer [1]. These films featured a high interface trap density, which was most likely a result of the diffusion.

This study aims to improve the structural quality of the Ba<sub>2</sub>SiO<sub>4</sub> films by employing a co-deposition growth method, in which Ba and Si are evaporated simultaneously in an oxygen atmosphere. This eliminates the need for the Si diffusion and allows for control of the interface and the exact stoichiometry.

The chemical composition and the crystallinity of the films are investigated using XPS and SPA-LEED, respectively. The chemical shift of the O 1s peak in XPS enables the detection of excess Ba or Si and can thus be used to adjust the Si/Ba deposition ratio. The films are grown at RT to avoid Si diffusion from the substrate. Growth at higher temperatures is also possible, but the Si deposition rate has to be reduced to offset the diffusion. The epitaxial growth succeeded without any surface passivation or interface layer. However, even with correctly adjusted deposition rates, annealing to 680°C is needed in order to obtain crystalline films. During the annealing process the film is partially evaporated but the relative concentration of Ba to Si remains unchanged.

[1] S. Islam et al. Phys. Rev. Applied 5, 054006 (2016)