# DS 20: Poster

Time: Wednesday 16:00–18:00

## Location: P3

demonstrate that this background pressure strongly affects the resulting film\*s stoichiometry. Using two different vacuum setups, we are able to show that significant changes are imposed, e.g. on the optimized co-evaporation rates, by the specific vacuum chamber setup. Our results have important implications for the optimized evaporation of FA-based perovskites as they identify key issues related to the deposition of the FAI precursor.

DS 20.4 Wed 16:00 P3 In situ surface X-ray diffraction studies at high temperatures of Co oxide model catalysts for electrochemical water splitting — •CARL HENDRIC SCHARF<sup>1</sup>, CANRONG QIU<sup>1</sup>, JOCHIM STETTNER<sup>1</sup>, OLVIDO IRRAZÁBAL-MOREDA<sup>2</sup>, MATHILDE BOUVIER<sup>3</sup>, FOUAD MAROUN<sup>3</sup>, and OLAF MAGNUSSEN<sup>1</sup> — <sup>1</sup>Institute of Experimental and Applied Physics, Kiel, Germany — <sup>2</sup>European Synchrotron Radiation Facility (ESRF), Grenoble, France — <sup>3</sup>Physique de la Matière Condensée, Ecole Polytechnique, Palaiseau, France

The development of low-cost electrocatalysts for electrochemical water splitting is of great interest for hydrogen technology. Among the best precious-metal-free electrode materials for the anodic oxygen evolution reaction (OER) in alkaline electrolysis are Co oxides such as Co<sub>3</sub>O<sub>4</sub> and CoOOH. It was shown previously that a sub-nm thick  $CoO_x(OH)_y$  skin layer is formed in the pre-OER potential range, which forms the active phase during OER. Furthermore, reversible and irreversible structural changes in the oxide bulk were detected in the pre-OER regime. So far the vast majority of publications on Co oxide OER electrolysis have been performed at room temperature. We present first results up to 60°C (typ. operating temperatures of commercial electrolysers). Using operando surface X-ray diffraction Co<sub>3</sub>O<sub>4</sub> and CoOOH epitaxial films electrodeposited on Au(111) were studied in 0.1M NaOH at Petra III, Desy. These data are correlated with the electrochemical properties, determined by Cyclic Voltammetry and Optical Reflectivity, in order to provide insights into the temperature-dependence of skin layer thickness, bulk lattice changes and the stability of the oxides.

DS 20.5 Wed 16:00 P3

Growth of CoO Thin Films for Application in Superconductor - Magnet Heterostructures — •AMY McGLINCHEY — Trinity College Dublin, Ireland

Cobalt monoxide, CoO, is an antiferromagnet (AF) with a Néel temperature of 293K. It is utilised to pin the magnetisation of Co layers via exchange bias and is employed in magnetic heterostructures. The interaction between ferromagnet (F) and AF layers is predicted to generate long-range spin-triplet superconductivity in F-S-AF heterostructures [1]. CoO is a good candidate for the AF due to its strong magnetism, stability and low Neel temperature, which facilitates in-field cooling through the transition, improving magnetic uniformity. For the most part, CoO is synthesized by the oxidation of Co thin films. A fundamental understanding of how the Co phase (fcc or hcp) and oxidation environment influence the crystalline quality and surface morphology of the resultant CoO is lacking. In this work, we investigate the crystalline quality of the CoO as a function of Co phase and oxidation environment. As a second step towards a F-S-AF heterostructure, we also investigate the superconducting properties of superconducting Nb grown on the different CoO films. The properties of the niobium - especially at low thickness relevant to heterostructures - will, in theory, be influenced by the CoO magnetic and surface structure. 1. L. G. Johnsen et al., Phys. Rev. B, 103, L060505 (2021).

DS 20.6 Wed 16:00 P3

Pseudo-2-dimensional Ga<sub>2</sub>O<sub>3</sub> structures grown on Al<sub>2</sub>O<sub>3</sub> using metal-oxide catalyzed epitaxy (MOCATAXY) — •JUSTIN ANDREAS BICH<sup>1</sup>, MARCO SCHOWALTER<sup>1</sup>, TJARK LIESTMANN<sup>1</sup>, SUSHMA RAGHUVANSY<sup>1</sup>, JONATHAN MCCANDLESS<sup>2</sup>, MANUEL ALONSO-ORTS<sup>1</sup>, ANDREAS ROSENAUER<sup>1</sup>, MARTIN EICKHOFF<sup>1</sup>, and PATRICK VOGT<sup>1</sup> — <sup>1</sup>Institute of Solid-State Physics, Bremen University, Otto-Hahn-Allee 1, 28359 Bremen, Germany — <sup>2</sup>School of Electrical and Computer Engineering, Cornell University, Ithaca, New York 14853, USA

 $Ga_2O_3$  has attracted attention as a new wide-bandgap semiconductor—which can be alloyed with  $Al_2O_3$ —for high-power applications. However, the growth of group-III sesquioxides by

DS 20.1 Wed 16:00 P3 Thickness effect on ferroelectric domain formation in compressively strained K0.65Na0.35NbO3 epitaxial films — •YANKUN WANG<sup>1,2</sup>, SAUD BIN ANOOZ<sup>1</sup>, GANG NIU<sup>2</sup>, MAR-TIN SCHMIDBAUER<sup>1</sup>, LINGYAN WANG<sup>2</sup>, WEI REN<sup>2</sup>, and JUTTA SCHWARZKOPF<sup>1</sup> — <sup>1</sup>Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany — <sup>2</sup>Electronic Materials Research Laboratory, Xi'an Jiaotong University, Xi'an, China

Ferroelectrics are of increasing interest for a broad range of applications such as nonvolatile memory devices, transducers and MEMS sensors. Herein, the influence of thickness in epitaxial K0.65Na0.35NbO3 ferroelectric thin films grown on (110) TbScO3 substrate is systematically studied. By combining piezoresponse force microscopy and high-resolution x-ray diffraction, the occurrence of 90° stripe domains was demonstrated for the films with a thickness above 11 nm, while the domain periodicity is in good agreement with Kittel\*s law. Furthermore, up to a thickness of 93 nm, elastic strain relaxation induced by the formation of ferroelectric domains is observed, whereas plastic strain relaxation plays only a minor role. With increasing film thickness three successive phases of ferroelectric domains were observed: i) Irregularly arranged orthorhombic c domains in the thinnest film, ii) periodically arranged  $90^{\circ}$  monoclinic MC domains up to a thickness of 25 nm and iii) flux closure vortex-like structure in thicker films to achieve the lowest equilibrium energy. These results demonstrate the importance of understanding the lattice relaxation mechanisms for intentional tuning of ferroelectric thin film properties.

DS 20.2 Wed 16:00 P3 X-ray characterization of an above-RT bi-stable sublimable molecular spin-crossover Fe(II)-complex — •YAHYA SHUBBAK<sup>1</sup>, MIGUEL GAVARA EDO<sup>2</sup>, ARNO EHRESMANN<sup>1</sup>, and EUGENIO CORON-ADO MIRALLES<sup>2</sup> — <sup>1</sup>Institute of Physics & Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, D-34132 Kassel — <sup>2</sup>Institute of Molecular Science (ICMol), University of València, S-46980 Paterna

Spin crossover (SCO) molecules are a promising type of material that can undergo reversible switching between low-spin (LS)- and high-spin (HS)-states upon external stimuli (heat, light, pressure, etc.)[1], making them useful for information technology, data storage and optoelectronics[2]. However, most SCO molecules need to be cooled significantly for this transition to be observable. We have investigated the hitherto unknown electronic structure of the complex molecule bis[hydrotris(1,2,4-triazol-1-yl)borate]iron(II) ([Fe(HB(tz)3)2])[3] capable of above-RT transition by XPS and XAS measurements, since the distinct electronic structure in both spin-states unmistakably prove the transition between them.

[1]P. Gütlich and H. A. Goodwin. "Spin Crossover in Transition Metal Compounds I." Springer Berlin Heidelberg, May 2004. 356 pp. [2]E. P. Geest et al.,"Contactless Spin Switch Sensing by Chemo\*Electric Gating of graphene". In: Advanced Materials (2020), p. 1903575. [3]S. Rat et al.,"Solvatomorphism and structuralspin crossover property relationship in bis[hydrotris(1,2,4-triazol-1yl)borate]iron(ii)". In: CrystEngComm 19.24 (2017).

DS 20.3 Wed 16:00 P3 Insights into the evaporation behaviour of FAI: material degradation and consequences for perovskite solar cells — MARTIN KROLL<sup>1</sup>, SEREN DILARA ÖZ<sup>3</sup>, ZONGBAO ZHANG<sup>1</sup>, RAN JI<sup>1</sup>, •TIM SCHRAMM<sup>1,2</sup>, TOBIAS ANTRACK<sup>1</sup>, YANA VAYNZOF<sup>1,2</sup>, SELINA OLTHOF<sup>3</sup>, and KARL LEO<sup>1</sup> — <sup>1</sup>Dresden Integrated Center for Applied Physics and Photonic Materials, IAPP — <sup>2</sup>Center for Advancing Electronics Dresden, CFAED — <sup>3</sup>Department of Chemistry, University of Cologne

Thermal co-evaporation is a promising method for large-scale uniform perovskite deposition. In this work, we look at the decomposition of formamidinium iodide (FAI) upon evaporation in high vacuum by tracking the composition of the residual gas with a mass spectrometer. We find that the precursor material degrades during the evaporation process into hydrogen cyanide (HCN) and sym-triazine (C3H3N3), leading to an increase in pressure, which is commonly observed during the deposition of FAI. Using optical characterization as well as x-ray photoelectron spectroscopy on co-deposited perovskite films, we molecular-beam epitaxy differs substantially from other material systems, e.g., III-V materials.

In this work, we present the growth of ultra-thin  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> (0001) on  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> (0001) in a controlled self-passivating manner. Using MO-CATAXY, we observe the formation of this 'pseudo' 2-dimensional (2D)  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> thin film and its growth passivation after reaching 2 nm thickness. This  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> 2D thin film serves as a template for growing  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub>/ $\alpha$ -Al<sub>2</sub>O<sub>3</sub> quantum wells.

We present reflection-high energy electron diffraction, x-ray photoelectron spectroscopy, atomic force microscopy, x-ray diffraction, x-ray reflectivity, and transmission electron microscopy data, showing the existence and characteristics of this 'pseudo' 2D  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> thin film grown by MOCATAXY, and explain our results using a kinetic and thermodynamic framework.

DS 20.7 Wed 16:00 P3 An unconventional octahedral metal: AgSnTe2 — •SOPHIA WAHL, CHRISTIAN TEICHRIB, CARL-FRIEDRICH SCHÖN, MARIA HÄSER, YUAN YU, and MATTHIAS WUTTIG — 1. Institute of Physics (Ia), RWTH Aachen University, Aachen, Germany

Phase-change materials (PCMs) provide a unique combination of properties. Switching from the amorphous to crystalline structural phase, their optical and electrical properties change significantly. While conventional PCMs undergo a change from covalent to metavalent bonding upon crystallization accompanied by a dielectric behavior in both phases [1], we observe a change from dielectric to metallic in the optical and electrical properties for the unconventional metal AgSnTe2 (AST).

We analyze the dielectric properties of amorphous and crystalline AST samples by employing optical spectroscopy from the infrared to UV/Vis range. Through a Kramers-Kronig analysis of the data, we can separate the contributions of the optical functions accordingly and yield insight into the nature of bonding. Transport measurements and the investigation of bond rupture in atom probe tomography support the findings and all imply a non-conventional bonding mechanism in crystalline AST.

This work is aiming to define a whole set of new plasmonic PCMs which are all located in one region of the materials bonding map[2].

[1] Wuttig et al., Nat. Photonics, 11, 2017

[2] Raty et al., Adv. Mater., 31, 2019

## DS 20.8 Wed 16:00 P3 $\,$

Structural and electronic investigations of Bismuth multilayers with DFT — •FABIAN TEICHERT<sup>1</sup>, CHITRAN GHOSAL<sup>1</sup>, UWE GERSTMANN<sup>2</sup>, CHRISTOPH TEGENKAMP<sup>1</sup>, and ANGELA THRÄNHARDT<sup>1</sup> — <sup>1</sup>Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — <sup>2</sup>Department of Physics, Paderborn University, Paderborn, Germany

Bismuth shows a variety of interesting properties as bulk material but also as thin film, e.g. it is a topological insulator, shows strong spinorbit coupling effects and has a semimetal-semiconductor transition concerning film thickness. The focus of this presentation will be on density functional theory (DFT) calculations, which have been done for Bi(110) multilayers to get insights into the concrete structure and electronic states. We compare the results with Bi multilayers, which have been grown epitaxially on graphene substrate and where (110) slabs have been figured out. They are treated with scanning tunneling microscopy (STM) measurements for various slab thicknesses. We found an even/odd scheme concerning the number of monolayers as well as concerning the number of bilayers indicating a structural relaxation like the black phosphorus allotrope. Further calculations with graphene and highly oriented pyrolytic graphite (HOPG) substrate have be performed to figure out if structurally separated and electronically decoupled layers are present at the substrate interface. Concerning the electronic properties, we present the calculated bandstructures and density of states and comparisons with the measured differential conductance, which are in good agreement.

#### DS 20.9 Wed 16:00 P3

Twisted bilayer antimonene — •STEFAN WOLFF, ROLAND GILLEN, and JANINA MAULTZSCH — Department of Physics, Chair of Experimental Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany

Antimony has proven to be a promising candidate for two-dimensional (2D) mono-elemental materials. In bulk form, it is a layered crystal comprising sheets of antimony atoms arranged in a hexagonal buckled honeycomb lattice called antimonene. The natural stacking order

follows an ABC-pattern, in which each subsequent layer is shifted by one third. Other than many other 2D materials, the interlayer bonds in few-layer antimonene show partially covalent character. Due to this covalent character, changes of the local stacking order via rotation and translation may lead to new interesting features and properties of the material. Density functional theory (DFT) is used to simulate twisted bilayer antimonene structures with different rotation angels and to investigate their physical properties. Moiré patterns and local stacking orders can be found, which lead to a non-uniform bond length distribution. Additionally, our investigation of the charge density shows how the overlap of atomic orbitals in certain areas changes, depending on the proximity of atoms from neighboring layers. A comprehensive understanding of how the properties of twisted bilayer antimonene are modified compared to naturally stacked bilayer antimonene may lead to future applications making use of well-constructed, favorable stacking orders in layered materials.

DS 20.10 Wed 16:00 P3

**Determination of circularly polarized light-triggered chiral excitons in organic light harvesting devices** — •OTGONBAYAR ERDENE-OCHIR, DIRK HERTEL, and KLAUS MEERHOLZ — Chemistry Department, University of Cologne, Cologne, Germany

Organic-chiroptics have not been a focus of the research area due to the trace amount of circular dichroism (CD) nature has provided in most chiral molecules. However, aggregation of chiral prolinol functionalized squaraine offers giant intrinsic CD behavior. The CD effect is related not only to the difference of left- and right-handed circularly polarized (CP) light absorption for the organic chiral molecule, but also associated with their excitonic nature based on the formation of molecular aggregates. This work discusses the determination of the selective chiral excitons via direct right- and left-handed CP laser radiation. The enantiomer of squaraine derivative (S,S)-ProSQ-C16 is a strongly CD-active material featuring maximum absorbance at ca. 780 nm after thermal annealing of a thin film. We introduced (S,S)-ProSQ-C16 as a p-type active material in a planar heterojunction (PHJ) and bulk heterojunction (BHJ) blend for the photovoltaic devices, together with the fullerenes C60 and PCBM as acceptors, respectively. We used normal-incident transmission Mueller Matrix method to determine the intrinsic CD effects of the thin film. An electronic characterization of the chiral exciton within the PHJ and BHJ systems are quantified. The efficiency of the chiroptical response is estimated by the dissymmetry factor. A systematic correlation between optical and electronic dissymmetry factors will be discussed.

DS 20.11 Wed 16:00 P3

Molecular dynamics simulations of carbon nanomembranes (CNMs): Formation and mechanical properties — •LEVIN MIHLAN, JULIAN EHRENS, and JÜRGEN SCHNACK — Universität Bielefeld, Universitätsstrasse 25, D-33615 Bielefeld

CNMs are made by electron-induced crosslinking of aromatic selfassembled monolayers (SAMs) [1,2]. Their supposedly irregular internal structure cannot be adequately investigated by standard spectroscopic techniques, however, a determination of, e.g. Young's moduli is possible. In order to propose possible internal structures obtained from various initial configurations of the SAM and irradiation processes, we investigate the monolayers with respect to the Young's modulus in terms of classical molecular dynamics calculations using LAMMPS and compare to experimental values. We present three distinct methods to calculate the Young's modulus: Global scaling of all coordinates, stress-strain response from clamped straining and barostatted dynamics. Discrepancies among the methods with regard to vastly different outcomes will be discussed considering finite size effects. CNMs can be used for water filtration, a property that is closely related to the distribution of holes in the membrane [3]. With a hole-detection algorithm for our simulated CNMs we can investigate the hole distributions too and use this as a second observable for comparison with experimental data.

[1] Dementyev, Petr, et al. ChemPhysChem 21.10 1006, 2020

[2] Ehrens, Julian, et al. Phys. Rev. B 103 115416, 2021

[3] Y. Yang, et al. ACS Nano vol. 12 no. 12 pp. 4695-4701, 2018

DS 20.12 Wed 16:00 P3

Microscopic theory of X-ray absorption spectroscopy — •JORIS STURM, DOMINIK CHRISTIANSEN, MALTE SELIG, and ANDREAS KNORR — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany X-ray absorption near-edge spectroscopy (XANES) and extended Xray absorption fine structure (EXAFS) are two widely used methods to investigate the structure of solid states. Unfortunately, for both techniques, mostly heuristic models are available [1,2,3].

In this contribution, we present the first self-consistent Maxwell-Bloch approach based on Heisenberg equation of motion formalism for the unified description of XANES and EXAFS for 2D solid-state materials and apply it to the exemplary material graphene. For XANES we reproduce the experimentally observed absorption peaks and polarization-dependent selection rules of the included orbitals. Furthermore, the rigorous treatment of the Bloch theorem allows us to calculate the Fourier transformed EXAFS spectrum [2] predicting so far uninterpreted features which have not been assigned within scattering theory [1].

[1] Sayers, Dale E., et al., PRL 27 (1971): 1204

 $\left[2\right]$ Buades, Bárbara, et al., Optica 5 (2018): 502

[3] Chowdhury, M. T., R. Saito, and M. S. Dresselhaus, PRB 85 (2012): 115410.

DS 20.13 Wed 16:00 P3

Confinement induced coherent phonon softening in Sb2Te3 thin films — •JONATHAN FRANK<sup>1</sup>, JULIAN MERTENS<sup>1</sup>, FELIX HOFF<sup>1</sup>, MOHIT RAGHUWANSHI<sup>2</sup>, and MATTHIAS WUTTIG<sup>1</sup> — <sup>1</sup>1. Institute of Physics (IA), RWTH Aachen University, Aachen, Germany — <sup>2</sup>Forschungszentrum Jülich, Jülich, Germany

Femtosecond reflection-type optical pump-probe experiments on a thickness-series of MBE-grown Sb2Te3 thin films were carried out to study confinement effects of coherent optical phonons. Therefore, an isotropic detection scheme was applied to investigate the ultrafast dynamics of the LO-phonon mode of A1g-symmetry in Sb2Te3 thin films ranging from 1.3 to 55 nm. The ultrafast response of each thin film contains a distinct coherent feature uncovered by damped harmonic oscillations in the transient reflectivity traces. It is shown that coherent optical phonons are efficiently photoexcited in thin films of only a few quintuple layers. This finding supports the hypothesis that electronphonon coupling in ultrathin sesqui-chalcogenide films does not fundamentally differ from bulk which is essential for the performance in strongly scaled applications as for example in topological insulators. Furthermore, a slight decrease in phonon-frequency accompanied by a more pronounced decrease in phonon-lifetime is observed in films smaller than ten nanometers; both quantities nearly monotonously decrease with film thickness. We ascribe this phonon softening to a decreased interlayer coupling in films of a few quintuple layers compared to a more bulk-like behavior observed in the thicker films.

DS 20.14 Wed 16:00 P3

Characterization of layer systems by combination of X-ray reflectivity and hyperspectral imaging — •STEFFEN BIEDER<sup>1</sup>, FLORIAN GRUBER<sup>2</sup>, PATRICK SCHLENZ<sup>3</sup>, PHILLIPP WOLLMANN<sup>2</sup>, CHRISTIAN ALBERS<sup>1</sup>, SUSANNE DOGAN<sup>1</sup>, MICHAEL PAULUS<sup>1</sup>, NICOLA THIERING<sup>1</sup>, CHRISTIAN STERNEMANN<sup>1</sup>, and STEFFEN CORNELIUS<sup>3</sup> — <sup>1</sup>TU Dortmund, 44227 Dortmund, Germany — <sup>2</sup>Fraunhofer IWS, Winterbergstrasse 28, 01277 Dresden, Germany — <sup>3</sup>Fraunhofer FEP, Winterbergstrasse 28, 01277 Dresden, Germany

Different thin film multilayers consisting of indium tin oxide, zinc tin oxide and silver deposited on flexible PET foils were studied using Xray reflectivity and hyperspectral imaging aiming for an online quality control of the coatings' manufacturing process. The X-ray reflectivity data measured at beamline BL9 of the DELTA synchrotron radiation source provide detailed information on layer thickness with Angström resolution, roughness and electron density. These results are used to establish statistical models in order to analyze and interpret the data obtained from hyperspectral imaging. Latter is foreseen to be implemented into the foils' production line for in-situ detection of thickness changes during the production process.

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DS 20.15 Wed 16:00 P3

Surface second harmonic generation in dielectric nanofilms — •FATEMEH ALSADAT ABTAHI<sup>1</sup>, PALLABI PAUL<sup>1,2</sup>, SEBASTIAN BEER<sup>1</sup>, ADRIANA SZEGHALIMI<sup>1,2</sup>, STEFAN NOLTE<sup>1,2</sup>, and FALK EILENBERGER<sup>1,2,3</sup> — <sup>1</sup>Institute of Applied Physics, Friedrich-Schiller-University, Jena, Germany — <sup>2</sup>Fraunhofer-Institute for Applied Optics and Precision Engineering IOF, Jena, Germany — <sup>3</sup>Max Planck School of Photonics, Jena, Germany Second-harmonic generation (SHG) is a second-order nonlinear optical process that is not allowed in media with inversion symmetry. However, due to the broken symmetry at the surface, surface SHG can still occur in such materials. We experimentally investigate the surface SHG in the periodic stacks of ultrathin dielectric layers. Uniform, dense and optically homogeneous multilayer stacks of SiO2/TiO2were grown by Plasma Enhanced Atomic Layer Deposition (PEALD) on fused silica substrates. With this technique individual layers of a thickness of less than 2 nm can be fabricated, increasing the number of SHG-active surfaces substantially. Because of the material discontinuity, in each surface of this structure, the symmetry is broken and surface SHG will occur. By changing the Angle of Incidence (AOI) and having constructive interference between all fundamental/SHG signals from different surfaces, we are able to enhance the surface SHG. We experimentally show that under large angles of incidence > 20 degrees there is substantial SHG, well beyond the level, which can be expected for simple surfaces.

DS 20.16 Wed 16:00 P3

Surface-Enhanced Raman Spectroscopy and Transient Reflectivity of Strained LSMO Thin Films — •LEONARD SCHÜLER, TIM TITZE, STEFAN MATHIAS, DANIEL STEIL, and VASILY MOSH-NYAGA — I. Physikalisches Institut, Georg-August-Universität Göttingen

The effect of lattice strain on the structural and electronic surface reconstruction of epitaxial  $La_{0.7}Sr_{0.3}MnO_3/LaAlO_3$  (LSMO/LAO) thin films has been studied by surface-enhanced optical measurements. Surface sensitivity is achieved by deposition of gold nanoparticles, in which the localized surface plasmon resonance enhances laser electric fields at the surface, enabling surface-enhanced Raman spectroscopy (SERS) and pump-probe reflectivity (SE-PPR) studies of the LSMO films. For this system, SERS reveals a structural surface reconstruction and signals an insulating surface state characterized by strong Jahn-Teller modes which are not present in the conventional Raman spectra of the ferromagnetic metallic LSMO/LAO films. Furthermore, a structural transition of the insulating surface is shown at T\*=200-220 K possibly related to charge ordering (CO). SE-PPR indicates that it is possible to photoinduce a ferromagnetic metallic phase at the surface above the assumed CO transition temperature.

DS 20.17 Wed 16:00 P3 In-situ spectroscopic ellipsometry analysis of SiO2 on Si under different atmosphere and temperature — •XINYU ZHOU, YOUNES SLIMI, STEFAN KRISCHOK, and RÜDIGER SCHMIDT-GRUND — Technische Universität Ilmenau, Fachgebiet Technische Physik I, Weimarer Strafte 32, 98693 Ilmenau, Germany

In-situ Spectroscopic ellipsometry has been applied to obtain optical constants and thin film thicknesses of SiO2 on Si under different atmospheres (nitrogen, dry air) and temperatures. We found changes in refractive index and thickness of the SiO2 layer under different conditions due to oxidation and material ablation. We further present our recent developments in building up an in-situ ellipsometry system for photo-electrochemical applications.

DS 20.18 Wed 16:00 P3

Spectroscopic Ellipsometry of transition metal oxide thin films — ●NAHID AHMADIAN<sup>1,2</sup>, TERESA I. MADEIRA<sup>1,2</sup>, and DIET-RICH R.T. ZAHN<sup>1,2</sup> — <sup>1</sup>Chemnitz University of Technology, Chemnitz, Germany — <sup>2</sup>Center for Materials, Architectures and Integration of Nanomembranes (MAIN), D-09107, Chemnitz, Germany

Transition metal oxides such as  $HfO_2$  or  $TiO_2$  with bandgaps of 5.3-5.9 eV and 3.0-3.4 eV, are transparent in the visible range of the spectrum, i.e. their extinction coefficient in this range is very low close to zero while the refractive index varies as a function of photon energy. In this work, we tested four dispersion models: Sellmeier, Cauchy, extended Cauchy, and Tauc-Lorentz aiming at understanding the mathematical and physical differences of these approximations, their robustness and limitations in addressing amorphous and crystalline phases of thin films of  $HfO_2$  deposited by atomic layer deposition (ALD) on Si(100) and  $TiO_2$  thin films prepared on Si(100) by magnetron sputtering and spin coating. The spectroscopic ellipsometry measurements were performed using a M-2000 T-Solar from J.A. Woollam. Spectra covering a range of energies 0.7 (IR) -5 eV (UV) were taken in air at room temperature and analyzed using CompleteEASE. We conclude that multiple oscillators are required to treat the crystalline phases in comparison to the amorphous, and when very good solutions are obtained from all oscillators, the choice to use one or the other is based on complexity:

the less the fit parameters the best.

DS 20.19 Wed 16:00 P3 Reaction of Tetrapyrrole Thin Films with Alkali Metals — •LEONARD NEUHAUS<sup>1</sup>, STEFAN RENATO KACHEL<sup>1</sup>, PE-TER SCHWEYEN<sup>2</sup>, MARK HUTTER<sup>1</sup>, MAIK SCHÖNIGER<sup>1</sup>, FLORIAN MÜNSTER<sup>1</sup>, LUKAS RUPPENTHAL<sup>1</sup>, JAN HERRITSCH<sup>1</sup>, MARIE-IRENE ALBUS<sup>1</sup>, MARTIN BRÖRING<sup>2</sup>, and J. MICHAEL GOTTFRIED<sup>1</sup> — <sup>1</sup>Fachbereich Chemie, Philipps-Universität Marburg, Germany — <sup>2</sup>Institut für Anorganische und Analystische Chemie, Technische Universität Braunschweig, Germany

Tetrapyrroles such as porphyrins play an import role in living organism and for various modern technologies. While most previous publications related to tetrapyrrole thin films focus on transition metal complexes, we want to expand the field by exploring the reaction of various tetrapyrrole films with alkali metals. For this purpose, we prepared multilayer films of tetraphenylporphyrin and an octaalkylcorrol on a Au(111) surface and studied their reactions with Li and Cs, thus covering the extremes of the lightest and heaviest stable alkali metal. For all studied systems, X-ray photoelectron spectroscopy (XPS) showed, changes in the N 1s region that indicate formation of the corresponding tetrapyrrole metal complexes. Complementary studies with temperature programmed reaction (TPR) provided unambiguous mass spectrometric evidence for the formation of the metal complexes. TPR also showed that the number of alkali metal atoms attached to a tetrapyrrole ligand can exceed the number of pyrrolic hydrogen atoms in the free-base tetrapyrrole.

DS 20.20 Wed 16:00 P3 Thermoelectric Characterization of Polymer Thin Films with Ag-nanowire Additives —  $\bullet$ Sohraab Scherzad<sup>1</sup>, Marie SIEGERT<sup>1</sup>, and JENS PFLAUM<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, University of Würzburg, 97074 Würzburg — <sup>2</sup>ZAE Bayern, 97074 Würzburg Along the process of power conversion from primary energy carriers vast amounts of waste heat in the low and mid temperature range occur. A possible solution to recover this waste heat is offered by thermoelectric generators which rely on the Seebeck effect and are able to directly convert thermal into electrical energy. Polymeric semiconductors, operating in this temperature regime, offer a sustainable and low-cost alternative to inorganic thermoelectrics. Their characteristics include a sufficiently low thermal conductivity  $\kappa$ , but also a low electrical conductivity  $\sigma$ , due to the low charge carrier concentration and generic disorder. Here we report on composite thin films made of Agnanowires embedded in PEDOT:PSS polymer matrices, which lead to changes in the electrical conductivity compared to pure PEDOT:PSS. Ag-nanowires are considered to be a suitable additive for increasing  $\sigma$  of the resulting composite and its impact on  $\kappa$  will also be studied. First results on the thermoelectric properties of this material combination will be presented together with structural information obtained by X-ray diffraction and atomic force microscopy. Based on this complementary information we will critically discuss the potential of the presented approach for application in TEGs.

#### DS 20.21 Wed 16:00 P3

Plasmonic-induced Thermoelectric Effects in Metal-organic Hybridstructures — •Lucca Macher<sup>1</sup>, Paul Hoppstock<sup>1</sup>, Max-IMILIAN FRANK<sup>1</sup>, MAXIMILIAN RÖDEL<sup>1</sup>, and JENS PFLAUM<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, University of Würzburg, 97074 Würzburg — <sup>2</sup>Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Local heat generation by plasmonic excitations in noble metal nanoparticles is of high technological interest for numerous applications such as photo-thermal chemistry or cancer therapy. In this work we utilize this approach to create a thermal gradient by the absorption of light in metal-organic hybrid structures. The latter are based on arrays of nanostructured gold and silver triangles in combination with solution processed p-type PEDOT:PSS films. As we can demonstrate, a defined temperature enhancement and thus, gradient evolves upon resonantly exciting local plasmons in the Au or Ag nanoparticle arrays. The amplitude of this enhancement amounts to  $\Delta T = 0.5$  K for an incident light power of 1.4 mW/mm<sup>2</sup>. Accordingly, this plasmon-induced temperature gradient which is aligned along the PEDOT:PSS polymer layers results in a significant enhancement of the thermovoltage to  $V_T = 24 \,\mu\text{V/K}$  as compared to neat PEDOT:PSS ( $V_T = 12 \,\mu\text{V/K}$ ). An application-oriented approach was carried out as well, using arrays of nanostructured gold triangles covered by a transparent polymer-gel electrolyte PEGMA/BEMA in a window-like device architecture. A temperature gradient of  $\Delta T=0.1~{\rm K}$  for an incident light power of 1.8  $\rm mW/mm^2$  was determined along the PEGMA/BEMA layer.

DS 20.22 Wed 16:00 P3

Self-assembled monolayers of molecular spin-crossover (SCO) switches — •FABIAN STRELLER<sup>1</sup>, STEPHEN GOODNER<sup>2</sup>, MARAT KHUSNIYAROV<sup>2</sup>, and RAINER FINK<sup>1</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II, Friedrich Alexander Universität Erlangen Nürnberg, Germany — <sup>2</sup>Lehrstuhl für Anorganische und Allgemeine Chemie, Friedrich Alexander Universität Erlangen Nürnberg, Germany

Spin-crossover (SCO) complexes are regarded as promising materials in applications such as spintronics, molecular electronics and ultra-highdensity memory systems. They can be switched by external stimuli, e.g., change of temperature, pressure, or illumination with light. In the investigated complexes switching occurs between diamagnetic lowspin (LS) and paramagnetic high-spin (HS) species by either a simple SCO, or a valence tautomeric (VT) transition accompanied by a SCO. While the mentioned applications seem promising, one big challenge that needs to be overcome is the transfer of the systems from solution or bulk towards thin films or even monolayers on well-defined surfaces. Six-coordinate iron(II) complexes have been used as SCO materials, whereas six-coordinate Co complexes with redox active dioxolene ligands were chosen as VT materials. Both materials can be attached to the surface via a bidental phenanthroline ligand containing mojeties suitable for bonding to the substrate. Here we report a step by step formation of single-layer films on Au(111) surfaces. The thus created specimens were characterized by atomic force microscopy (AFM), xray photoelectron spectroscopy (XPS) and near edge x-ray absorption fine structure (NEXAFS).

DS 20.23 Wed 16:00 P3 Chern number control in quantum anomalous Hall insulators by external fields — •YURIKO BABA<sup>1,2</sup>, FRANCISCO DOMÍNGUEZ-ADAME<sup>1</sup>, and RAFAEL A. MOLINA-FERÁNDEZ<sup>2</sup> — <sup>1</sup>GISC, Departamento de Física de Materiales, Universidad Complutense, E–28040 Madrid, Spain — <sup>2</sup>Instituto de Estructura de la Materia, IEM-CSIC, E–28006 Madrid, Spain

Topological magnetic insulators have been discovered as a new platform for observing Quantum Anomalous Hall states with high Chern number C. In three-dimensional structures of stacking layers of magnetically doped and undoped topological insulators of Bi2(Se,Te)3, the number of chiral edge channels can be controlled by the width and number of layers and by the doping concentration. This has been recently measured by Zhao et al. [1] in Cr doped samples, showing this feature up to C = 5.

In this theoretical work, we explore the possibilities of tuning the chiral channels of the aforementioned materials in the presence of electric fields in multilayered structures. The external field tunes the Chern number and changes the number of topological channels dynamically without the need of replacing the sample to modify the Chern number. The tuneability has a remarkable impact on the transport properties of pristine and disordered samples.

[1] Zhao, Y. F. et al., Nature, 588 (2020) 419

DS 20.24 Wed 16:00 P3

topological magnons and thermal hall conductivity in 2D magnets — •HAMID NOURI and HONGBIN ZHANG — Technical University of Darmstadt, 64287 Darmstadt, Germany

Two-dimensional (2D) materials provide a fascinating playground for emergent phenomena driven by enhanced thermal and quantum fluctuations, in particular the nontrivial topological phases with the associated dissipationless transport properties. For 2D magnetic insulators, magnons can also host Dirac and Weyl points with nonzero Berry curvature, leading to finite thermal Hall conductivities. In this work, based on the linear response spin-wave theory, we investigated a Hamiltonian formulated on 2D lattices comprising the Heisenberg exchange, Dzyaloshinskii-Moriya interaction (DMI) interactions, singleion anisotropy, external magnetic fields, and found that the gapped magnon bands exhibit nonzero Chern numbers of \*1 due to finite DMI which acts like effective spin-orbit coupling. The thermal Hall conductivity is evaluated based on the Boltzmann transport theory, suggesting a novel approach to designing 2D thermal management materials. The realization of such Hamiltonians in experimentally available 2D materials will be discussed as well.

DS 20.25 Wed 16:00 P3 Bottom-up preparation of large area van-der-Waals het-

Wednesday

erostructures by the subsequent growth of 2D transition metal dichalcogenides layers — •DEVENDRA PAREEK<sup>1</sup>, MARCO A. GONZALEZ<sup>1</sup>, NEDAL GREWO<sup>1</sup>, MARTEN L. JANSSEN<sup>1</sup>, LEON A. GRÄPER<sup>1</sup>, KUMARAHGIRI ARUNAKIRI<sup>1</sup>, KAYODE. L. ALIMI<sup>1</sup>, MARTIN SILIES<sup>1,2</sup>, JÜRGEN PARISI<sup>1</sup>, LEVENT GÜTAY<sup>1</sup>, and SASCHA SCHÄFER<sup>1</sup> — <sup>1</sup>Ultrafast Nanoscale Dynamics, Institute of Physics, Carl von Ossietzky University of Oldenburg, Oldenburg, Germany — <sup>2</sup>Institute for Lasers and Optics, University of Applied Sciences Emden/Leer, Emden, Germany

We report the preparation of as-grown two-dimensional transition metal dichalcogenides (2D-TMDC) heterostructures from a processing route employing a combination of atomic layer deposition of monolayer MoS<sub>2</sub> and solution-based processing of ultrathin Mo(S/Se)<sub>2</sub> and W(S/Se)<sub>2</sub> films. Grown on centimeter-scale sapphire substrates, spatially uniform optoelectronic characteristics of the individual TMDC layers and heterostructures are demonstrated down to micrometer length scales using photoluminescence, Raman spectroscopy, and light-beam-induced current measurements. Preliminary observations on enhanced photogenerated currents in MoS<sub>2</sub>-MoS<sub>2</sub>/WS<sub>2</sub> lateral heterostructures demonstrate the suitability of this approach for the preparation of functional devices on macroscopic length scales. Finally, we also discuss the possibilities to synthesize these compounds at temperatures below 400 °C, making them suitable for a broad range of substrate materials.

DS 20.26 Wed 16:00 P3 Twist-angle dependent proximity induced spin-orbit coupling in graphene/transition-metal dichalcogenide and graphene/topological insulator heterostructures — •THOMAS NAIMER<sup>1</sup>, KLAUS ZOLLNER<sup>1</sup>, MARTIN GMITRA<sup>2</sup>, and JAROSLAV FABIAN<sup>1</sup> — <sup>1</sup>Uni Regensburg, Regensburg, Germany — <sup>2</sup>Pavol Jozef Šafárik University, Košice, Slovakia

We investigate the proximity-induced spin-orbit coupling in twisted heterostructures of graphene/transition-metal dichalcogenides ( $MoS_2$ ,  $WS_2$ ,  $MoSe_2$ , and  $WSe_2$ ) as well as graphene/topological insulators ( $Bi_2Se_3$  and  $Bi_2Te_3$ ) from first principles. To correct for strain induced band offsets, we apply a perpendicular electric field. The resulting corrected band structure is then fitted around the Dirac point to an established spin-orbit Hamiltonian, yielding the twist angle dependencies of the (Rashba and valley-Zeeman) spin-orbit coupling. This work was funded by the Elite Network of Bavaria, the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), SFB 1277, SPP 2244 and by the European Union Horizon 2020 Research and Innovation Program under contract number 881603 (Graphene Flagship). M.G. acknowledges VEGA 1/0105/20.

### DS 20.27 Wed 16:00 P3

Valley depolarization of excitons in encapsulated MoSe<sub>2</sub>-WSe<sub>2</sub> heterostructures with controlled moiré potentials — •ANDREAS BEER<sup>1</sup>, ANNA WEINDL<sup>1</sup>, NICLAS MAIER<sup>1</sup>, ANTONY GEORGE<sup>2</sup>, ANDREY TURCHANIN<sup>2</sup>, and CHRISTIAN SCHÜLLER<sup>1</sup> — <sup>1</sup>Universität Regensburg — <sup>2</sup>Friedrich-Schiller-Universität Jena

Our focus is the investigation of the temporal and spatial dynamics of interlayer excitons in MoSe<sub>2</sub>-WSe<sub>2</sub> heterostructures with well-defined moiré potentials, based on CVD grown samples. The so called hot pickup method enables us to fabricate such heterostructures out of CVD grown triangulars in a controlled, dry, PDMS-free and easy way.

To understand the valley depolarization mechanism in TMDC monolayers and heterostructures we perform time resolved pump probe measurement. First measurements on twisted TMDC exfoliated heterostructures reveal twist-angle-dependent decay times of the interlayer exciton.

### DS 20.28 Wed 16:00 P3

Protection of QSHI indenene from air via intercalation — •CEDRIC SCHMITT<sup>1,2</sup>, JONAS ERHARDT<sup>1,2</sup>, SIMON MOSER<sup>1,2</sup>, and RALPH CLAESSEN<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — <sup>2</sup>Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany

In the search for new quantum materials, ultrathin metals are interesting as they push bulk properties to the 2D limit and foster novel quantum effects. Unfortunately, these systems are prone to oxidation in air, making them useless for quantum transport devices. Metal intercalation is a relatively new capping method, that utilizes graphene, an inert quantum material that can be easily produced by heating of a SiC substrate [1,2]. Hereby, the metal is intercalated between the SiC/graphene layer, thus forming freestanding graphene, which is believed to protect the intercalated layers against oxidation [3]. Hitherto studies focused mainly on identifying stable allotropes but lacking a detailed investigation of metal coverage and oxidation [3]. Here, we study the intercalation of indenene, a recently discovered QSHI on a triangular lattice [4]. First experiments indicate the indium layer to remain intact upon air exposure, indeed pointing to an effective protective function of the overlayer graphene.

[1] K. S. Novoselov et. al. Science 306, 666 (2004)

- [2] C. Berger et. al. J. Phys. Chem. B 108, 19912 (2004)
- [3] N. Briggs et al. Nat. Mater. 19, 637-643 (2020)
- [4] M. Bauernfeind et al. Nat. Commun. 12, 5396 (2021)

DS 20.29 Wed 16:00 P3

Electronic Structure of  $[(SnSe)_{1+\delta}]_m(TiSe_2)_n$  investigated by Photoelectron Spectroscopy — •NIELS RÖSCH<sup>1</sup>, FABIAN GÖHLER<sup>1</sup>, DANIELLE M. HAMANN<sup>2</sup>, DAVID C. JOHNSON<sup>2</sup>, and THOMAS SEYLLER<sup>1</sup> — <sup>1</sup>Technische Universität Chemnitz, Institut für Physik, 09126 Chemnitz — <sup>2</sup>University of Oregon, Department of Chemistry, Eugene OR 97401

The Modulated Elemental Reactants (MER) synthesis is a new method for producing multilayer heterostructures. A precursor is created in MER by using consecutive physical vapour deposition. The precursor's structure and composition can be deliberately changed to mimic the desired heterostructure. After that, the precursor is crystallized by annealing it at low temperatures in an inert environment. Low temperatures allow thermodynamically metastable films to form, albeit at the cost of turbostratic rotational disorder between layers. By systematically modifying the stacking sequence of individual layers, this approach can be used to create a succession of layered heterostructures.

X-ray photoelectron spectroscopy was used to investigate the electrical structure of a sequence of  $[(SnSe)_{1+\delta}]_m(TiSe_2)_n$  heterostructures [1]. It is demonstrated that electrons are transferred from the SnSe layers to the TiSe<sub>2</sub> layers. Understanding charge transfer in heterostructures is important for future applications, as controlled stacking of the heterostructure may allow for targeted doping.

[1] Göhler, F., Hamann, D. M., Rösch, N., et al., J. Mater. Res. 34 (12): (2019)

### DS 20.30 Wed 16:00 P3

Atomistic Simulations of Defects Production Under Ion Irradiation in Epitaxial Graphene on SiC — •MITISHA JAIN<sup>1</sup>, SILVAN KRETSCHMER<sup>1</sup>, KATJA HÖFLICH<sup>2,3</sup>, JOAO MARCELO J. LOPES<sup>4</sup>, and ARKADY KRASHENINNIKOV<sup>1</sup> — <sup>1</sup>Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — <sup>2</sup>Ferdinand-Braun Institut gGmbH, Leibniz-Institut für Höchstfrequenztechnik, Berlin, Germany — <sup>3</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — <sup>4</sup>Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany

In this work, using atomistic simulations at the analytical potential and density-functional theory (DFT) levels, we theoretically study defect production in EG on SiC by ion beams (He and Ne ions). We explicitly consider the effects of the substrate (bulk SiC) on the response of graphene to irradiation. Since the substrate affects the number of displaced carbon atoms and vacancy types in EG, we present information about the number, types and location of defects produced in each layer of EG to guide the experiment in tailoring the defect production. Motivated by the He FIB experiments (aiming at nucleation sites of h-BN growth, operating at 30 keV), our considerations apply to the typical ion energies used in HIM, that is 10-30 keV.

### DS 20.31 Wed 16:00 P3

Low energy ion induced effects on core-shell nano particles — •JULIAN LISSON, SHIVA CHOUPANIAN, and CARSTEN RONNING — Institute of Solid State Physics, Friedrich Schiller University Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Ion irradiation can be used for manipulating the shape and properties of nanomaterials. However, the comportment of nano materials irradiated with energetic ions differs from bulk and thin films due to the mesoscopic properties of nanoparticles. The succeeding effects such as sputtering and ion beam mixing are strongly coupled and are dependent on the properties of the irradiated target. In this study, the effect of Ga+ ions with an energy range of 10-30 keV on different nanomaterials of Au, Ag, Au-Ag mix, and core-shell nanoparticles dispersed on Si substrates has been investigated. The sputter yield for each nanomaterial has been measured. Comparing the sputter yield and morphology changes of the nanoparticles, we observe that the ion beam mixing at the interface of the Au-Ag core-shell nano particles is prominent. The sputter yield dependence is changing when ion beam mixing is occurring and leads to dissimilar morphology changes of the core-shell nanoparticles due to preferential sputtering.

## DS 20.32 Wed 16:00 P3

Lattice dynamics in tuneable thin films with Ruddlesden-Popper structure — •VERONICA GOIAN<sup>1</sup>, NATALIE DAWLEY<sup>2</sup>, JING-SHU ZHANG<sup>2</sup>, CHRISTELLE KADLEC<sup>1</sup>, NATHAN D. ORLOFF<sup>3</sup>, REIN-HARD UECKER<sup>4</sup>, STEFFEN GANSCHOW<sup>4</sup>, DARRELL G. SCHLOM<sup>2,5</sup>, and STANISLAV KAMBA<sup>1</sup> — <sup>1</sup>Institute of Physics ASCR, Prague, Czech Republic — <sup>2</sup>Department of Materials Science and Engineering, Cornell University, Ithaca, NY, USA — <sup>3</sup>National Institute of Standards and Technology, Boulder, CO, USA — <sup>4</sup>Leibniz-Institut für Kristallzüchtung, Berlin, Germany — <sup>5</sup>Kavli Institute at Cornell for Nanoscale Science, Ithaca, NY, USA

In this work, we will compare the phonon dynamics of  $(SrTiO_3)_6SrO$ (SrRP6) thin film with  $(SrTiO_3)_5(BaTiO_3)_1SrO$  (BaRP6) and Sr<sub>5/6</sub>Ba<sub>1/6</sub>TiO<sub>3</sub> (SBT) thin films, all deposited on (110)DyScO<sub>3</sub> substrates. The XRD measurements and the rocking curves prove the thin films are single phase and epitaxially grown on the substrates. The lattice dynamics of the thin films were determined using THz and IR spectroscopies down to 10 K. Many phonons exhibit anomalies near temperatures of the ferroelectric phase transitions. We found out that the 100 nm BaRP6 and SBT thin films, which is due to slightly relaxed strain in the thin films. We will also compare the temperature behavior of the complex permittivity of BaRP6 and SBT thin films with behavior of Ba<sub>x</sub>Sr<sub>1-x</sub>TiO<sub>3</sub> (x=0.1..0.6) ceramics and will discuss the reason for high tuneability of permittivity and low dielectric loss in strained thin films.

#### DS 20.33 Wed 16:00 P3

Stabilized ferromagnetism in LPCMO thin films by using buffer layers —  $\bullet$ PIA HENNING<sup>1</sup>, KAREN STROH<sup>1</sup>, VI-TALY BRUCHMANN-BAMBERG<sup>1</sup>, OLEG SHAPOVAL<sup>2</sup>, and VASILY MOSHNYAGA<sup>1</sup> — <sup>1</sup>Erstes Physikalisches Institut, Georg-August-Universitat-Göttingen, Gottingen, Germany — <sup>2</sup>IIEN, Academy of Sciences of Republic Moldova, Chisinau, Republic of Moldova

 $(La_{0.6}Pr_{0.4})_{0.7}Ca_{0.3}MnO_3$  (LPCMO) is an A-site substituted perovskite manganite and is mostly known for the colossal magnetoresistance (CMR) effect. Relatively thick LPCMO films ( $d \approx 50 - 100$  nm) with a coupled ferro-to-paramagnet and a metal-to-insulator transition (MIT) and CMR can be heteroepitaxially grown on MgO(200) substrates, where a relaxed growth due to misfit dislocations is achieved. However, very thin LPCMO films with  $d \lesssim 20$  nm on MgO(200) do not show a MIT and CMR. On the alternative substrate SrTiO<sub>3</sub> (100), LPCMO grows coherently strained and with good surface morphology, but lacks an MIT and CMR even for  $d \lesssim 50$  nm.

To enable high-quality LPCMO thin film growth on  $SrTiO_3$  substrates, the introduction of a buffer layer to bridge the lattice mismatch of film and substrate is inevitable. Based on this, we investigate the growth of LaAlO<sub>3</sub> (LAO) buffer layers on  $SrTiO_3$  and the influence of LAO buffer layers on the growth of LPCMO in order to improve the magnetic and electric properties. Specifically, the interplay of buffer and film thickness is studied. It is demonstrated the possibility of high quality thin film growth of LPCMO on buffered STO and a stabilization of the ferromagnetic-metallic phase.

## DS 20.34 Wed 16:00 P3

Electronic Reconstruction and Anomalous Hall Effect at the LaAlO<sub>3</sub>/SrRuO<sub>3</sub> Interface — •MERIT SPRING<sup>1</sup>, JI SOO LIM<sup>1</sup>, MARTIN KAMP<sup>1</sup>, LOUIS VEYRAT<sup>2</sup>, PAVEL POTAPOV<sup>2</sup>, AXEL LUBK<sup>2</sup>, BERND BÜCHNER<sup>2</sup>, MICHAEL SING<sup>1</sup>, and RALPH CLAESSEN<sup>1</sup> — <sup>1</sup>Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, 97074 Würzburg, Germany — <sup>2</sup>Leibniz Institute for Solid State and Materials Research and Würzburg-Dresden Cluster of Excellence ct.qmat, 01069 Dresden, Germany

4d and 5d transition metal oxides are a promising class of materials for topological phases in the context of electron correlations. Recently, the ferromagnetic metal  $SrRuO_3$  (SRO) grown on a  $SrTiO_3$  (STO) (001) substrate has been reported to exhibit electronic-reconstruction induced interfacial charge pinning accompanied by a topological transition of its electronic bands when capped with a LaAlO<sub>3</sub> (LAO) layer [1]. LAO is a polar oxide and the electronic reconstruction in a heterosystem of LAO/STO caused by the polar discontinuity at the interface is well known. For the LAO/SRO system a similar behaviour is expected and charge is thought to be accumulated at the very interface giving rise to strong inversion-symmetry breaking and hence change in the momentum-space topology [1]. Here we show the observation of signatures of an anomalous Hall effect in 4uc SRO films capped with LAO but also with non-polar STO. We correlate these findings with angle-dependent XPS data that allow for depth-profiling the oxidation state of ruthenium in both systems.

[1] Thiel, T. C. et al., Phys. Rev. Lett. 127, 127202 (2021)

DS 20.35 Wed 16:00 P3 Epitaxial growth of IrO2(110) thin films on TiO2(110) substrates by pulsed-laser-deposition — •Tim Waldsauer<sup>1</sup>, Philipp Kessler<sup>1</sup>, Theodore Pellegrin<sup>1</sup>, Christopher Reiser<sup>1</sup>, Ralph Claessen<sup>1</sup>, Vedran Jovic<sup>2</sup>, and Simon Moser<sup>1</sup> — <sup>1</sup>JMU Physikalisches Institut, am Hubland, Würzburg, Germany — <sup>2</sup>GNS National Isotope Center, Gracefield Rdd, Gracefield, New Zealand

Iridium dioxide (IrO2), a state-of-the-art catalyst for the electrocatalytic oxygen evolution reaction in water splitting, has recently been shown to exhibit exotic physical phenomena such as the inverse spin Hall effect. The latter is supposed to promote easy switching of its majority charge carriers. For both fundamental spectroscopic studies as well as device applications, IrO2 samples of high bulk and surface crystalline order are required. Here, we present a growth study of rutile IrO2(110) thin films on TiO2(110) substrates by pulsed-laserdeposition (PLD). Film characterization by AFM, RHEED and XPS shows stochiometric growth of thin films with high bulk crystallinity but a granular surface at higher thicknesses. Strategies to enhance the surface quality, e.g., through utilization of an oxygen plasma are outlined and first results are presented.

DS 20.36 Wed 16:00 P3

**2D** electronic states at  $Fe_xO_y/STO$  interfaces — •PIA M. DÜRING<sup>1</sup>, PAUL ROSENBERGER<sup>1,2</sup>, LUTZ BAUMGARTEN<sup>3</sup>, FATIMA ALARAB<sup>4</sup>, FRANK LECHERMANN<sup>5</sup>, VLADIMIR N. STROCOV<sup>4</sup>, and MARTINA MÜLLER<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — <sup>2</sup>Fakultät Physik, Technische Universität Dortmund, 44221 Dortmund, Germany — <sup>3</sup>FZ Jülich GmbH, PGI-6, 52425 Jülich, Germany — <sup>4</sup>PSI, Swiss Light Source, CH-5232 Villingen PSI, Switzerland — <sup>5</sup>Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany

Oxide interfaces play an important role in investigating phenomena like 2D electronic states which can feature properties like magnetism, superconductivity or the spin Hall effect. While 2DEGs have been reported for various oxide systems like LAO/STO or EuO/STO, the direct experimental evidence for the counterpart, the 2DHG, is still lacking. Using our UHV-MBE system, we grow high-quality oxide heterostructures to investigate these properties using synchrotron radiation. Here presented are the results of resonant photoelectron spectroscopy measurements that reveal the emergence of different 2DESs at FexOy/STO interfaces which suggests a dependence of the 2D interface properties on the oxidation state of Fe.

#### DS 20.37 Wed 16:00 P3

Stabilization of ferromagnetic metallic ground state in epitaxial  $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$  /SrTiO<sub>3</sub> thin films by using buffer layers — •PIA HENNING<sup>1</sup>, KAREN STROH<sup>1</sup>, VITALY BRUCHMANN-BAMBERG<sup>1</sup>, OLEG SHAPOVAL<sup>2</sup>, and VASILY MOSHNYAGA<sup>1</sup> — <sup>1</sup>Erstes Physikalisches Institut, Georg-August-Universitat-Göttingen, Gottingen, Germany — <sup>2</sup>IIEN, Academy of Sciences of Republic Moldova, Chisinau, Republic of Moldova

 $({\rm La}_{1-y}{\rm Pr}_y)_{0.7}{\rm Ca}_{0.3}{\rm MnO}_3$  (LPCMO) is an A-site substituted perovskite manganite, mostly known for the colossal magnetoresistance (CMR) effect. Relatively thick, d=50-100 nm, and stress-free LPCMO films with coupled ferro/paramagnetic and metal/insulator transition (MIT) and CMR  $\sim 10^4\%$  can be heteroepitaxially grown by the metalorganic aerosol deposition technique on MgO(200) substrates, where strain relief occurs due to misfit dislocations. However, thin LPCMO films  $d{<}20$  nm on MgO(200) do not show MIT and CMR. Alternatively, LPCMO/SrTiO3 (LPCMO/STO) films grow coherently strained and with smooth surface morphology, however lacking the MIT and CMR even for  $d{>}50$  nm. To obtain epitaxial LPCMO films with optimal metal-insulator transition sharpness and temperature we have employed a strain-engineered LaAlO<sub>3</sub> buffer layer to bridge the lattice mismatch of the LPCMO film and SrTiO<sub>3</sub>(100) substrate. The influence of LaAlO<sub>3</sub> buffers on the magnetic and electric properties of epitaxial LPCMO films was studied. A high-quality growth of LPCMO/LAO/STO films and stabilization of the ferromagnetic-metallic phase for 10 nm thick LPCMO films were demonstrated.

 $\bullet \mathrm{Christian}$  Teichrib and Matthias Wuttig — I. Physikalisches Institut (IA)

Metal-insulator transitions describe the localisation of charge carriers upon the change of a physical parameter. They can occur as a result of electron correlations (Mott transition) or disorder (Anderson transition) but a distinction between these two mechanisms is generally difficult and often both effects play a role in the transition. Phase change materials show a multitude of remarkable properties that make them suitable for the investigation of localisation phenomena. Their density of states at the Fermi level can be varied through chemical composition and disorder can be tuned through thermal annealing. This allows for the electrical resistivity to be modified over several orders of magnitude and a transition from a metallic to an insulating state to occur.

We present electrical transport and structural data for  $\operatorname{AgSb}_{1-x}\operatorname{Sn}_x\operatorname{Te}_2$  alloys where a metal-insulator transition is observed upon variation of the stoichiometry. The nature of the transition is investigated using the temperature dependence of the resistivity, magnetoresistance data, and the Hall effect.

DS 20.39 Wed 16:00 P3

Cryogenic Transport And Dielectric Properties Of Atomically Thin 2D-Polar Metals — •Sven Bökemeier<sup>1</sup>, Pierre-Maurice Piel<sup>1</sup>, Jakob Henz<sup>1</sup>, Margaux Lassunière<sup>1</sup>, Joshua Robinson<sup>2</sup>, Siavash Rajabpour<sup>2</sup>, Alexander Vera<sup>2</sup> und Ursula Wurstbauer<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, — <sup>2</sup>MatSE; Center for 2DLM; Atomic; 2D Crystal Consort, PennState University, USA

2D layered materials are of great interest due to their electronic and optical properties that can be manipulated to a high degree. A novel class of atomically thin materials are 2D polar metals such as 2D Ga or 2D In and their ternary alloys that exhibit fascinating properties like strong nonlinear optical properties emerging by giant second harmonic generation [1], epsilon near zero behavior in the visible and NIR range [2] and alloy dependent superconductivity [3]. Intriguingly, 2D Ga exhibits a superconducting phase transition around 4K, while 2D In remains a metal down to < 800mK [3]. The 2D polar metals are prepared via confinement hetero-epitaxy (CHet) by intercalating metals between epitaxial graphene and the hosting SiC crystal resulting in atomically thin half-van der Waals materials [1]. We report on combined temperature dependent transport and spectroscopic ellipsometry experiments in order to a develop a better understanding of the alloy dependent emerging superconductivity of thin 2D Ga and 2D GaIn films. [1] M. A. Steves et al. Nano Lett. 2020, 20, 11, 8312\*8318. [2] K. Nisi et al. Adv. Mater. 2021, 2104265 [3] S. Rajabpour et al. Adv. Funct. Mater. 2020, 2005977

## DS 20.40 Wed 16:00 P3

Magnetic Field-Dependent Thermal Conductivity in Manganite Thin Films — •VITALY BRUCHMANN-BAMBERG, KAREN STROH, PIA HENNING, and VASILY MOSHNYAGA — I. Physik. Inst. Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

In perovskite manganites strong electron-phonon and spin-phonon coupling give rise to intriguing magneto-electric phenomena like colossal magnetoresistance (CMR), i.e. reduction of electrical resistivity by several orders of magnitude in an applied magnetic field of few Tesla. Since thermal conductivity of a solid contains both lattice and electronic contributions, a question of its manipulation by an external magnetic field can be addressed in CMR manganites.

Here we present temperature- and magnetic-field-dependent measurements of thermal conductivity by means of  $3\omega$ -technique in  $(La_{0.6}Pr_{0.4})_{0.7}Ca_{0.3}MnO_3/MgO(100)$  thin films with a CMR ratio of  $[R(0T)-R(5T)]/R(5T)\approx 10^4\%$ . The observed significant change of the thermal conductivity,  $\kappa$ , in magnetic field  $[\kappa(5T)-\kappa(0T)]/\kappa(0T) = 16\%$  close to  $T_C \approx 200$ K is caused by the electronic contribution in agreement with the Wiedemann-Franz law.

DS 20.41 Wed 16:00 P3 Phonon-dominated energy transport in purely metallic thin films — •Marc Herzog<sup>1</sup>, Alexander von Reppert<sup>1</sup>, JanETIENNE PUDELL<sup>1,2</sup>, CARSTEN HENKEL<sup>1</sup>, MATTHIAS KRONSEDER<sup>3</sup>, CHRISTIAN BACK<sup>3,4</sup>, ALEXEI MAZNEV<sup>5</sup>, and MATIAS BARGHEER<sup>1,6</sup> — <sup>1</sup>Inst. f. Physik & Astronomie, Universität Potsdam, Germany — <sup>2</sup>European XFEL, Schenfeld, Hamburg, Germany — <sup>3</sup>Inst. f. Experimentelle & Angewandte Physik, Universität Regensburg, Germany — <sup>4</sup>Fakultät f. Physik, Technische Universität München, Germany — <sup>5</sup>Departent of Chemistry, MIT, Cambridge, USA — <sup>6</sup>Helmholtz-Zentrum Berlin, Germany

In various branches of physical sciences it is assumed that electrons are the main carriers of thermal energy in metals. We use ultrafast x-ray diffraction to quantify the energy exchange among the metallic constituents in nanoscale thin films after laser excitation. Modeling the data with two-temperature models describing the energy exchange between non-equilibrium electrons and phonons provides clear evidence that phonons dominate the heat transport within gold films thinner than approx. 10 nm. Our fundamental experimental findings shifts the paradigm of energy being solely transported by electron in noble metals. These results may be relevant for the description of nonequilibrium thermal transport in diverse fields ranging from thermal management in nanoelectronics, spin-caloritronics and ultrafast spin dynamics to photothermal processes and plasmonic chemistry.

> DS 20.42 Wed 16:00 P3 of Pb<sub>1</sub> SpuSe Films with Sputter

Combinatorial Synthesis of Pb<sub>1-x</sub>Sn<sub>x</sub>Se Films with Sputter Deposition — •THOMAS SCHMIDT, PETER KERRES, and MATTHIAS WUTTIG — RWTH Aachen University, Aachen, Germany

PbSe and SnSe are two chalcogenides with a wide range of applications of their properties, in particular as thermoelectrics. Interestingly, these two iso-electronic materials employ different bonding mechanisms. While at room temperature SnSe utilizes covalent bonds, PbSe is characterized by a more unconventional bonding mechanism, coined metavalent bonding. Therefore, we expect significant property changes upon crossing the border between those two bonding mechanisms. Such a change opens up the possibility to tailor material properties with sample stoichiometry. We have thus studied optical and electrical properties of  $Pb_{1-x}Sn_xSe$  films as a function of stoichiometry. Effective sample-production has been employed to facilitate this analysis. In this study the compositions around x=0.5, at which a structural transition is expected, are confocally sputtered and subsequently analyzed. The two targets PbSe (cubic structure) and SnSe (orthorhombic structure) were focused on the different ends of the 7.5 cm long Si-substrate. The resulting stoichiometry gradient in the sample was determined by energy dispersive X-ray spectroscopy and linked to the evolution of structure (X-ray diffraction) and optical properties (spectroscopic ellipsometry and reflectometry).

DS 20.43 Wed 16:00 P3 Growth of Crystalline High-Entropy Alloy thin Films by Magnetron Sputtering — •HOLGER SCHWARZ<sup>1</sup>, THOMAS UHLIG<sup>2</sup>, ERIC WONG<sup>1</sup>, PETER HENNING<sup>1</sup>, GUNTRAM WAGNER<sup>2</sup>, and THOMAS SEYLLER<sup>1</sup> — <sup>1</sup>Institute of Physics, Faculty of Natural Sciences, TU Chemnitz, 09126 Chemnitz, Germany — <sup>2</sup>Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, TU Chemnitz, 09126 Chemnitz, Germany

Multicomponent alloys of at least four elements with near equimolar percentage were first reported and investigated by Cantor et al. in 2004 [1] and are nowadays often referred to as High-Entropy Alloys (HEAs) [2]. This group of materials has raised high attention in the field of material research due to its almost infinite possibilities of element combination and resulting physical properties. We demonstrate the fabrication of crystalline HEA thin films on MgO(100) and  $Al_2O_3(0001)$  single crystal substrates from homemade targets via magnetron sputtering. Low electron energy diffraction and X-ray diffraction experiments confirmed the formation of single phase crystalline HEA films. The surface elemental composition is investigated by Xray photoelectron spectroscopy whereas the bulk stoichiometry is measured by energy dispersive X-ray spectroscopy. Angle resolved photoemission spectroscopy was used to investigate the band structure of the thin films.

 B. Cantor, I. Chang, P. Knight, A.Vincent, Mat. Sci. Eng. A, 213-218, 375-377 (2004)

[2] D.B. Miracle, JOM, 2130-2136, 69 (2017)

DS 20.44 Wed 16:00 P3

Different approaches to deposit tungsten-doped vanadium dioxide by ion-beam sputter-deposition — •JILL KESSLER, SEBASTIAN LEONARD BENZ, ISABEL MÜLLER, MARTIN BECKER, and

SANGAM CHATTERJEE — Institute for Exp. Physics I and Center for Materials Research (LaMa), Justus Liebig University Giessen, Germany

The complexity of the phase diagram of vanadium oxides makes the reproducible growth of thin films of defined phases by nonequilibrium techniques challenging. Here, we discuss thermochromic VO<sub>2</sub>, which exhibits a significant change in optical transparency and reflectivity and, thus, is an ideal candidate for the use in smart windows. However, the bulk phase transition temperature of  $68\,^\circ\mathrm{C}$  is too high for useful applications. Doping  $VO_2$  with tungsten drives the thermochromic key measures close to the desired range.

We present different approaches for tungsten doping of  $VO_2$  based on ion-beam sputter-deposition. We employ tungsten screws that are inserted into the vanadium target. Furthermore, a pre-doped vanadium target is used. In another approach we employ two targets of vanadium and tungsten, respectively, to be sputtered simultaneously. Here, a compositional gradient allows for identification of the optimum doping concentration. The different approaches are compared regarding thin film properties and overall reproducibility of the growth process.

Raman spectroscopy and X-ray photoelectron spectroscopy provide structural and compositional analysis. UV/Vis/NIR spectroscopy yields the thermochromic performance.

DS 20.45 Wed 16:00 P3 Enhanced amorphization of Cu-Sn-I alloy thin films fabricated by reactive magnetron sputtering — •CHRISTIANE DETHLOFF, SOFIE VOGT, TILLMANN STRALKA, DANIEL SPLITH, HOL-GER VON WENCKSTERN, and MARIUS GRUNDMANN — Universität Leipzig, Leipzig, Deutschland

CuI is a promising p-type semiconductor for optoelectronical applications due to various advantageous material properties such as transparency in the visible spectrum [1] and its earth abundant, cheap and non-toxic constituents. Growth of amorphous layers of CuI by solution processing has already been reported [2, 3]. The feasibility of deposition of the amorphous Cu-Sn-I alloy has not yet been demonstrated for a physical, scalable process, such as sputtering.

We present our investigations of the influence of the process parameters during the deposition of a Cu-Sn-I-alloy using reactive co-sputtering of Cu and Sn in a reactive iodine ambient. A dependence of the growth rate, the thin films morphology and the electrical properties on the process parameters i.e. the magnitude of the electrical power applied at the sputtering sources, the iodine partial pressure and the chamber pressure. A decrease of crystallinity was observed by XRD measurements for increasing sputtering power applied on the tin target as well as with increasing chamber pressure. LSM and AFM measurements yielded root-mean-square surface roughnesses below 10 nm.

[1] M. Grundmann et al. Phys. Status Solidi A 210, 1671 (2013);

[2] H. Wu et al. Appl. Phys. Lett. 118, 222107 (2021);

[3] T. Jun et al. Advanced materials 30, e1706573 (2018).

#### DS 20.46 Wed 16:00 P3

Overcoming the integration issues between 2D materials and waveguides — •Oscar Camacho Ibarra<sup>1</sup>, Ioannis Caltzidis<sup>1</sup>, SELIM SCHARMER<sup>2</sup>, SAMUEL GYGER<sup>2</sup>, MARC SARTISON<sup>1</sup>, and KLAUS D. Jöns<sup>1</sup> — <sup>1</sup>HQPD lab, Department of Physics, Paderborn University, Germany — <sup>2</sup>Quantum Nanophotonics, KTH Royal Institute of Technology, Sweden

To achieve fully operational quantum photonic integrated circuits, developing a scalable platform capable of supplying an efficient coupling between single-photon emitters and photonic circuitry is essential. A hybrid approach is the most favorable to integrate single-photon emitters with other on-chip components since the advantages of each material platform are exploited. Single-photon emitters hosted in 2D materials are emerging technologies and promising candidates for future scalable photonic circuits. However, the coupling of light from these emitters into waveguides remains challenging: In particular, higher coupling efficiency and reduction of spectral jitter are needed. Both issues can be simultaneously overcome by implementing a cavity in the photonic circuit. In this work, 1D photonic crystal cavities were designed and simulated for later integration of 2D emitters. These photonic crystal cavities are designed to be efficiently coupled to waveguide modes, and they possess high\*quality factors and small mode volumes, resulting in prominent Purcell factors. Furthermore, the cavity geometrical structure can act as nucleation sites for strain\*driven singlephoton emitters, allowing a self-alignment process between emitter and cavity.

DS 20.47 Wed 16:00 P3 Propagation and manipulation of Bloch Surface Waves and Bloch Surface Wave Polaritons in ZnO — • SEBASTIAN HENN, SI-MON BRIESENICK, CHRIS STURM, and MARIUS GRUNDMANN - 1Universität Leipzig, Faculty of Physics and Earth Sciences, Felix Bloch Institute for Solid State Physics, Linnéstr. 5, 04103 Leipzig, Germany In this contribution we demonstrate experimentally the control of the propagation of Bloch Surface Waves (BSW) in the transparent spectral range and Bloch Surface Wave Polaritons (BSWP) in the vicinity of excitonic transitions in ZnO. BSWP are bosonic quasi-particles originating from the strong coupling between BSW and excitons and exist along the ambient interface of a distributed Bragg reflector (DBR) with a thin ZnO top layer [1]. Using shallow optical diffraction gratings with sub-micron sized lattice constant, incident light is coupled into and out of the Bloch modes, which propagate along the surface interface between the gratings. Depending on the geometry of the sample and roughness of the surface layer the low-loss nature of evanescent BSW allows long-range lateral propagation of BSWP, on the order of micrometers, making this an interesting candidate for on-chip polaritonic devices. We determine the propagation lengths and test the coupling efficiency of the gratings, which are modelled using RCWA computions.

[1] S. Henn et al., New J. Phys. 23, 093031 (2021)

DS 20.48 Wed 16:00 P3

Improvement of the Architecture of Water-Based Dye-Sensitized Solar Cells —  $\bullet$ Sara Domenici, Andreas Ringleb, and DERCK SCHLETTWEIN — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik

Dye-sensitized solar cells (DSSCs) have emerged as a possible alternative technology for the conversion of sunlight into electrical energy. Aqueous electrolytes would considerably increase their sustainability. Aside from chemical instabilities, the power conversion efficiencies of aqueous DSSCs remain significantly lower compared to other DSSCs. One main problem which is dealt with in the present work, consist in low diffusion coefficients of appropriate redox couples. Aqueous DSSCs were assembled using screen-printed  $TiO_2$  semiconducting layers sensitized with an organic dye, XY1b. The redox couple was  $TEMPO/TEMPO^+$  dissolved in aqueous  $LiClO_4$  with MBI added as organic corrosion inhibitor. To improve the accessibility of the photo anodes for the redox couple, the size of  $TiO_2$  nanoparticles was varied. Further, this helps to add a scattering layer. In a second approach, the sealing method for the cells was adjusted. For instance, the distance between the working electrode and the counter electrode was tuned by using different sealant materials, such as hotmelt foils or UV glue, in order to allow short pathways for ion conduction. In this context, interactions of different sealant materials and the organic redox mediators have to be considered. The influence of the different approaches on cell efficiency will be discussed.

DS 20.49 Wed 16:00 P3

Development of a Transport Layer for the Integration of a TiO2-based Photoanode on a Silicon Wafer for Solar Water Splitting — •LUISA BUSCH, DENNIS BERENDS, and KAI GEHRKE DLR Institut für Vernetzte Energiesysteme, Oldenburg, Germany

Recently, Segev et al. [1] proposed a three-terminal hybrid photoelectrochemical (PEC) / photovoltaic (PV) device for improved solar spectrum utilization. The concept integrates a TiO2 photoanode on an IBC silicon wafer in tandem configuration. To overcome the rather large bandgap of TiO2, which still limits the absorption of the solar spectrum and therefore the efficiency of the PEC, a sub-stochiometric TiO2 layer is advantageous. However, contacting the two semiconductors directly would result in a high recombination of the free charge carriers and thus low currents in the cell, due to band mismatch. By adding a transport layer between the two materials, for example a tunnel recombination junction, an improved current flow can be achieved. Within this work, the development of such a transport layer is presented in order to integrate a sub-stochiometric TiO2 photoanode on a Si wafer. For this purpose, the optoelectronic properties of the two semiconductor materials are characterized to select a suitable transport layer material by simulating the band alignment with AFORS-HET. Based on these results, a possible transport layer is developed and integrated into the tandem structure for electrochemical characterization.

[1] G. Segev et al., In: Nature materials, 17(12):1115-1121, 2018. doi: 10.1038/s41563-018-0198-y

Hybrid thin film for H2 evolution applications — •MORGAN LE Dû<sup>1</sup>, MANUEL ANDREE REUS<sup>1</sup>, KUN SUN<sup>1</sup>, ZERUI LI<sup>1</sup>, CRISTIANE HENSCHEL<sup>2</sup>, ANDRE LASCHEWSKY<sup>2,3</sup>, SIGIRD BERNSTORFF<sup>4</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,5</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — <sup>2</sup>Universität Potsdam, Institut für Chemie, 14476 Potsdam-Golm — <sup>3</sup>Fraunhofer Institut für Angewandte Polymerforschung, 14476 Postdam-Golm — <sup>4</sup>Elettra-Sincrotrone Trieste, Basovizza, 34149 Trieste, Italy — <sup>5</sup>MLZ, TU München, 85748 Garching

Photocatalysis via water splitting reaction is a way to implement the sun to produce hydrogen-based energy. Recently, Pt loaded graphitic carbon nitride (g-CN) has been found has a promising photocatalyst for H2 evolution under visible light. The aim of this work is to bring this material in a polymer thin film configuration to make it suitable for industrial purposes. Poly(N-isopropylacrylamide) exhibits good swelling capacity of water vapor and seems to be suitable for such a hybrid thin film system. A new isomer of PNIPAM, poly(N-vinylisobutyramide) (PNVIBAM) raised our attention due to its higher lower critical solution temperature (LCST) in aqueous solution ( $\approx 39^{\circ}C$ ) which makes it more stable in ambient environment. Spray coating has been chosen to be the deposition technique of PNVIBAM/g-CN/Pt hybrid films. A comparative study of the photocatalyst concentrations is presented. Grazing incident small angle x-ray scattering is the main tool of this work. G-CN/Pt blended polymer films structure is analysed under light irradiation condition.

DS 20.51 Wed 16:00 P3 Fabrication and electrochemical characterization of 2D membranes — •YOSSARIAN LIEBSCH — Universität Duisburg-Essen, AG Schleberger, Germany

Membranes are critical components in widely used industrial and technical processes, *e.g.*, water filtration, desalination and energy storage and conversion. With their extreme thinness of only a few angstrom, two-dimensional (2D) materials have the potential to be used as highly efficient membranes, possibly outperforming conventional membranes by orders of magnitude. We fabricated two different types of 2D membranes: Membranes made of commercially available CVD-grown graphene and membranes made of self grown CVD MoS<sub>2</sub>. The membranes were made by transferring the 2D material onto a  $3\,\mu m$  micropore. Subsequently the membranes were plasma etched (graphene) or irradiated by highly charged ions  $(MoS_2)$  in order to create nanopores. Raman and photoluminescence spectroscopy was used to analyse the membranes in terms of doping, stress and defects density. Additionally an electrochemical characterization of the membranes was done in a custom build membrane potential measurement stand. In case of the graphene membranes the measured membrane potentials were in good agreement to the well-known Theorell-Meyer-Sievers Theory. However for the  $MoS_2$  membranes no potential could yet be measured. In upcoming experiments with this electrochemical cell we aim to investigate the correlations between the pore creation mechanisms and intrinsic membrane properties like pore size, pore chemistry and surface charge density.

### DS 20.52 Wed 16:00 P3

Laser-assisted polarization switching dynamics in ferroelectric thin films —  $\bullet$ REKIKUA ALEMAYEHU<sup>1</sup>, MATTHIAS RÖSSLE<sup>2</sup>, and MATIAS BARGHEER<sup>1,2</sup> — <sup>1</sup>Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — <sup>2</sup>Helmholtz Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany

Nucleation and growth of domains with opposite polarization moderates the electric field-induced polarization reversal process in ferroelectric materials. Accordingly, the domain wall velocity governs the timescale of polarization switching. Achieving the ultimate switching time in ferroelectrics is a fundamental quest to improve the device response time. Here we show laser-assisted polarization switching dynamics in metal-ferroelectric-metal heterostructure via heat and strain waves induced by a femtosecond laser pulse.