

## DS 12: Poster

Time: Wednesday 17:00–19:00

Location: P3

DS 12.1 Wed 17:00 P3

**Growth and structural investigation of the SnBiTe stoichiometric series via MBE and TEM** — ●XIAO HOU<sup>1</sup>, ABDUR REHMAN JALIL<sup>2</sup>, DETLEV GRÜTZMACHER<sup>2</sup>, CLAUS CLAUS MICHAEL SCHNEIDER<sup>1</sup>, and LUKASZ PLUCINSKI<sup>1</sup> — <sup>1</sup>PGI-6, Forschungszentrum Jülich, Germany — <sup>2</sup>PGI-9, Forschungszentrum Jülich, Germany

A topological phase transition (TPT) can be induced to engineer the band structure. This TPT is a fascinating, yet complex phenomenon in condensed matter research. Upon changing the stacking order of layers having different spin-orbit coupling (SOC) strengths, one can achieve a topological phase transition between trivial and nontrivial states [1,2]. Here, the Sn<sub>x</sub>Bi<sub>y</sub>Te<sub>z</sub> (SBT) stoichiometric series is a classical example, in which a stacking-dependent topological phase transformation group is explored.

The epitaxial growth of three distinct compositions i.e. SnBi<sub>2</sub>Te<sub>4</sub>, SnBi<sub>4</sub>Te<sub>7</sub>, Sn<sub>2</sub>Bi<sub>2</sub>Te<sub>5</sub> is conducted on Si (111) substrates via molecular beam epitaxy (MBE). X-ray diffraction (XRD) is employed to characterize the crystal quality of the grown thin films. We have also used advanced transmission electron microscopy (TEM) to investigate the stacking order. High-angle annular dark-field imaging provided detailed information about the crystallinity and atomic arrangements of the layer stacks and also of various types of structural defects in the thin films. The link between the stacking order and the topological characteristics requires further investigation that is ongoing.

[1] B.-J. Yang and N. Nagaosa, *Nature Comm.* 5, 4898 (2014). [2] R. Peng et al. *Phys. Rev. B* 101,115427 (2020).

DS 12.2 Wed 17:00 P3

**Thin film growth characterization of a multipurpose physical vapor deposition apparatus with the goal of investigating tailored perpendicular magnetic anisotropy systems** — ●FLORIAN OTT, CHRISTIAN JANZEN, ARNE SCHRÖDER, and ARNO EHRESMANN — Institute of Physics, University of Kassel, D-34132 Kassel

In recent years, systems of multilayered (ML) magnetic thin films consisting of ferromagnetic transition metals (TM) with noble metallic spacers displaying perpendicular magnetic anisotropy (PMA) have gained increased interest for applications in magnetic particle transport [1], controlled domain movement [1,2] and sensor technologies [3]. These TM-based PMA systems may rely on the precise modulation of layer growth additionally to the already very low thickness requirements [1]. As a result, a precise control of the growth conditions is necessary in order to produce these systems. This work focuses on the characterization of growth conditions and parameters inside a multipurpose physical vapor deposition (PVD) apparatus with the ultimate goal of creating and investigating engineered TM-based PMA systems. [1] M Urbaniak, et al. Magnetization reversal of Co/Au multilayer stripes with keV-He<sup>+</sup> ion bombardment induced coercivity. *J. Phys. D: Appl. Phys.* 48 (2015) 335003 (7pp) gradient, [2] A. Jarosz, et al. Magnetic domain propagation in Pt/Co/Pt micro wires with engineered coercivity gradients along and across the wire, *Journal of Magnetism and Magnetic Materials*, Volume 435 (2017) [3] M. Matczak, et al. Co/Au multilayers with graded magnetic anisotropy for magnetic field sensing. *applied physics letters* 100, 162402 (2012)

DS 12.3 Wed 17:00 P3

**Strain and Lattice-Relaxation Effects of (Al,Ga)N/GaN Interfaces on 4D-STEM Signals** — ●FREDERIK OTTO, LAURA NIERMANN, TORE NIERMANN, and MICHAEL LEHMANN — Technical University of Berlin, Berlin, Germany

The immense increase in computation power over the past decades can be attributed to the decreasing size of semiconductor device structures. Preceding this trend, semiconductor research focuses on thin films and their interfaces with the surrounding substrate material.

At these interfaces of heterogeneous device structures, the atomic lattices are strained due to the mismatch of lattice constants of interfacial materials. Scanning-Transmission Electron-Microscopy (STEM) is capable of resolving strain at a nanometer scale, however, investigated specimens must be sufficiently thin to be electron transparent. For such thin specimens, the relaxation of the strained lattice at its surfaces cannot be neglected when measuring strain in an electron microscope.

Here, knowledge about the underlying strain and relaxation effects

at the interface of (Al,Ga)N/GaN Quantum Wells (QWs) is obtained by comparing 4D-STEM measurements with simulations. By carefully choosing the experimental parameters, i.e., convergence angle and tilt, features of multiple scattering events are found in the measured diffraction discs perpendicular to the QW structure at every position of a 2D scanned area. These features are evaluated by comparison with corresponding simulations considering a strain field and relaxation effects as obtained from finite element calculations.

DS 12.4 Wed 17:00 P3

**Comparative evaluation of EDS quantification methods for the analysis of Sc<sub>x</sub>Al<sub>1-x</sub>N films** — ●HAUKE HONIG<sup>1</sup>, REBECCA PETRICH<sup>2</sup>, LORENZ STEINACKER<sup>1</sup>, YOUNES SLIMI<sup>2</sup>, DANIEL GLÖSS<sup>3</sup>, STEPHAN BARTH<sup>3</sup>, HAGEN BARTZSCH<sup>3</sup>, RAPHAEL KÜHNEN<sup>4</sup>, DIETMAR FRÜHAUF<sup>4</sup>, STEFAN KRISCHOK<sup>2</sup>, and KATJA TONISCH<sup>2</sup> — <sup>1</sup>Technische Universität Ilmenau, Fachgebiet Werkstoffe der Elektrotechnik, IMN MacroNano<sup>®</sup>, 98693 Ilmenau — <sup>2</sup>Technische Universität Ilmenau, Fachgebiet Technische Physik I, IMN MacroNano<sup>®</sup>, 98693 Ilmenau — <sup>3</sup>Fraunhofer-Institut für Organische Elektronik, Elektronenstrahl- und Plasmatechnik FEP, 01277 Dresden, Germany — <sup>4</sup>Endress+Hauser SE+Co. KG, TTD Technologieentwicklung, 79689 Maulburg, Germany

The quantitative analysis of Sc<sub>x</sub>Al<sub>1-x</sub>N films with energy dispersive x-ray spectroscopy (EDS) poses some challenges due to peak overlaps and the thin film character. Standard-free and standard-based methods are compared regarding their reliability for the quantification of the Sc-content in sputtered films with  $0 \leq x \leq 0.35$  and evaluated using reference samples that have been quantified with GDOES and EDS by Fraunhofer FEP. Therefore, parameters such as acceleration voltage, selection of standard materials and quantification models are considered. Theoretical spectrums generated with Monte-Carlo simulations are used to improve the selection of excitation energy in the small range between substrate influence and limits of the quantification models. The crystalline hexagonal structure is confirmed with XRD.

DS 12.5 Wed 17:00 P3

**From Doping to Dilution: Local Chemistry and Collective Interactions of La in HfO<sub>2</sub>** — ●OLIVER REHM<sup>1</sup>, THOMAS SZYJKA<sup>1,2</sup>, LUTZ BAUMGARTEN<sup>2</sup>, CLAUDIA RICHTER<sup>3</sup>, YURY MATVEYEV<sup>4</sup>, CHRISTOPH SCHLUETER<sup>4</sup>, THOMAS MIKOLAJICK<sup>3,5</sup>, UWE SCHROEDER<sup>3</sup>, and MARTINA MÜLLER<sup>1</sup> — <sup>1</sup>Uni Konstanz, Konstanz, Germany — <sup>2</sup>FZJ, Jülich, Germany — <sup>3</sup>NaMLab, Dresden, Germany — <sup>4</sup>DESY, Hamburg, Germany — <sup>5</sup>TU Dresden, Dresden, Germany

HfO<sub>2</sub>-based thin films exhibit huge potential for the next generation of nonvolatile memory applications, such as FeRAM or FeFET. The application of HfO<sub>2</sub>-based thin films as active ferroelectrics (FE) in these devices face reliability issues like wake-up, imprint, and fatigue. The FE phase of HfO<sub>2</sub> is the metastable orthorhombic structure, for which La doping is considered a promising route for stabilization.

La:HfO<sub>2</sub> samples were grown by ALD with a range of La doping, from 3.5% to 33%, i.e., from the doping to dilution level. We link the local chemistry at the La lattice sites with local and collective electronic properties of the La:HfO<sub>2</sub> matrix using HAXPES. The satellite structure of La 3d core level, the plasmonic excitation energies, and core-level rigid binding energy (BE) shifts are investigated. The emerging chemical phases and electronic properties are discussed as a function of La doping. From the evolution of the plasmon excitation energies and rigid BE shifts, it is concluded that electronic charge compensation by oxygen vacancies occurs for increasing La content.

[1] T. Szyjka, et al., *Phys. Status Solidi RRL* 2022, 16, 2100582

DS 12.6 Wed 17:00 P3

**Molecular Dynamics - Two Temperature Model simulations of gold** — ●OTHMANE BENHAYOUN<sup>1</sup>, EMILIANO PRINCIPPI<sup>3</sup>, BERND BAUERHENNE<sup>1</sup>, DMITRY S. IVANOV<sup>2</sup>, and MARTIN E. GARCIA<sup>1</sup> — <sup>1</sup>University of Kassel, Theoretical physics II, Kassel, Germany — <sup>2</sup>Moscow, Russia — <sup>3</sup>Elettra-Sincrotrone Trieste S.C.p.A., Trieste, Italy

We aim to explain the results obtained from a recent Ultrafast Electron Diffraction (UED) experiment that showed periodic oscillations in both height and width of the (311) Au diffraction peak. The same

effect is however not observed in polycrystalline gold. We have thus performed Molecular Dynamics - Two Temperature Model (MD-TTM) simulations to model more than 11 million atoms, enabling us to understand the underlying physical processes. In our simulations, we obtain similar peak oscillations and determine the major mechanisms that lead to such lattice dynamics.

DS 12.7 Wed 17:00 P3

**In situ X-Ray Total Scattering Investigation of Thermal Annealing in FeCoSiB Metallic Glass Films** — ●NICOLAS HAYEN<sup>1</sup>, PHILIPP JORDT<sup>1</sup>, LARS THORMÄHLEN<sup>2</sup>, MATHIS MEWES<sup>1</sup>, ANN-CHRISTIN DIPPPEL<sup>3</sup>, OLOF GUTOWSKI<sup>3</sup>, NIKLAS WOLFF<sup>2</sup>, LORENZ KIENLE<sup>2</sup>, and BRIDGET MURPHY<sup>1,4</sup> — <sup>1</sup>Institute of Experimental and Applied Physics, Kiel University, Germany — <sup>2</sup>Institute of Material Sciences, Kiel University, Germany — <sup>3</sup>Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — <sup>4</sup>Ruprecht Haensel Laboratory, Kiel University, Germany

Thin films of the iron-based metallic glass (Fe<sub>0.9</sub>Co<sub>0.1</sub>)<sub>78</sub>Si<sub>12</sub>B<sub>10</sub> (Fe-CoSiB) are seen as a promising candidate for technical applications in high sensitivity magnetic field sensors and have been utilized extensively within the CRC 1261 "Biomagnetic Sensing". Thermal annealing of these films leads to a decrease in quality of the desired magnetic properties depending on the parameters of the annealing process.

*In situ* grazing incidence high-energy x-ray total scattering experiments were used to investigate the onset of structural changes occurring in the material. Films of thickness ranging from 0.05 to 1 μm were investigated under varied annealing conditions with temperatures up to 700°C. From these measurements we were able to observe two separate crystallization phase transitions and the emergence of textured structures. Further analysis of the scattering from the amorphous phase may give further insight into the initial structural changes the material undergoes during annealing and their influence on magnetic properties.

DS 12.8 Wed 17:00 P3

**Synthesis of structurally defined graphene nanoribbons: Peritetracene and it's corresponding 1,1'-bitetracene precursor** — ●MAREN KLEIN<sup>1,2</sup>, JOHN B. BAUER<sup>2</sup>, MARIE WAGNER<sup>1,2</sup>, HOLGER F. BETTINGER<sup>2</sup>, THOMAS CHASSÉ<sup>1</sup>, and HEIKO PEISERT<sup>1</sup> — <sup>1</sup>Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany — <sup>2</sup>Institute of Organic Chemistry, University of Tübingen, Germany

Band gap engineering of precise nanographenes has attracted much attention in the field of organic electronics as they show great electronic properties. One class of these promising nanographenes are acenes and their related peri-acenes. Acenes are linearly condensed polycyclic hydrocarbons whereas peri-acenes exhibit a two-dimensionally enlarged π system. As peri-acenes possess a diradical open-shell character, the synthesis is quite challenging. Here we demonstrate that peritetracene can be formed on-surface by annealing the deposited precursor molecule 1,1'-bitetracene on a Cu (111) surface. The unique 1,1'-bitetracene undergoes a surface-assisted cyclodehydrogenation which was investigated by microscopic and spectroscopic techniques, as well as by DFT calculations. In the XAS spectra we could observe that the as-deposited molecule shows a vanishing intensity of π\* transitions at normal incidence (90°), which indicates a planarization of the molecule already before annealing and an almost flat lying adsorption geometry.

DS 12.9 Wed 17:00 P3

**Study of cadmium-based thin films obtained by pulsed laser deposition** — ●CRISTINA POSTOLACHI<sup>1</sup>, GEORGIANA BULAI<sup>1</sup>, SANDU CIBOTARU<sup>2</sup>, ALEXANDRU COCEAN<sup>1</sup>, BOGDAN SILVESTRU MUNTEANU<sup>3</sup>, NICANOR CIMPOESU<sup>1,4</sup>, SILVIA GAROFILDE<sup>1</sup>, GEORGIANA COCEAN<sup>1</sup>, IULIANA COCEAN<sup>1</sup>, and SILVIU GURLUI<sup>1</sup> — <sup>1</sup>Alexandru Ioan Cuza University of Iasi, Faculty of Physics, Atmosphere Optics, Spectroscopy and Laser Laboratory (LOASL), 11 Carol I Bld. 700506 Iasi, Romania — <sup>2</sup>Petru Poni Institute of Macromolecular Chemistry, Gr. Ghica Voda Alley, 41A, 700487 Iasi, Romania — <sup>3</sup>Alexandru Ioan Cuza University of Iasi, Faculty of Physics, 11 Carol I Bld. 700506 Iasi, Romania — <sup>4</sup>Gheorghe Asachi Technical University of Iasi, Faculty of Material Science and Engineering, 59A Mangeron Bld., Iasi, Romania

This study investigates the processes that occur when different chemical compounds of cadmium are mixed with selenium and are further used as targets for thin film growth by pulsed laser deposition. Here the interactions between these compounds in the laser induced plasma plume will be analyzed.

The aim of the investigation of the reactions that take place in the

plasma plume at high vacuum is to obtain thin films of cadmium selenide. The thin films proprieties will be investigated with different techniques, such as Scanning Electron Microscopy coupled with Energy Dispersive Spectroscopy (SEM-EDX), X-ray Diffraction (XRD), profilometry, UV-VIS spectroscopy and others.

DS 12.10 Wed 17:00 P3

**Fabrication of copper halide thin films by combinatorial PLD** — ●CHRISTOPHER WALTER, FELIX-FLORIAN DELATOWSKI, MICHAEL BAR, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

Copper halides are promising p-type materials for transparent device applications due to their large direct band gaps ( $E_g = 3-3.4\text{ eV}$ ) [1]. Here we present the deposition of copper halide thin films by combinatorial pulsed laser deposition (PLD) and discuss their structural, morphological and optical properties as a function of different growth parameters [2]. At ambient conditions, CuI crystallizes in the cubic zinc-blende structure. XRD shows <111>-orientation for CuI independent from the used substrate material. CuBr and CuCl grow polycrystalline with the same crystal structure as CuI. However, with the incorporation of low iodine concentration, the crystallinity improves significantly. We find that the thin films exhibit very smooth surfaces with a roughness of  $R_{RMS} = 0.8-1.6\text{ nm}$  for the binary CuI, CuBr and CuCl systems under optimal parameters. Furthermore, using combinatorial PLD and a segmented target with one segment each of CuBr and CuI, ternary CuBr<sub>x</sub>I<sub>1-x</sub> alloys were grown. Based on the resulting locally varying composition, the influence on structural and optical properties can be directly observed.

[1] M. Grundmann *et al.* : phys. stat. sol. (a) 210, 9, 1671 (2013)

[2] H. von Wenckstern *et al.* : phys. stat. sol. (b) 257, 7, 1900626 (2019)

DS 12.11 Wed 17:00 P3

**Electrical characterization of SnTe thin film topological crystalline insulator** — ●NEGIN BERYANI NEZAFAT, SEPIDEH IZADI, and GABI SCHIERNING — Department of physics, Experimental physics, Bielefeld University, 33615, Bielefeld, Germany

Topological crystalline insulators (TCIs) with gapless metallic states and protected carrier transport offer unique electrical features. Band structure of these materials consists of conventional parabolic band diagram together with linear surface transport. In this work, SnTe thin film as a promising TCI is considered to be our model system. Therewith, SnTe thin films with different thicknesses are deposited on silicon substrate using RF magnetron sputtering. The resulting morphology characterization for rock-salt SnTe crystalline thin film fulfills stoichiometric ratio. Electrical characterization including temperature dependent resistivity, magnetoresistance and Hall analysis are performed using Van der Pauw configuration. These findings introduce SnTe thin film as a promising candidate for technical applications such as device fabrication.

DS 12.12 Wed 17:00 P3

**Current probe AFM measurements on reactively co-sputtered Ag<sub>x</sub>Cu<sub>1-x</sub>I thin films** — TILLMANN STRALKA, ●SOFIE VOGT, CHRISTIANE DETHLOFF, JORRIT BREDOW, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Universität Leipzig, Felix-Bloch-Institut, Germany

CuI exhibits a high hole mobility of up to 44 cm<sup>2</sup>/Vs in bulk crystals and of about 19 cm<sup>2</sup>/Vs in polycrystalline thin films<sup>[1,2]</sup>. This, combined with high transparency in the visible light range, renders CuI an interesting material for transparent complementary devices. However, grain boundary (GB) conduction is dominating electrical properties and might inhibit device performance<sup>[3]</sup>. Annadi *et al.* showed that alloying with silver reduces the conductivity of Ag<sub>x</sub>Cu<sub>1-x</sub>I thin films and even results in switching from p-type to n-type<sup>[4]</sup>.

We present topological and current probe (cp)-atomic force microscopy measurements on reactively sputtered Ag<sub>x</sub>Cu<sub>1-x</sub>I thin films with silver contents from x=0.1 to x=0.6. A strong decrease of the grain size with increasing silver content is observed. In addition, a decrease of the overall surface current is observed, which agrees well with electrical bulk characterizations. For x ≥ 0.39 we observed that the current from tip to sample is mainly injected at grain boundaries while for large Ag content the injected current at GBs is negligible.

[1] D. Chen *et al.*, Crystal Growth Design, 10, 2057\*2060, 2010.

[2] C. Yang *et al.*, ACS Appl. Electr. Mater., 2, 3627-3632, 2020.

[3] Kneif *et al.*, Adv. Mater. Interfaces, 5, 1701411, 2018.

[4] A. Annadi *et al.*, *Appl. Mater. Today*, 20, 100703, 2020.

DS 12.13 Wed 17:00 P3

**Analysis of the structural properties of  $\text{Li}(\text{Ni}_{1/3}\text{Co}_{1/3}\text{Mn}_{1/3})\text{O}_{2-d}$  (NCM) thin film model cathodes** — JULIUS KONSTANTIN DINTER and •MATTHIAS ELM — Center for Materials Research, Justus-Liebig-University Giessen Germany, Heinrich-Buff-Ring 16, 35392 Giessen

Lithium ion batteries often suffer from capacity fading due to undesired side reactions occurring at the cathode surface. To get a deeper understanding of these side reactions, 2D model system are necessary. For this purpose, NCM thin film cathodes were prepared via spin coating followed by annealing at high temperatures. Using these thin film cathodes allow us to perform various surface sensitive measurements such as Raman microscopy, AFM, ESM, SEM and EDX. As no additives are used, we are able to study the surface reaction occurring at the cathode active material in more detail using in-situ measurements. The results reveal structural changes of the surface accompanied by an increase of the cell resistance, which confirms the formation of an SEI. Furthermore, the electrochemical performance of thin films coated with  $\text{Al}_2\text{O}_3$  using atomic layer deposition (ALD) were investigated. The analysis of the surface properties confirm that coating of the NCM-thin film suppresses the undesired surface reactions resulting in an improved long-term cycling stability.

DS 12.14 Wed 17:00 P3

**Nanosopic Investigation of the Monolayer  $\text{MoSe}_2$ - $\text{WSe}_2$  Lateral Heterostructures under Illumination** — •ALEXANDER TURCHANIN<sup>1</sup>, TOBIAS NÖRENBERG<sup>1</sup>, ZIYANG GAN<sup>2</sup>, ANTONY GEORGE<sup>2</sup>, ANDREY TURCHANIN<sup>2</sup>, SUSANNE C. KEHR<sup>1,3</sup>, and LUKAS M. ENG<sup>1,3</sup> — <sup>1</sup>TU Dresden — <sup>2</sup>Friedrich Schiller University Jena — <sup>3</sup>Würzburg-Dresden Cluster of Excellence - EXC 2147 (ct.qmat)

Transition metal dichalcogenides (TMDCs) such as  $\text{MoSe}_2$  and  $\text{WSe}_2$ , are inorganic semiconductor monolayers with great potential for integration into nanoscale devices. Monolayers of different TMDCs can be engineered into lateral or vertical heterostructures forming, e.g., 1D or 2D p-n junctions that strongly respond to light [1]. Here, lateral heterostructures of monolayer  $\text{MoSe}_2$  and  $\text{WSe}_2$  grown by chemical vapor deposition are studied at the nanometer length scale by Kelvin Probe Force Microscopy (KPFM) under visible to near-infrared light illumination, i.e. photon energies between 1.45 and 1.95 eV. This approach enables for the simultaneous recording of both the sample surface morphology and the local photoinduced surface potential. By employing the side-band KPFM demodulation [2], quantification of the local band-bending of this in-plane heterostructure is possible with superior sensitivity. Different alterations of the local surface potential are observed when choosing the light exposure above and below the individual TMDCs bandgap energies.

[1] P.A. Markeev *et al.*, *J. Phys. Chem. C* **125**, 13551 (2021).

[2] T. Wagner *et al.*, *Beilstein J. Nanotechnol.* **6**, 2193 (2015).

DS 12.15 Wed 17:00 P3

**Electronic structure of MXenes determine from angle-resolved photoelectron spectroscopy** — •WEI YAO<sup>1</sup>, DONGQI LI<sup>1,2</sup>, JONAS A. KRIEGER<sup>1</sup>, MIHIR DATE<sup>1</sup>, EMILY C. MCFARLANE<sup>1</sup>, MINGHAO YU<sup>1,2</sup>, XINLIANG FENG<sup>1,2</sup>, and NIELS B.M. SCHRÖTER<sup>1</sup> — <sup>1</sup>Max-Planck Institute of Microstructure Physics, Halle (Saale), 06120, Germany — <sup>2</sup>Center for Advancing Electronics Dresden (cfaed) and Faculty of Chemistry and Food Chemistry, TU Dresden, Dresden, 01062, Germany

Transition metal carbides, also known as MXenes, have been one of the most fascinating two-dimensional material systems beyond graphene. Chemical substitution of the transition metal elements and terminal function groups have resulted in versatile and tunable electronic, optical and mechanical properties, with applications in energy storage, multifunctional sensors, transparent and flexible electrodes, electromagnetic interference shielding, or hydrogen evolution reaction catalysis [1]. However, to reveal the origins of the MXenes' exceptional properties, a deeper understanding of their electronic structure is required. Here we report the first micro-focused angle-resolved photoemission spectroscopy (ARPES) measurements of single MXene flakes, which will reveal the influence of the chemical environment on the the single-particle electronic band structure, as well as many-body effects reflected in its spectral function.

[1]. A. VahidMohammadi, J. Rosen, and Y. Gogotsi. The world of two-dimensional carbides and nitrides (MXenes). *Science* 372, eabf1581 (2021)

DS 12.16 Wed 17:00 P3

**Mode-selective Raman Signal Enhancement in  $\text{MoS}_2/\text{WS}_2$  Heterostructures** — •ANNIKA BERGMANN<sup>1</sup>, MUSTAFA HEMAID<sup>1</sup>, RICO SCHWARTZ<sup>1</sup>, ZIYANG GAN<sup>2</sup>, ANTONY GEORGE<sup>2</sup>, ANDREY TURCHANIN<sup>2</sup>, and TOBIAS KORN<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Rostock, Germany — <sup>2</sup>Institute of Physical Chemistry, Friedrich Schiller University Jena, Germany

In the family of van der Waals materials, transition metal dichalcogenides (TMDCs) have attracted much attention in recent years. Stacking various TMDC materials forms heterostructures in which new phenomena, such as interlayer charge transfer and interlayer excitons [1] occur. However, for the observation of interlayer effects good contact between the constituent monolayers is crucial.

Here, we investigate bilayer heterostructures that were formed by combining Chemical Vapor Deposition (CVD) grown  $\text{MoS}_2$  and exfoliated  $\text{WS}_2$  monolayers. Photoluminescence quenching is used as an indicator to evaluate the interlayer coupling. In addition, the out-of-plane ( $A_{1g}$ ) phonon mode provides information on the interfacial contact [2]. We observe a selective enhancement of the  $\text{WS}_2$   $A_{1g}$  Raman mode in well-coupled  $\text{MoS}_2/\text{WS}_2$  heterostructures compared to  $\text{WS}_2$  monolayers or heterostructures with only poor contact. A systematic study of this phenomenon is presented to elucidate its microscopic origin.

[1] Fang *et al.*, *Proc. Natl. Acad. Sci. USA* 111 (2014)

[2] Zhou *et al.*, *ASC Nano* 8 (2014)

DS 12.17 Wed 17:00 P3

**Exfoliation of 2D materials for nanooptics** — •JAKOB WETZEL<sup>1</sup>, MAXIMILIAN OBST<sup>1,2</sup>, SUSANNE C. KEHR<sup>1,2</sup>, and LUKAS M. ENG<sup>1,2</sup> — <sup>1</sup>TU Dresden, Dresden, Germany — <sup>2</sup>Würzburg-Dresden Cluster of Excellence - EXC 2147 (ct.qmat), Dresden, Germany

The desire for smaller and more energy efficient optical components leads to the necessity of light confinement below the diffraction limit. This can be achieved e.g by phonon polaritons (PhPs) which are quasiparticles formed by the coupling of infrared photons with the optical phonons of a crystal. Particularly the related light confinement is enhanced when the PhPs are generated in anisotropic, 2D van der Waals materials such as  $\text{MoO}_3$  and  $\text{GeS}$  [1, 2]. Therefore, flat and  $\mu\text{m}$ -sized nanosheets of such materials are required, which can be realized by mechanical exfoliation.

Here, we present an optimized exfoliation technique for  $\text{MoO}_3$  and  $\text{GeS}$  resulting in the reproducible generation of 20 to 100  $\mu\text{m}$ -sized flakes with a thickness of about 100 nm. We present a quick and easy to implement adaptation of the scotch-tape exfoliation technique as well as exemplary results based on optical microscopy images and atomic force microscopy.

[1] T.V.A.G de Oliveira *et al.*, *Adv. Mater.* **33**, 2005777 (2021).

[2] T. Nörenberg *et al.*, *ACS Nano*, published online (2022),

DOI: 10.1021/acsnano.2c05376.

DS 12.18 Wed 17:00 P3

**hybrid resonant circuits with van der Waals materials** — •HAOLIN JIN<sup>1</sup>, GIUSEPPE SERPICO<sup>2</sup>, CHRISTIAN N. SAGGAU<sup>2</sup>, SANAZ SHOKRI<sup>2</sup>, MICKEY MARTINI<sup>2</sup>, YEJIN LEE<sup>2</sup>, POYA YANG<sup>1</sup>, SEBASTIAN SEIFERT<sup>1</sup>, URI VOOL<sup>1</sup>, and NICOLA POC CIA<sup>2</sup> — <sup>1</sup>Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — <sup>2</sup>Leibniz Institute for Solid State and Materials Science Dresden (IFW Dresden), Dresden, Germany

Van der Waals superconductors, especially heterostructures, are believed to exhibit novel superconducting phases. However, the standard measurement techniques designed for bulk superconductors are challenging to apply in 2D materials which cannot be grown in sufficient size and quality. Herein, we introduce an efficient method to explore the properties of 2D materials, by combining them into hybrid resonant circuits. The resonator can have a strong inductive interaction with a small-size superconducting sample, affecting its frequency response. However, creating superconducting contacts between the resonator and the 2D material is challenging, especially for air-sensitive materials where evaporation must be done in a protected glovebox. Here, we present a technique to make robust superconducting contacts to a 2D sample by using a flexible nanomembrane. The Niobium resonator circuit is fabricated on top of the nanomembrane, and via contacts connect it to the 2D materials. Through the circuit response, we can explore the properties of novel unconventional superconductors. Moreover, this hybrid circuit is a new type of quantum device for future quantum technology applications.

DS 12.19 Wed 17:00 P3

**Phase transformations in few-layer transition metal phosphorus trichalcogenides studied by low-voltage TEM** — •ALEXANDER STORM<sup>1</sup>, JANIS KÖSTER<sup>1</sup>, MAHDI ASL-GOHRBANI<sup>2</sup>, SILVAN KRETSCHMER<sup>2</sup>, TATIANA GORELIK<sup>1</sup>, MICHAEL K. KINYANJUI<sup>1</sup>, ARKADY KRASHENINNIKOV<sup>2</sup>, and UTE KAISER<sup>1</sup> — <sup>1</sup>Central Facility Materials Science Electron Microscopy, Ulm University, 89081 Ulm, Germany, — <sup>2</sup>Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany,

In this work we study phase transformations in freestanding few-layer transition metal phosphorus trichalcogenides (TMPTs) induced by electron irradiation as well as thermal annealing in vacuum, using various analytical transmission electron microscopy techniques (TEM). In addition, our results are supported by ab-initio calculations.

We show that due to knock-on damage, first sulphur atoms are ejected in sulphur-based TMPTs at common TEM acceleration voltages (60kV - 300kV), which in turn leads to the formation of defects and strong modifications of the TMPT's properties [1]. For instance, we show that in few-layer MnPS<sub>3</sub> and MnPSe<sub>3</sub>, stable, ultrathin  $\alpha$ - and  $\gamma$ -MnS/MnSe phases are formed showing the reliability of this transformation in Mn based TMPTs. Eventually, we elucidate the emerging phases and transition temperatures for few-layer MnPS<sub>3</sub>, MnPSe<sub>3</sub>, FePS<sub>3</sub>, FePSe<sub>3</sub>, and NiPS<sub>3</sub> induced by thermal annealing.

[1] Köster, Storm et al., J. Phys. Chem. C, 126, 36, 15446 (2022).

DS 12.20 Wed 17:00 P3

**Encapsulating high-temperature superconducting twisted van der waals heterostructures blocks detrimental effects of disorder** — •YEJIN LEE<sup>1,2</sup>, MICKEY MARTINI<sup>1,2</sup>, TOMMASO CONFALONE<sup>1</sup>, SANAZ SHOKRI<sup>1,2</sup>, CHRISTIAN SAGGAU<sup>1</sup>, DANIEL WOLF<sup>1</sup>, GENDA GU<sup>3</sup>, KENJI WATANABE<sup>4</sup>, TAKASHI TANIGUCHI<sup>4</sup>, DOMENICO MONTEMURRO<sup>5</sup>, VALERII VINOKUR<sup>6</sup>, KORNELIUS NIELSCH<sup>1,2</sup>, and NICOLA POCIA<sup>1</sup> — <sup>1</sup>IFW Dresden, Dresden, Germany — <sup>2</sup>TU Dresden, Dresden, Germany — <sup>3</sup>Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, NY, USA — <sup>4</sup>NIMS, Tsukuba, Japan — <sup>5</sup>University of Naples Federico II, Naples, Italy — <sup>6</sup>Terra Quantum AG, Gallen, Switzerland

Van der Waals (vdW) heterostructures based on cuprate superconductors attract substantial interest of novel topological phases as well as technological applications. One of the hindrances for the progress is the detrimental effect of disorder on the properties of the vdW device-based Josephson junctions. This work reports a novel method of fabricating twisted vdW heterostructures made of Bi<sub>2</sub>Sr<sub>2</sub>CuCa<sub>2</sub>O<sub>8+x</sub>, combining the employed cryogenic stacking using a solvent-free stencil mask technique and additionally covering the interface with insulating hexa boron nitride layers. We find that encapsulating the interface in the stacked systems overcomes detrimental effects of disorder providing highly coherent Josephson junction. This finding enables crucial improvement of its critical current and the T<sub>c</sub> of the junctions up to their magnitudes in bulk intrinsic junctions.

DS 12.21 Wed 17:00 P3

**In-situ formation of Mo<sub>6</sub>Te<sub>6</sub> nanowire in single-layer 2H-MoTe<sub>2</sub> by annealing and electron irradiation** — •JANIS KÖSTER<sup>1</sup>, SILVAN KRETSCHMER<sup>2</sup>, MICHAEL K. KINYANJUI<sup>1</sup>, ALEXANDER STORM<sup>1</sup>, FABIAN RASPER<sup>1</sup>, ARKADY V. KRASHENINNIKOV<sup>2</sup>, and UTE KAISER<sup>1</sup> — <sup>1</sup>Electron Microscopy of Materials Science, Ulm University, Albert Einstein Allee 11, 89081 Ulm, Germany — <sup>2</sup>Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Up to now, the fundamental understanding of transformations in 2D materials at the atomic scale are not fully characterized. Here, we demonstrate a route to locally transform freestanding single-layer (1H-) MoTe<sub>2</sub> [1] into 1D-Mo<sub>6</sub>Te<sub>6</sub> nanowires [2] under electron beam irradiation and by heating. (HR)TEM at the Cc/Cs-corrected SALVE [3] microscope at 80 kV is used to analyse structural changes in the material. Combining the experimental data with the results of first-principles calculations, we explain energetics and stabilities of MoTe<sub>2</sub> monolayers and Mo<sub>6</sub>Te<sub>6</sub> nanowires due to an interplay of electron-beam-induced energy input, atom ejection, and oxygen absorption. A detailed understanding of high-temperature solid-to-solid phase transformation in the 2D limit provides insights into the material's applicability for future device fabrication.

[1] J. Köster, et al. The Journal of Physical Chemistry C 125.24 (2021): 13601-13609.

[2] H. Kim, et al. Small 16.47 (2020): 2002849

[3] M. Linck, et al. Physical review letters 117.7 (2016): 076101

DS 12.22 Wed 17:00 P3

**structural and magnetic properties of two dimensional (2D) Fe<sub>x</sub>GeTe<sub>2</sub> and Fe<sub>x</sub>GaTe<sub>2</sub> grown by molecular beam epitaxy (MBE)** — •ATEKELTE KASSA, HUA LV, NEHA AGRAWAL, MICHAEL HANKE, ABBES TAHRAOUI, MANFRED RAMSTEINER, and MARCELO LOPES — Paul-Drude-Institut für Festkörperelektronik, Leibniz Institut im Forschungsverbund Berlin e.V., Berlin, Germany

2D materials with intrinsic functionality showed importance in fundamental condensed-matter science and for the development of advanced technologies, where 2D ferromagnetic materials have raised interest for developing low dimensional magnetic/spintronic devices. Yet maintaining 2D ferromagnetism at /above room temperature remains a challenge. This work presents our recent results on 2D ferromagnets of Fe<sub>x</sub>GeTe<sub>2</sub> and Fe<sub>x</sub>GaTe<sub>2</sub> ( $3 \leq x \leq 5$ ) prepared using MBE. Films were grown at 300 °C using elemental fluxes of Fe, Ge (Ga), and Te on epitaxial graphene on SiC (0001). Epitaxial films with good structural quality were confirmed by reflection high-energy electron diffraction and X-ray Diffraction. Atomic force microscopy confirmed continuous and smooth surface growth. Raman spectroscopy results showed that the graphene layers remain structurally unaltered after MBE growth. Anomalous Hall effect investigations through Magneto-transport studies identified a perpendicular magneto anisotropy as well as a Curie temperature (T<sub>c</sub>) above 300 K for both films with Fe composition close to x=5. For Fe<sub>x</sub>GaTe<sub>2</sub>, T<sub>c</sub> values around 380 K were obtained. These results make the studied ferromagnets promising for the development of novel spintronic devices based on 2D materials and heterostructures.

DS 12.23 Wed 17:00 P3

**Towards engineering of tailored 2D single photon emitters (SPE) by encapsulating single dye molecules into few layer hexagonal boron nitride (hBN)** — •NILS LE COUTRE, TIM VÖLZER, PAUL WEINBRENNER, LISA BÖHME, FRANZISKA FENNEL, TOBIAS KORN, STEFAN LOCHBRUNNER, and FRIEDEMANN REINHARD — University of Rostock, Rostock, Germany

We hypothesize that encapsulating dye molecules into multilayer hBN flakes overcomes photobleaching, for example by improved thermal conduction and airtight sealing. This would tackle one of the biggest barriers to the application of fluorescent dyes in various methods like optical nearfield microscopy or quantum sensing. I will present work to deposit dyes on exfoliated multilayer hBN flakes by different methods of physical vapor deposition (PVD) and liquid deposition, as well as initial studies on photostability by confocal microscopy. The large variety of available dye molecules will provide a rich toolbox for engineering of 2D SPEs, with greater flexibility than the limited set of intrinsic defects in 2D materials and bulk crystals.

DS 12.24 Wed 17:00 P3

**Epitaxy and transfer of freestanding oxide perovskites** — •JEREMY MALTITZ, DUC NGUYEN, ALEV YUVANC, JENS MARTIN, and JUTTA SCHWARZKOPF — Leibniz Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Deutschland

Fabrication of artificial 3D heterostructures is of increasing interest for a broad range of application, such as flexible sensor, memristors, or electronic skins. Layer transfer of thin films has established a new paradigm of material assembly and design in context of 2D-van-der-Waals crystals. Recently, freestanding oxide perovskites have been achieved by introducing a perovskite-like sacrificial layer (Sr<sub>3</sub>Al<sub>2</sub>O<sub>6</sub>) between substrate and functional film. In combination with layer transfer, the functional film can be placed on arbitrary substrates (e.g. silicon wafers). Additionally, two functional layers (same or different) can be stacked with the opportunity to create moiré patterns by rotating the layers with respect to each other. Therefore, the influence of PLD growth parameter and thickness of SrTiO<sub>3</sub>/Sr<sub>3</sub>Al<sub>2</sub>O<sub>6</sub> heterostructures are studied to improve the quality of freestanding SrTiO<sub>3</sub> thin films. Furthermore, the solid-solution family of (Ba,Ca,Sr)<sub>3</sub>Al<sub>2</sub>O<sub>6</sub> enables the possibility to tune the lattice parameter. This property was used to adjust the lattice parameter of the sacrificial layer to closely match the lattice parameter of SrTiO<sub>3</sub>. With improved growth parameter and lattice matched sacrificial layer, the crackformation of the freestanding film was reduced, paving the path towards the stacking of freestanding thin films.

DS 12.25 Wed 17:00 P3

**Characterization of structural and magnetic properties of**

**SrRuO<sub>3</sub> thin films** — •VITOR DE OLIVEIRA LIMA<sup>1</sup>, MAI HUSEIN HAMED<sup>1</sup>, CONNIE BEDNARSKI-MEINKE<sup>1</sup>, MICHAEL FALEY<sup>2</sup>, EMANUEL KENTZINGER<sup>1</sup>, and THOMAS BRÜCKEL<sup>1</sup> — <sup>1</sup>Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institute (PGI-4), JARA-FIT, Forschungszentrum Jülich GmbH, Germany. — <sup>2</sup>Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ERC), Forschungszentrum Jülich GmbH, Germany.

Proximity effects in Ferromagnet/Superconductor Heterostructures (F/S-H) have demonstrated high potential for development of new devices for spintronic and quantum computing application. SrRuO<sub>3</sub> (SRO) has attracted much attention among transition metal oxides for being the only 4d oxide to show itinerant ferromagnetism and metallic conductivity. In this work, we are characterizing the crystal structure as well the magnetic properties of SRO thin films for further application in F/S-H with YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub> superconducting films. The samples were prepared on STO (001) single crystals by High-Oxygen Pressure Sputtering. SRO thin films are epitaxial and have smooth surface. Magnetometry indicate that samples have out-of-plane magnetic anisotropy and paramagnetic-ferromagnetic transition at approximately 150 K, which corresponds to the SRO with Ru<sup>4+</sup> Curie temperature, and two transitions at lower temperatures, that may be related to another Ru oxidation state. The samples stoichiometry will be further investigated by Rutherford Backscattering Spectroscopy.

DS 12.26 Wed 17:00 P3

**Charge-to-spin conversion in the quasi-two-dimensional electron gas emerging at the doped interface between LiNbO<sub>3</sub> and LaAlO<sub>3</sub>** — •IGOR MAZNICHENKO<sup>1,2</sup>, SERGEY OSTANIN<sup>1</sup>, INGRID MERTIG<sup>1</sup>, and PAWEŁ BUCZEK<sup>2</sup> — <sup>1</sup>Institute of Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany — <sup>2</sup>Department of Engineering and Computer Sciences, Hamburg University of Applied Sciences, Berliner Tor 7, D-20099 Hamburg, Germany

We anticipate that the functional use of a solid electrolyte lithium niobate in LaAlO<sub>3</sub>/LiNbO<sub>3</sub> heterostructure allows one to tune the quasi-two-dimensional electron gas (q2DEG) which emerges there. This phenomenon can be achieved by charging and discharging LiNbO<sub>3</sub>. Here, on the basis of *ab initio* calculations of the hydrogen-doped LaAlO<sub>3</sub>/LiNbO<sub>3</sub> interface, we demonstrate how the q2DEG and its spin polarization appear. The out-of-plane electric polarization of LaAlO<sub>3</sub>/LiNbO<sub>3</sub> forces the H dopants to accommodate at the Al-terminated interface. This results in the formation of the q2DEG, whose spatial extent is about 1.5 nm along the stacking direction.

DS 12.27 Wed 17:00 P3

**Preparation of oxide ferroelectric membranes by epitaxial sacrificial layers** — •JONAS WAWRA<sup>1,2</sup>, ROBIN ADLUNG<sup>1,2</sup>, KORNELIUS NIELSCH<sup>1,2</sup>, and RUBEN HÜHNE<sup>1</sup> — <sup>1</sup>Institute for Metallic Materials, Leibniz IFW Dresden, Germany — <sup>2</sup>Institute of Applied Physics, TU Dresden, Germany

Oxide ferroelectric thin films are used in a variety of applications due to their strong remnant polarization and excellent dielectric, piezoelectric and optoelectric properties. However, well performing and robust materials require a high crystalline quality and orientation, which is commonly achieved by growing the desired ceramic on comparably thick and rigid substrates at high temperatures. This procedure prohibits in most cases the incorporation in advanced organic heterostructures and limits their utilization in flexible devices. One idea to overcome the discrepancy between processing and implementation is the use of a sacrificial layer during growth, which allows to release the functional material as a thin membrane afterwards and enables a transfer to flexible substrates. Here, we present our approach by growing different fully epitaxial hetero-structures of La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> (which can be wet-etched in a hydrochloric acid solution), conducting SrRuO<sub>3</sub> and ferroelectric Ba<sub>1-x</sub>Sr<sub>x</sub>TiO<sub>3</sub> on oxide single crystal substrates by pulsed laser deposition. Different sample architectures were used to obtain a diversity of membranes that allow us to study their microstructure and functional properties with methods like X-ray diffraction, scanning probe microscopy, dielectric and ferroelectric measurement techniques to compare them to similar films still clamped on a substrate.

DS 12.28 Wed 17:00 P3

**Resistive switching and oscillations in NdNiO<sub>3</sub> and SmNiO<sub>3</sub> planar thin film devices** — •FARNAZ TAHOUNI-BONAB<sup>1</sup>, THEODOR LUIBRAND<sup>1</sup>, CLARIBEL DOMÍNGUEZ<sup>2</sup>, JENNIFER FOWLIE<sup>2</sup>, STEFANO GARIGLIO<sup>2</sup>, RODOLFO ROCCO<sup>3</sup>, SOUMEN BAG<sup>3</sup>, LORENZO FRATINO<sup>3</sup>, MARCELO ROZENBERG<sup>3</sup>, JEAN-MARC TRISCONI<sup>2</sup>, REINHOLD KLEINER<sup>1</sup>, DIETER KOELLE<sup>1</sup>, JAVIER DEL VALLE<sup>2</sup>, and STE-

FAN GUÉNON<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Center for Quantum Science (CQ) an LISA<sup>+</sup>, Universität Tübingen, 72076 Tübingen, Germany — <sup>2</sup>Department of Quantum Matter Physics, Université de Genève, 1211 Geneva, Switzerland — <sup>3</sup>Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405 Orsay, France

Recently, there has been growing interest in strongly correlated materials that undergo a temperature-driven insulator-to-metal transition in the emerging research field of neuromorphic computing. Of particular interest are resistive switching phenomena for emulating integrate-and-fire behavior or self-sustained oscillations for spike train generation. In this study, we used a combination of wide field microscopy and electrical transport measurements to investigate thin film devices of the charge transfer insulators NdNiO<sub>3</sub> and SmNiO<sub>3</sub>. Current-voltage characteristics and photomicrographs reveal resistive switching via an intermediate state with a blurry metallic filament. The intermediate state is accompanied by oscillations in the 10 kHz frequency range that have a characteristic saw-tooth shape indicative of a relaxation oscillator. The intermediate state can be suppressed by changing the slew rate of the current source.

DS 12.29 Wed 17:00 P3

**Determining the brazeability of copper surfaces via spectroscopic ellipsometry** — •FRIEDRICH BÜRGER, LIENHARD WEGEWITZ, and WOLFGANG MAUS-FRIEDRICH — Clausthal Centre of Material Technology, Clausthal University of Technology, Agricolastr. 2, 38678 Clausthal-Zellerfeld

In Brazing, surface conditions play a fundamental role in determining the joint strength. Not all changes of the surface, like thick oxide layers or oil films, may be immediately apparent and therefore will only be noticed when the brazing process failed. Since most methods of determining brazeability work by performing a brazing process and evaluating the results they can only be performed on samples. This does not represent variation of surfaces within a batch of material. To fill this gap a nondestructive method to determine brazeability is needed. Spectroscopic ellipsometry (SE) is an optical measurement method commonly used to characterize the optical properties of surfaces and thin films. To evaluate if SE can be used to distinguish surface states of copper surfaces that negatively impact the joint strength, different surfaces were prepared. The selected surface states were a reference condition, ground surfaces, oxidized surfaces and different oil films on the reference surface. Those surfaces were characterized by confocal laser scanning microscopy (CLSM) and X-Ray photoelectron spectroscopy (XPS) to determine their morphology and chemical composition. SE-measurements were performed subsequently. Except for the ground states all surfaces showed distinct features in their SE-spectra, suggesting identification via SE is possible.

DS 12.30 Wed 17:00 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 X-ray absorption fine structure (EXAFS) are two widely used methods to investigate the structure of solid states. [1,2,3].

In this contribution, we present a self-consistent Maxwell-Bloch approach based on Heisenberg equations of motion for a 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 wave interference allows us to calculate the Fourier transformed EXAFS spectrum [2] predicting so far uninterpreted features which have not been assigned within point-scattering theory [1].

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

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

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

DS 12.31 Wed 17:00 P3

**Ultrafast vibrational dynamics of CH-stretch modes of surface adsorbates** — •TIM LÄMMERZAHN, NELLI KREMER, and ECKART HASSELBRINK — University Duisburg-Essen

The understanding of energy transfer between different modes in one molecule, which is called internal vibrational energy redistribution

(IVR), is crucial for further development in the field of rate theory and for applications in molecular electronics. As a model we study adsorbate monolayers of a single species using time-resolved two-color pump probe sum frequency spectroscopy.

Previously, we revealed that the coupling between valence vibrations is faster than a few ps and equilibrates with bending and torsion modes on a tens of ps time scale in fatty acid monolayers [1]. Now we moved on to conducting surfaces (e.g. gold) and used different terminated alkanethiols. Since gold surfaces exhibit a strong non-resonant (NR) signal, which is usually the dominant source of noise, we used the technique by Dlott et al. [2] to suppress the NR signal. Results from a study of alkylthiols with different headgroups on gold will be presented.

[1] Lackner, M., Hille, M., Hasselbrink, E. (2019), Phys. Chem. Lett., 11, 108-112.

[2] Lagutchev, A., Hambir, S. A., Dlott, D. D. (2007). J. Phys. Chem. C., 111, 13645-13647.

DS 12.32 Wed 17:00 P3

**Dynamics of the response of thiol monolayers to rapid heating** — ●MATTHIAS LINKE and ECKART HASSELBRINK — Universität Duisburg-Essen, 45141 Essen, Germany

Energy transport between metal substrates and molecules as well as intramolecular energy transport between vibrations is still not well understood, even though systems such as thiols on gold were studied extensively. Self-assembled molecular films are an ideal model system such as their characterization attracted much interest over the last decades, especially in the field of nanotechnology. It is well established that thiols adsorb easily and reproducibly on gold substrates by self-assembly. Sum-frequency generation vibrational spectroscopy (SFGvS) can be used for characterization of such systems, since it is inherently sensitive to surface species, interfaces at which centrosymmetry is broken. We adsorbed different thiols on Au-surfaces and heated the substrate by focussing an additional 25 ps 532 nm laser beam on the backside of the sample. Absorption of the photons leads to temperature jumps in the metal which can be assessed by tracking the reflectivity changes of the sample. Tracking the spectral changes via SFGvS at different delays between the pump and probe pulses can be done to assess the temperature effects induced in the substrate and the molecules and time constants can be extracted. The effect of the probing of different head groups ( $NO_2$ ,  $CN$ ,  $CH_3$ ) and variation of the spacer group are studied in this work.

DS 12.33 Wed 17:00 P3

**In-situ spectroscopic ellipsometry measurement and analysis of native SiO<sub>2</sub> behavior under different atmosphere and temperature** — ●YOUNES SLIMI<sup>1,2</sup>, JANNIS WALDMANN<sup>1</sup>, RÜDIGER SCHMID-GUND<sup>1</sup>, and STEFAN KRISCHOK<sup>1</sup> — <sup>1</sup>Technische Universität Ilmenau, Fachgebiet Technische Physik I, Weimarer Straße 32, 98693 Ilmenau, Germany — <sup>2</sup>Ferhat Abbas University, Institut of optics and precision mechanics, Optics and Applied Photonics laboratory 19000 Setif, Algeria

the most common wafer used in the semiconductor industry nowadays is silicon (Si), the latter oxidizes when left to its own devices. these silicon oxide layers' behavior was investigated using In-situ Spectroscopic ellipsometry to obtain optical constants and thin film thicknesses under different atmospheres (nitrogen, dry air) and temperatures. We found changes in the refractive index and thickness of the SiO<sub>2</sub> layer under different conditions due to oxidation and material ablation. These results are meant to be used as possible references for future Electrochemical cells for in-situ Spectroscopic ellipsometry measurement for water splitting devices.

DS 12.34 Wed 17:00 P3

**Sprayed hybrid nanocellulose fibril-silver nanowire transparent electrodes** — ●MARIE BETKER<sup>1,2</sup>, CONSTANTIN HARDER<sup>1,3</sup>, ELISABETH ERBES<sup>1,4</sup>, JULIAN HEGER<sup>3</sup>, ALEXANDROS E. ALEXAKIS<sup>2,5</sup>, BENEDIKT SOCHOR<sup>1</sup>, QING CHEN<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>1</sup>, ANDREI CHUMAKOV<sup>1</sup>, PETER MÜLLER-BUSCHBAUM<sup>3,6</sup>, KONRAD SCHNEIDER<sup>7</sup>, SIMONE TECHERT<sup>1</sup>, L. DANIEL SÖDERBERG<sup>2,5</sup>, and STEPHAN V. ROTH<sup>1</sup> — <sup>1</sup>DESY, 22607 Hamburg — <sup>2</sup>Fibre and Polymer Technology, KTH, 10044 Stockholm, Sweden — <sup>3</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching — <sup>4</sup>Institute for X-ray Physics, Goettingen University, 37077 Goettingen — <sup>5</sup>WWSC, KTH, 10044 Stockholm, Sweden — <sup>6</sup>MLZ, TUM, 85748 Garching — <sup>7</sup>Leibniz-Institut für Polymerforschung Dresden e.V., Abteilung Werkstofftechnik, 01069 Dresden

The fabrication of sustainable, thin, and flexible electrical devices on an industrial scale will be an important challenge in the future. Nanocomposites, consisting of conductive nanoparticles like silver nanowires (AgNWs) and a sustainable matrix material like cellulose nanofibrils (CNFs), can meet these requirements. Here, we report on the nanoscale structure and the corresponding optoelectronic properties of a sprayed CNFs-AgNWs nanocomposite electrode. Adding CNF to the aqueous AgNW-based spray ink improves the dispersion and distribution of the AgNWs. This, and the cold-welding of the AgNW junctions enhance the conductivity of the electrode greatly. Finally, we demonstrate the electrode's high transmittance, resilience under multiple cycles of bending deformations, and its long-term stability.

DS 12.35 Wed 17:00 P3

**Detecting nitrogen-vacancy-hydrogen centers on the nanoscale using nitrogen-vacancy centers as local sensors in CVD-diamond** — ●CHRISTOPH FINDLER, GERHARD WOLFF, KAROLINA SCHÜLE, RÉMI BLINDER, PRIYADHARSHINI BALASUBRAMANIAN, JOHANNES LANG, CHRISTIAN OSTERKAMP, and FEDOR JELEZKO — Institute for Quantum Optics, Ulm University, Albert-Einstein-Allee 11, D-89081 Ulm, Germany

The negatively-charged nitrogen-vacancy center (NV) in diamond has attracted a lot of attention in the field of quantum technologies as it shows coherence times up to milliseconds at room temperature and enables optical polarization and coherent control of the electron spin. Apart from NV centers, the spin bath in diamond grown by chemical vapor deposition (CVD) consists mainly of substitutional nitrogen (P1) and negatively charged nitrogen-vacancy-hydrogen (NVH) defects which are usually analyzed by electron paramagnetic resonance (EPR) spectroscopy. In nm-thick epitaxial layers, however, the total number of paramagnetic spins becomes eventually too low for state-of-the-art EPR spectrometers. This problem can be solved by switching to a confocal microscope and studying the NV centers optically. Here, we show that 15NV ensembles can be employed as local sensors to estimate the density of non-fluorescent 15NVH and P1 centers in 15N-doped (100)-diamond layers and even get insight into the spatial distribution and correlation of P1 and 15NVH on the micrometer scale using a wide-field microscope.

DS 12.36 Wed 17:00 P3

**Tailoring Optical Properties in Transparent Highly Conducting Perovskites by Cationic Substitution** — ●MAHDAD MOHAMMADI, RUIWEN XIE, NILOOFAR HADAEGHI, ALDIN RADETINAC, ALEXEY ARZUMANOV, PHILIPP KOMISSINSKIY, HONGBIN ZHANG, and LAMBERT ALFF — Institute of Materials Science, Technische Universität Darmstadt

SrMoO<sub>3</sub>, SrNbO<sub>3</sub>, and SrVO<sub>3</sub> are remarkable highly conducting  $d^1$  (V, Nb) or  $d^2$  (Mo) perovskite metals with an intrinsically high transparency in the visible. A key scientific question is how the optical properties of these materials can be manipulated to make them suitable for application as transparent conductors and emergent plasmonics. In this work, it is demonstrated for the first time how  $3d/4d$  cationic substitution in perovskites shifts the optical transition energy and plasma frequency. At the example of the solid solution SrV<sub>1-x</sub>Mo<sub>x</sub>O<sub>3</sub> we show that the absorption and reflection edges can be shifted to the edges of the visible, resulting in a material that has the potential to outperform ITO due to its extremely low sheet resistance. For  $x = 0.5$ , a resistivity of 32  $\mu\Omega\text{cm}$  ( $12 \Omega/\text{sq.}$ ) is paired with a transmittance above 84 % in the whole visible spectrum. Quantitative comparison between experiments and electronic structure calculations show that the shift of the plasma frequency is governed by the interplay of  $d$ -band filling and electronic correlations.

[1] M. Mohammadi *et al.*, "Tailoring Optical Properties in Transparent Highly Conducting Perovskites by Cationic Substitution", Adv. Mater. (2022), Accepted Author Manuscript 2206605

DS 12.37 Wed 17:00 P3

**Influence of dielectric Layers on the optomechanical Properties of Polymer Membranes in a Fiber Cavity** — ●ANDREAS REUSS<sup>1</sup>, STEFAN LINDEN<sup>1</sup>, HANNES PFEIFER<sup>2</sup>, LUKAS TENBRAKE<sup>2</sup>, and ALEXANDER FASSBENDER<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Bonn, Germany — <sup>2</sup>Institut für Angewandte Physik, Universität Bonn, Germany

Fiber cavities are an attractive platform for optomechanical experiments as they can combine direct fiber-coupled optical access, small cavity lengths, high optical finesse, and an open resonator volume. Direct laser writing allows for a fast and flexible way to add polymer

drums as mechanical resonators directly on the end facets of a fiber cavity. These membrane-in-the-middle systems show a rather large optomechanical coupling strength despite of the low reflectivity due to the maximized intensity differences on the two membrane interfaces. A disadvantage of direct laser written structures are the comparatively large mechanical losses of the used resist, which limit the mechanical quality factor of the membranes to several hundred at cryogenic temperatures. Therefore, we are interested how the deposition of different dielectric layers influences the optomechanical response of the polymer membranes. By using materials with high young's modulus, like  $\text{MgF}_2$ , we aim to reduce overall mechanical losses and therefore increase the optomechanical response.

DS 12.38 Wed 17:00 P3

**IST 312 - an unconventional phase change material?** — ●MARIA HÄSER, PETER KERRES, SOPHIA WAHL, CARL-FRIEDRICH SCHÖN, and MATTHIAS WÜTTIG — I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen Germany

Chalcogenide-based Phase Change Materials (PCM) are a prominent candidate for energy-efficient memory devices. This material class shows a significant difference in its optical properties between the amorphous and crystalline phases: The former phase shows more insulating characteristics. In contrast, the almost metallic properties characterise the crystalline state. However, enabling fast switching between insulators and a real metal would broaden the field of application of PCMs.

In this study, the unusual phase change material  $\text{In}_3\text{SbTe}_2$  (IST) has been investigated, which shows a metallic-like behaviour in its crystalline phase. The dielectric functions of both phases were determined using optical measurements (FTIR, Ellipsometry). Additionally, DFT calculations and XRD measurements were performed to better understand the unusual property change.

DS 12.39 Wed 17:00 P3

**Characterization of the interaction of acrylic polymers with gold and silica surfaces** — ●SASCHA JAN ZIMMERMANN, PHILIPP MORITZ, and WOLFGANG MAUS-FRIEDRICH — Clausthal Centre of Material Technology, Clausthal University of Technology, Agricolastr. 2, 38678 Clausthal-Zellerfeld

Adhesives play a key role in the 21st century. In particular, hybrid material composites can be joined in this way while saving weight. To advance this technology, a fundamental understanding of adhesive interactions, particularly to metal (oxide) substrates, is required.

In order to investigate these interactions, nanometer thin planar polymer films were deposited on the model substrates of silicon oxide and gold. This was done for the polymers poly(methyl methacrylate) and poly(glycidyl methacrylate) applying a spin coating process. X-ray photoelectron spectroscopy (XPS), Metastable Impact Electron Spectroscopy (MIES) and Ultraviolet photoelectron spectroscopy (UPS) were used to analyze the chemical interactions at the interface.

In the case of PMMA, the XPS measurements show the presence of a carboxylate ion, which indicates probable ionic interactions. A varying chemical shift and the changes in the MIES spectra indicate additional hydrogen bonds. In the case of PGMA, no interactions were detected by the applied measurement methods.

DS 12.40 Wed 17:00 P3

**Photoinduced charge injection into single-layer WSe<sub>2</sub> via deposited dye molecules** — ●TIM VÖLZER<sup>1,2</sup>, ALINA SCHUBERT<sup>1,2</sup>, JULIAN SCHRÖER<sup>1</sup>, RICO SCHWARTZ<sup>1</sup>, TOBIAS KORN<sup>1,2</sup>, and STEFAN LOCHBRUNNER<sup>1,2</sup> — <sup>1</sup>Institute of Physics, University of Rostock, Albert-Einstein-Str. 23, 18059 Rostock, Germany — <sup>2</sup>Department "Life, Light and Matter", University of Rostock, Albert-Einstein-Str. 25, 18059 Rostock, Germany

The deposition of molecules allows the functionalization of 2D semiconductors as well as the fabrication of hybrid structures exhibiting charge separation after optical excitation that can be exploited in optoelectronic devices. Here, we investigate the charge transfer from optically excited molecules of the dye Perylene Orange (PO) into a monolayer of tungsten diselenide (1L-WSe<sub>2</sub>) by means of low-temperature micro-photoluminescence spectroscopy: In comparison to the blank 1L-WSe<sub>2</sub>, the proportion of charged trion versus neutral exciton emission is expected to change as the PO molecules are deposited and excited. In contrast, when reducing the pump photon energy below the PO absorption band, the emission spectrum would remain identical. Thus, we aim to control the light-induced charge injection into the WSe<sub>2</sub> by tuning the pump wavelength.

DS 12.41 Wed 17:00 P3

**Theoretical insights into the monolayer adsorption and characterization of HB238 Merocyanine on Ag(100) surface** — ●RITU TOMAR, THOMAS BREOW, ANNA KNY, and MORITZ SOKOŁOWSKI — Clausius Institute of Physical and Theoretical Chemistry, University of Bonn, Germany

Merocyanines (MCs) are intriguing compounds that can be used as efficient absorbers for organic solar cells. We studied the adsorption of HB238 merocyanine on the surface of Ag (100) using STM and SPA-LEED experiments, which suggested that HB238 self-organizes as chiral tetramers upon adsorption. The molecular structure was significantly different from the typical configuration in the bulk phases of HB238. It is critical to control the structure and morphology of merocyanine films to enhance light absorption and optimize their optoelectronic properties. Therefore, we performed quantum chemical calculations to corroborate our experimental findings. Initially, we screened the HB238 conformers and used the most stable structure to determine the optimal adsorption orientation of HB238 on the Ag surface using the semi-empirical method GFN1-XTB in DFTB+. HB238 preferentially adheres face-on to the Ag surface. Next, we optimized the tetramer models at the DFT level to analyze the assembly of chiral tetramers while maintaining supercell lattice constant values, as in the experiment. We then relaxed the HB238 molecules on the Ag 3-layer slab model and fixed the bottom two layers using the GGA method in VASP. However, rapid and effective system convergence was achieved only using the ASE/LBFGS optimization algorithm.

DS 12.42 Wed 17:00 P3

**Modelling liquid flow through nanopores on the nanoscale** — ●RUSTAM DURDYEV<sup>1</sup>, CHRISTIAN R. WICK<sup>1</sup>, and ANA-SUNČANA SMITH<sup>1,2</sup> — <sup>1</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg, PULS Group, Institute for theoretical physics, Interdisciplinary Center for Nanostructured Films (IZNF), Cauerstrasse 3, 91058 Erlangen, Germany — <sup>2</sup>Division of Physical Chemistry, Ruder Bošković Institute, Zagreb, Croatia

Liquid chromatography is one of the most important separation techniques and has proceeded mainly along empirical knowledge from the expansive collection of experimental data by using chromatographic methods, spectroscopic methods and technical innovations in column packing, particle technology and equipment design. However, a classic liquid chromatography column, is a cylinder densely packed with mesoporous silica particles whose surface has been mostly chemically modified. In this work, we investigated the physisorption of water to functionalized silica surfaces and hydrophilicity properties of surface by molecular dynamics simulations. We built on previously gathered knowledge on chromatography to establish a unified picture of stationary phase and solute mobility in liquid chromatography. In analogy to previous studies, we utilized a crystalline SBA-15 structure as starting point for our modeling approach. Furthermore, we investigate the effect of functionalization using different loadings with silanol group (Si-OH) and trimethylsilyl groups (O-Si-(CH<sub>3</sub>)<sub>3</sub>). With this strategy, we hope to understand the effect of functionalization of silica on the physisorption of water molecules at the nanometer scale.

DS 12.43 Wed 17:00 P3

**Optimizing two-dimensional materials for biomolecule detection using machine learning techniques** — ●CALIN-ANDREI PANTIS-SIMUT<sup>1,2,3</sup>, AMANDA TEODORA PREDĂ<sup>1,2,3</sup>, NICOLAE FILIPOIU<sup>1,2</sup>, and GEORGE ALEXANDRU NEMNES<sup>1,2,3</sup> — <sup>1</sup>Horia Hulubei National Institute of Physics and Nuclear Engineering (IFIN-HH), Str. Reactorului no.30, P.O.BOX MG-6, Magurele, Romania — <sup>2</sup>University of Bucharest, Faculty of Physics, 077125 Magurele-Ilfov, Romania — <sup>3</sup>Research Institute of the University of Bucharest (ICUB), Sos. Panduri 90, Bucharest Romania.

The problem of correctly identifying the biomarkers associated with specific pathologies is of great interest nowadays for rapid diagnoses. The transport properties of different active layers like beta-arsenate, phosphorene, graphene, or Al-doped MoSe<sub>2</sub> were investigated in the presence of certain biomolecules. Additionally, predictions of biomolecular compounds with tunable gaps were reported as well as carbon nanotube-based. Our study brings a detailed analysis of 2D semiconductor heterostructures in contact with biomarkers of respiratory diseases, which exhibit large tunabilities in transport properties. As a first step, by using DFT simulations, the electronic properties of the systems are analyzed under different doping conditions and nanostructuring. In a second step, a large number of systems will be considered

for transport calculations and the results will define the input for machine learning procedures. This involves the mapping between structural information and transport properties. In the end, an analysis of the sensor's limit of detection and regeneration is performed.

DS 12.44 Wed 17:00 P3

**Microstructure investigation of pulsed laser deposited GeTe-Sb<sub>2</sub>Te<sub>3</sub> heterostructures** — ●SONJA CREMER<sup>1</sup>, LENNART VOSS<sup>2</sup>, NILS BRAUN<sup>1</sup>, LORENZ KIENLE<sup>2</sup>, and ANDRIY LOTNYK<sup>1,3,4</sup> — <sup>1</sup>Leibniz Institute of Surface Engineering, Leipzig — <sup>2</sup>Faculty of Engineering, University of Kiel — <sup>3</sup>Laboratory of Infrared Materials and Devices, Ningbo University — <sup>4</sup>College of Physics and Optoelectronic Engineering, Harbin Engineering University

Heterostructured phase change materials are an auspicious candidate to overcome high power consumption and resistance drift, hindering the implementation of Ge-Sb-Te based thin films for neuromorphic computing. Aiming at future systematic performance improvement, the impact of deposition parameters on the microstructure of GeTe-Sb<sub>2</sub>Te<sub>3</sub> heterostructures (HSs) was investigated. HSs were grown at RT onto SiO<sub>2</sub>/Si by PLD. Combining advanced TEM with XRD the microstructure was investigated in-depth. Energy and number of laser pulses affect the layer thickness and composition. The low energy and number of pulses lead to pronounced intermixing and hence to the formation of a single GeSb<sub>2</sub>Te<sub>4</sub> layer. Besides, the local structure of the layers within the HS differs. While GeTe layers are amorphous, Sb<sub>2</sub>Te<sub>3</sub> layers are polycrystalline and contain nanocrystals featured by varying sizes, defects and multiple phases. Thus, deposition parameters mainly affect the morphology and chemical composition of GeTe-Sb<sub>2</sub>Te<sub>3</sub> HSs. However, the main factor influencing the crystallinity of the HS layers is the alloy itself. Financial support by the DFG (No. 445693080) is acknowledged. We thank A. Mill for assistance in FIB preparation.

DS 12.45 Wed 17:00 P3

**Dynamics of ion beam-induced defects in phase-change materials investigated by in-situ optical measurements** — ●SEBASTIAN GRATZ, MARCEL BUCH, MARTIN HAFERMANN, and CARSTEN RONNING — Institute of Solid State Physics, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

Phase-change materials (PCMs) provide the ability of reversible, repeatable and rapid switching between amorphous and crystalline states. These transformations are accompanied with drastic changes of the electrical and optical properties, which is already been used in rewritable optical data storage or phase-change electronic memory. The transitions can be triggered by external thermal, optical, or electrical stimuli. The most extensively studied PCMs are pseudobinary (GeTe)<sub>m</sub>(Sb<sub>2</sub>Te<sub>3</sub>)<sub>n</sub> chalcogenide compounds (m, n being integer values), short GST. Ion irradiation was recently introduced to induce structural disorder and amorphize initially crystalline GST films. There are multiple studies that investigated the effect of defect engineering of GST compounds. However, there is still a lack of understanding of the dynamic effects, such as dynamic annealing of defects during the ion irradiation process. Furthermore, the direct impact of the specific GST stoichiometry on the ion-beam induced disorder has not been observed yet. Thus, we investigated the dynamics of defect formation for different GST stoichiometries, such as Ge<sub>1</sub>Sb<sub>2</sub>Te<sub>4</sub> (m=1, n=1), Ge<sub>1</sub>Sb<sub>4</sub>Te<sub>7</sub> (m=1, n=2), and Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> (m=2, n=1), via in-situ optical measurements during ion irradiation at different temperatures.

DS 12.46 Wed 17:00 P3

**Preparation and characterization of Cu-Te phases using focused ion beam** — ●NILS BRAUN<sup>1</sup>, VLADIMIR RODDATIS<sup>2</sup>, AGNES MILL<sup>1</sup>, SONJA CREMER<sup>1</sup>, HAGEN BRYJA<sup>1</sup>, LENNART VOSS<sup>3</sup>, LORENZ KIENLE<sup>3</sup>, and ANDRIY LOTNYK<sup>1,4,5</sup> — <sup>1</sup>Leibniz Institute of Surface Engineering e.V. (IOM) — <sup>2</sup>GFZ German Research Centre for Geosciences — <sup>3</sup>Institute for Materials Science, Faculty of Engineering, University of Kiel — <sup>4</sup>Laboratory of Infrared Materials and Devices, The Research Institute of Advanced Technologies, Ningbo University — <sup>5</sup>College of Physics and Optoelectronic Engineering, Harbin Engineering University

In this work, we prepared different nanoscale Cu-Te phases from Cu - Sb<sub>2</sub>Te<sub>3</sub> system using FIB. Copper chalcogenides have shown promising thermoelectric properties, e.g. high efficiency and tunability. Sb<sub>2</sub>Te<sub>3</sub> thin layers are epitaxially grown on p-type Si (111) substrates and polycrystalline Sb<sub>2</sub>Te<sub>3</sub> thin film are grown on a SiO<sub>2</sub> coated wafer using PLD. A standard cross-section FIB preparation method is used. Samples are investigated using advanced TEM methods and XRD. Depen-

dent on beam current used during FIB lamella preparation and Sb<sub>2</sub>Te<sub>3</sub> layer thickness, hole formation in the Cu layer, thickness change and chemical changes of the Sb<sub>2</sub>Te<sub>3</sub> layers are observed. In specimen prepared from the heated samples Sb<sub>2</sub>Te<sub>3</sub> and Cu-Te grains are found. In polycrystalline Sb<sub>2</sub>Te<sub>3</sub> specimen the intercalation of Cu and formation of new Cu-Te phases is observed. We thank P. Hertel for magnetron sputtering. We acknowledge the financial support by the German Research Foundation (DFG 448667535).

DS 12.47 Wed 17:00 P3

**Investigation of the insights of a TiN-PEALD process in a remote capacitively coupled plasma ALD reactor** — ●JAN BIEDINGER, JAN-MICHAEL SCHMALHORST, and GÜNTER REISS — Bielefeld University, Faculty of Physics, Germany

Atomic Layer Deposition (ALD) is a deposition technique of great interest due to precise and reproducible layer control, large-area uniformity and conformal coating. As it bases on chemical surface reactions, it is important to understand the mechanism of an ALD process. In the presented study, the effect of different process parameters (temperature, plasma power, plasma pulse length, NH<sub>3</sub> flow, plasma pressure) was studied in a titaniumnitride (TiN) plasma-enhanced ALD process, consisting of sequential pulsing of tetrakis(dimethylamido)titanium (TDMAT) and a NH<sub>3</sub> plasma. X-ray reflectivity and 4-point probe measurements were performed to determine the growth rate, roughness, density and electrical resistivity of all TiN films, respectively. Additionally, Auger electron spectroscopy revealed information about the chemical composition. By combining in-situ mass spectrometry data, where plasma species as well as reaction products could be identified during the process, with these ex-situ results, the process could be described in more detail. During the NH<sub>3</sub> step, the release of dimethylamine groups was observed, which decreased gradually with time. This correlates with the decline of carbon content by increasing the NH<sub>3</sub> step time. Moreover, it was observed that the plasma species (hydrogen and nitrogen radicals) seems to be responsible for decreasing the oxygen content and hence, improving thin film quality.

DS 12.48 Wed 17:00 P3

**Epitaxial growth of Ag<sub>x</sub>Cu<sub>1-x</sub>I on Al<sub>2</sub>O<sub>3</sub> (0001)** — ●E. KRÜGER<sup>1</sup>, V. GOTTSCHALCH<sup>2</sup>, G. BENNDORF<sup>1</sup>, R. HILDEBRANDT<sup>1</sup>, A.L. PEREIRA<sup>1</sup>, M. BAR<sup>1</sup>, E. ABO EL FADL<sup>1</sup>, S. BLAUROCK<sup>2</sup>, S. MERKER<sup>2</sup>, C. STURM<sup>1</sup>, M. GRUNDMANN<sup>1</sup>, and H. KRAUTSCHEID<sup>2</sup> — <sup>1</sup>Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany — <sup>2</sup>Universität Leipzig, Institut für Anorganische Chemie, Germany

Copper iodide (CuI) and related alloy compounds are of great interest as suitable materials for applications in fully transparent optoelectronic devices. While CuI exhibits intrinsic p-type conductivity with excessive high hole densities typically around 10<sup>18</sup> – 10<sup>19</sup> cm<sup>-3</sup>, it was recently shown that the carrier density can be strongly reduced for Ag<sub>x</sub>Cu<sub>1-x</sub>I alloy and even n-type conductivity can be achieved for high Ag contents [1]. Here we present the epitaxial growth of Ag<sub>x</sub>Cu<sub>1-x</sub>I thin films on Al<sub>2</sub>O<sub>3</sub> (0001) substrates using sublimation technique [2]. We demonstrate that Ag<sub>x</sub>Cu<sub>1-x</sub>I thin films with x ≤ 0.5 exclusively exhibit the zincblende γ-phase, while a coexistence of zincblende γ- and wurtzite β-phases is observed for Ag-rich alloy compositions. In addition we provide the epitaxial relationships between the different Ag<sub>x</sub>Cu<sub>1-x</sub>I phases and the Al<sub>2</sub>O<sub>3</sub> substrate. Moreover, we present another deposition approach based on a solid-state reaction between CuI and AgI, which allows the preparation of single-phase γ-Ag<sub>x</sub>Cu<sub>1-x</sub>I films up to x = 0.7.

[1] A. Annadi and H. Gong, Appl. Mater. Today **20**, 100703 (2020)

[2] E. Krüger et al., Phys. Stat. Solidi B (accepted)

DS 12.49 Wed 17:00 P3

**Growth of CoO Thin Films for Application in Superconductor - Magnet Heterostructures** — ●AMY MCGLINCHY — 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 low Néel temperature, which facilitates in-field cooling through the transition improving magnetic homogeneity. For the most part, CoO is synthesized by the oxidation of Co thin films or using techniques such as spray pyrolysis and pulsed laser deposition. In this work, we focus on



the growth of CoO by molecular beam epitaxy, investigating the crystalline quality of the CoO as a function of deposition conditions. We have optimised these conditions to grow single crystalline CoO(100) thin films on MgO(100) substrates. As a second step towards a F-S-AF heterostructure, we also investigate the superconducting properties of Nb grown on CoO films. Due to the proximity effect, the properties of the niobium - especially at low thickness relevant to heterostructures - will be influenced by the CoO magnetic and interface structure [2]. 1. L. G. Johnsen et al., Phys. Rev. B, 103, L060505 (2021). 2. G. A. Bobkov et al., Phys. Rev. B, 106, 144512 (2022).

DS 12.50 Wed 17:00 P3

**Potential of La-doped SrTiO<sub>3</sub> thin films grown by metal-organic vapor phase epitaxy for thermoelectric applications** — ●MOHAMED ABDELDAYEM<sup>1</sup>, AYKUT BAKI<sup>1</sup>, CARLOS MORALES SÁNCHEZ<sup>3</sup>, JAN INGO FLEGE<sup>3</sup>, DETLEF KLIMM<sup>1</sup>, ANDREAS FIEDLER<sup>1</sup>, OLIVER BIERWAGEN<sup>2</sup>, and JUTTA SCHWARZKOPF<sup>1</sup> — <sup>1</sup>Leibniz Institut für Kristallzüchtung, Berlin, Germany — <sup>2</sup>Paul Drude Institut für Festkörperelektronik, Berlin, Germany — <sup>3</sup>Brandenburgische Technische Universität Cottbus, Brandenburg, Germany

Conversion of waste heat energy into electrical energy by exploiting the thermoelectric effect in solids promises a great contribution to energy harvesting concepts. However, most thermoelectric materials use toxic Pb or Te. Recently, La-doped SrTiO<sub>3</sub> has gained a lot of interest as a potential candidate for thermoelectric devices for its good thermoelectric properties, chemical and thermal stability. In this paper, we report the homoepitaxial growth of La-doped SrTiO<sub>3</sub> thin films by metal-organic vapor phase epitaxy (MOVPE) technique, which works at high oxygen partial pressures and offers upscaling potential for industry. The adjustment of charge carrier concentration, necessary for thermoelectric power factor optimization, was performed by introducing a defined amount of the metal-organic precursor La(tmhd)<sub>3</sub> and tetraglyme to the liquid precursor solution. X-ray diffraction and atomic force microscopy verified a pure perovskite phase with high structural quality. The electrical conductivity increases linearly with the La concentration in the gas phase, which is attributed to the substitution of La+3 ions on the Sr+2 sites inferred from photoemission spectroscopy.

DS 12.51 Wed 17:00 P3

**Ultrathin alumina membrane: A new opportunity for constructing stable sodium metal anodes** — ●JIAJIA QIU, CHANGFAN XU, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Unstable solid electrolyte interphase (SEI) remains a major bottleneck for sodium metal batteries due to the mossy or dendritic growth of Na in the repetitive stripping/plating process. Recently, nanostructured modification of Na and Al<sub>2</sub>O<sub>3</sub> coatings have been reported as two effective solutions to address this issue. Accordingly, with almost identical pore regularity and precisely controlled geometrical structure, ultrathin alumina membrane (UTAM) is utilized as a functional layer to effectively protect the Na anode of Na-metal batteries for the first time in this work. The mossy or dendritic growth of Na has been suppressed due to the UTAM protection, resulting in a uniform electrodeposition interface. UTAM significantly improved the Coulombic efficiency while avoiding short circuit risks. And it has the potential to be applied to other metal anodes. The novel design of a UTAM-protected metal Na anode may bring in new opportunities for next-generation high performance Na metal batteries.

DS 12.52 Wed 17:00 P3

**Contact printed micro circuit boards for thermoelectric circuits in van der Waals high temperature twisted cuprate heterostructures** — ●SANAZ SHOKRI<sup>1,2</sup>, CHRISTIAN N SAGGAU<sup>1</sup>, KORNELIUS NIELSCH<sup>1,2</sup>, and NICOLA POC CIA<sup>1</sup> — <sup>1</sup>Institute for Metallic Materials, IFW Dresden, Dresden, Germany, IFW Dresden — <sup>2</sup>Institute for Materials Science, Dresden University of Technology

Recently, thermoelectric measurement has been established as an indicator of the topological nature of material due to its sensitivity to the Berry curvature. Nernst effect, which is defined as a generation of transverse electric field by a longitudinal temperature gradient in the presence of a magnetic field, in particular, is a powerful tool to investigate the area above superconductivity transition temperature where the transverse electrical signals become very small. Twisted Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+δ</sub> (BSCCO) van der Waals heterostructures have exhibited topological superconductivity. Nevertheless, the BSCCO is too fragile to make a complex circuit like thermoelectric. Therefore, we de-

veloped the whole thermoelectric circuit like Seebeck and Nernst, embedded within inorganic SiN so called nanomembrane and transferred it on the optimally doped BSCCO flake inside the Ar-filled glovebox to encapsulate the BSCCO flakes and contact it at the same time. We used Pt as a heater and gold as the thermocouples and will calibrate our measurements based on the heat losses through a thermal insulating substrate and nanomembrane as well.

DS 12.53 Wed 17:00 P3

**Preparation and characterization of Zn<sub>1-x</sub>Mg<sub>x</sub>O thin films obtained by the aerosol deposition method for UV radiation detector** — ●VADIM MORARI — Technical University of Moldova, D. Ghitu Institute of Electronic Engineering and Nanotechnologies, Chisinau, Republic of Moldova

Zn<sub>1-x</sub>Mg<sub>x</sub>O ternary oxide solutions with wide band gap were prepared by the aerosol spray deposition method [1] using zinc acetate and magnesium acetate as precursors. This technique offers the possibility of rapid deposition of homogeneous thin films with good electrical and optical properties. It is suitable for growing high-quality thin films on Si, quartz, glass or sapphire substrate, with relatively large areas at low cost due to vacuum-free equipment, low temperatures during deposition, low defect density and low environmental impact. The obtained thin films were characterized by scanning electron microscopy (SEM), energy dispersive X-Ray analysis (EDX), X-Ray Diffraction (XRD), Raman spectroscopy and optical absorption spectroscopy. The investigation of photosensitivity revealed that multilayer ZnMgO structures with different Mg content are more sensitive than single-layer films in a wide spectral range from visible to the ultraviolet (UV-C) radiation.

[1] Morari, V., et. All. Photosensitivity of heterostructures produced by aerosol deposition of ZnMgO thin films on Si substrates. In: Proceedings of SPIE - The International Society for Optical Engineering, vol. 11718, p. 1171818:1\*8, (2020). <https://doi.org/10.1117/12.2571189>.

DS 12.54 Wed 17:00 P3

**Heterostructure diodes based on reactively co-sputtered Ag<sub>x</sub>Cu<sub>1-x</sub>I thin films** — ●JORRIT BREDOW, SOFIE VOGT, CHRISTIANE DETHLOFF, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Universität Leipzig, Felix-Bloch-Institut, Germany

Copper iodide (CuI) is a transparent p-type semiconductor that exhibits high hole mobilities of up to 25 cm<sup>2</sup>/Vs in polycrystalline thin films<sup>[1]</sup>. This renders CuI an interesting candidate for the fabrication of transparent heterostructure diodes, such as p-CuI/n-ZnO<sup>[2]</sup>, or p-CuI/n-AgI<sup>[3]</sup>. CuI further exhibits a low resistivity, which was shown to be increased with an increasing fraction of silver (Ag) in Ag<sub>x</sub>Cu<sub>1-x</sub>I thin films<sup>[4]</sup>. Moreover, a transition from p-type to n-type material of the Ag<sub>x</sub>Cu<sub>1-x</sub>I thin films for  $x \approx 0.5$  was observed<sup>[4]</sup>. However, the Ag<sub>x</sub>Cu<sub>1-x</sub>I thin films were prepared with the Bädiker method, i.e. the iodization of metallic Ag<sub>x</sub>Cu<sub>1-x</sub> thin films.

We present transparent heterostructure diodes based on the ternary compound Ag<sub>x</sub>Cu<sub>1-x</sub>I. The Ag<sub>x</sub>Cu<sub>1-x</sub>I thin films were deposited using reactive co-sputtering of metallic Cu and Ag in Ar and I atmosphere. The feasibility of pn-heterojunction diodes with varying silver content is presented.

[1] C. Yang *et al.*, ACS Appl. Electr. Mater., 2, 3627-3632, 2020.

[2] F.-L. Schein *et al.*, Appl. Phys. Lett., 102, 092109, 2013.

[3] J.-H. Cha and D.-Y. Jung, ACS Appl. Mater. Interfaces, 9, 43807-43813, 2017.

[4] A. Annadi *et al.*, Appl. Mater. Today, 20, 100703, 2020.

DS 12.55 Wed 17:00 P3

**SnTe topological insulator thin film for field-effect transistors** — ●SEPIDEH IZADI, NEGIN BERYANI NEZAFAT, and GABI SCHIERNING — Department of physics, Experimental physics, Bielefeld University, 33615, Bielefeld, Germany

Topological insulators (TIs) as a new class of quantum materials are one of the potential interests for device fabrication. The unique electrical characteristics of TIs arises from robust metallic states passing through the bulk semiconducting band gap within the material. These surface states with high electrical mobility are considered as an efficient factor regarding high performance transistor. We herein present SnTe topological insulator as a potential candidate for active layer in field-effect transistor (FET). In this work the results of SnTe transistor device fabrication is reported using bottom gate approach. There-with, Si<sub>3</sub>N<sub>4</sub> and Al<sub>2</sub>O<sub>3</sub> are applied as gate insulating material which are deposited using magnetron sputtering and atomic layer deposition (ALD), respectively. The provided findings and analysis in this work

paves the way for SnTe electrical device characterization.

DS 12.56 Wed 17:00 P3

**Electric field induced laser-assisted polarization switching dynamics in ferroelectric thin films** — ●REKIKUA SAHILU ALEMAYEHU<sup>1</sup>, MATTHIAS RÖSSLE<sup>2</sup>, and MATIAS BAGRHEER<sup>1,2</sup> — <sup>1</sup>Institute for Physics & 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.

DS 12.57 Wed 17:00 P3

**Engineering Vertical Memristive Devices with TMDC Thin Films** — ●ANNA LINKENHEIL<sup>1,2</sup>, THERESA SCHELER<sup>3,2</sup>, OLE GRONENBERG<sup>4</sup>, HENDRIK GROSS<sup>4</sup>, MICHAELA BLUM<sup>3,2</sup>, TZVE-

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Transition metal dichalcogenides (TMDCs) represent a class of promising materials for memristive devices, which become increasingly important for emerging information processing approaches. In particular, homogeneous thin-films of few layers thickness have advantageous properties for memristive devices, such as excellent scaling behavior combined with the potential integration into planar wafer technology. Here, we assess the electrical properties of sputtered MoS<sub>2</sub> based devices and analyze the material. The devices were fabricated in a 4-inch wafer thin film technology, allowing for a systematic electrical investigation. Various electrode materials as well as oxidation treatments and their respective influences on device performance are evaluated using Transmission Electron Microscopy (TEM), revealing probable switching mechanisms and their origin.