

O 63: Poster DS (joint session DS/MM/O)

Time: Wednesday 17:00–19:00

Location: Poster B

O 63.1 Wed 17:00 Poster B

Tailoring Ti₃C₂ MXenes towards the Oxygen Evolution Reaction — ●ALINE ALENCAR EMERENCIANO and MICHELLE BROWNE — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Ti₃C₂ MXenes are promising materials for water splitting due to their high conductivity, hydrophilicity, and good mechanical properties when compared to other 2D-nanomaterials [1]. The possibility of tailoring MXenes in terms of functional groups, flake size/shape, presence of defects, and surface area makes them excellent candidates to be hybridized with transition metal oxides. MXenes/TMO catalysts can provide synergetic properties such as high conductivity in combination with active sites for Oxygen Evolution Reaction (OER). To reduce the mass loading by increasing the intrinsic activity and stability of MXenes, the surface functionalization and surface area must be controlled. In this work, in situ generated HF was utilized to remove Al-elements for the production of Ti₃C₂. Synthesis protocols utilizing different concentrations of HCl were investigated to evaluate the flake quality in terms of functional groups distribution, flake size towards the existence of multilayered and delaminated nanoflakes, as well as the concentration of pin-roles on their surface. Overall, this work provides a better understanding in how HCl concentration can influence the MXenes contribution in hybrid electrocatalysts considering functional groups distribution and presence of defects.

1.Zhang, C. J. et al. Adv. Mater. 29, 1-9 (2017).

O 63.2 Wed 17:00 Poster B

Chemical functionalisation of CuCo(2)-LDH on V(2)CT(x) for the oxygen evolution reaction — ●BASTIAN SCHMIEDECKE and MICHELLE BROWNE — Helmholtz-Zentrum Berlin, Berlin, Germany

MXenes, known for their exceptional surface area and high conductivity, serve as excellent catalyst supports, enhancing electrocatalytic performance in the oxygen evolution reaction (OER). Layered double hydroxide (LDH) materials, though promising for the OER, lack conductivity to ensure easy charge transfer during electrochemical processes. While, research on LDH materials has developed rapidly, there remains a high demand for refining the strategic combination of LDH with two dimensional (2D) materials, such as MXenes, which can significantly improve the water oxidation performance of LDH materials by inducing high conductivity, hydrophilicity and surface area.

This study introduces a hybrid catalyst, CuCo₂-LDH grown on delaminated vanadium carbide (V(2)CT(x)) nanosheets to enhance the OER performance. The synthesized CuCo₂-LDH@V(2)CT(x) electrocatalyst exhibited excellent activity with an overpotential of 289 mV at a catalytic current density of 10 mA cm⁻² with a Tafel slope value of 74 mV dec⁻¹. Furthermore, slight performance improvements were observed after 12 h of continuous operation. We propose that the enhanced performance is attributed to the conductivity of V(2)CT(x) and its synergistic interaction with CuCo₂-LDH, effectively minimizing aggregation, exposing more active sites. This work demonstrates the significant potential of combining LDH-based nanomaterials with V(2)CT(x) MXene for energy conversion applications.

O 63.3 Wed 17:00 Poster B

Analysis of polarization dependent IR spectra of thin films — ●KARSTEN HINRICHS¹, ANDREAS FURCHNER², FATIMA AKHTAR², NORBERT H. NICKEL², and JÖRG RAPPICH² — ¹Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Application Laboratories Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany — ²Helmholtz-Zentrum Berlin für Materialien und Energie GmbH 14109 Berlin, Germany

The interpretation of bands in polarization dependent infrared (IR) spectra of thin films is addressed. Several examples such as an isotropic polymer film and functionalized silicon surfaces will be discussed as case studies. It will be shown that the observed vibrational band properties depend on the measurement geometry, the film thickness, the materials dielectric functions, as well as the direction of the probing electromagnetic fields. Comparative Density Functional Perturbation Theory (DPFT) - calculations are used for analysis. The financial support by the Europäischer Fonds für regionale Entwicklung by EFRE 1.8/13 and ProFIT 10185407 as well as the Federal Ministry of Education and Research and the project CatLab (03EW0015A/B) is

acknowledged.

O 63.4 Wed 17:00 Poster B

Focused-Ion-Beam induced Defect Emission in Hexagonal Boron Nitride — ●FELIX SCHAUMBURG, DOMINIK KACZMAREK, DAVID PLITT, MARTIN GELLER, GÜNTHER PRINZ, and AXEL LORKE — Faculty of Physics, University of Duisburg-Essen and CENIDE, Germany

Defects in the wide bandgap material hexagonal boron nitride (hBN) exhibit single-photon emission at room temperature (RT) [1]. We used the gallium ion beam of a focused ion beam (FIB) to generate ensembles of defects that we associated with boron vacancies having a photoluminescence emission exceeding 800 nm [2]. After irradiation isolated point defects can also be found next to the irradiated areas. We show that our created defects exhibit a bright RT emission, an almost sublinear power dependence commonly associated with a two-level system and an increasing signal, a decreasing full width at half maximum (FWHM), and a minimal shift to lower wavelengths at lower temperatures. Our results show, that we can generate bright emitters in hBN by Ga-ion treatment that are in a wavelength range of up to 800 nm. Our next goals will be contacting these emitters by putting a gate structure on top of it, as well as creating single defects at higher wavelengths. [1] F. Hayee et.al., Nat.Mater.19 (2020) [2] C. Qian et.al., arXiv (2022)

O 63.5 Wed 17:00 Poster B

Optimizing electrical transport and SAW propagation in molybdenum disulfide — ●NOAH SPITZNER¹, PAI ZHAO¹, RENRONG LIANG², CHITHRA SHARMA¹, LARS TIEMANN¹, and ROBERT BLICK¹ — ¹Center of Hybrid Nanostructures, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg — ²School of Integrated Circuits, Tsinghua University, 100083 Beijing, China

Few-layered and monolayer MoS₂ has gained increasing significance in recent years, due to its large band gap of up to 1.9 eV at the K and K' valley of the hexagonal Brillouin zone. Surface acoustic waves (SAW) and transport measurements allow non destructive probing of the physics governing the material.

In this work we exfoliated MoS₂ flakes of a few layers onto a specially tailored substrate with LiNbO₃ as piezoelectric top layer. We can pass surface acoustic waves through the MoS₂ flake via an interdigitated transducer (IDT) electrode configuration and study the electrical response. To facilitate electron transport at low temperatures, liquid nitrogen physical vapor deposition (LNPVD) was utilized to deposit the contact metals. The cooled deposition reduces Fermi level pinning (FLP) in the contact interface and empowers us to measure longitudinal and transversal voltages with better contact quality.

Under acoustic excitation at 4.2 K, we observed acoustic currents and voltages in MoS₂ that depend on the power and frequency of the SAW. Hence, we were able to observe the acoustoelectric and acousto-galvanic effect. We also studied magnetotransport under perpendicular magnetic fields and the weak localization phenomenon.

O 63.6 Wed 17:00 Poster B

Creating realistic carbon nanomembranes using molecular dynamics model simulations — ●LEVIN MIHLAN¹, ANNA NIGGAS², FILIP VUKOVIC², JÜRGEN SCHNACK¹, and RICHARD A. WILHELM² — ¹Universität Bielefeld, Deutschland — ²TU Wien, Österreich

Inm thin carbon nanomembranes (CNMs) are synthesized from aromatic self-assembled monolayers (SAMs) by electron-induced crosslinking and supposedly of irregular internal structure, which renders standard spectroscopic characterization very difficult [1]. However MD simulations can offer insights into CNMs' internal structure. Recently, it was shown that the neutralisation dynamics of highly charged ions (HCIs) transmitting through thin materials are very sensitive to the material structure [2]. Hence, HCI spectroscopy may, together with accompanying simulations using a time dependent potential [3], be used to characterize CNMs. In order to obtain model membranes whose mechanical and spectral properties , fit to those of manufactured CNMs, a model process starting from a SAM is implemented as an MD simulation. Structures generated this way can be compared to alternative model structures, which are created by incorporating experimental mechanical properties as input parameters. This approach

helps to gain a better understanding of the internal structure of CNMs.

- [1] Demytyev et al. *ChemPhysChem* 21.10 1006 (2020)
 [2] Wilhelm, Richard A. *Surf.Sci.Rep.* Vol 77 Issue 4 (2022)
 [3] Wilhelm, Richard A; Grande, Pedro L. *Commun.Phys.*2,89 (2019)

O 63.7 Wed 17:00 Poster B

Rolle of Collective Behavior of Water Molecules in Robust Ferroelectricity in Graphene Nanoribbons — ●IGOR STANKOVIĆ¹, M. AWAIS ASLAM², and ALEKSANDAR MATKOVIĆ² — ¹Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, 11080 Belgrade, Serbia — ²Institute of Physics, Montanuniversität Leoben, Franz Josef Strasse 18, 8700 Leoben, Austria

An understanding of the water dynamics on the edges of one and two-dimensional structures is scarce. Still, such interactions can be sufficient to perturb local electric environments, therefore offering an opportunity to harness the effect of the local dipole moment of water. Combining experiments on nanoribbon field effect transistors and molecular dynamic simulations, we elucidate a collective behaviour of water within clusters adsorbed on graphene edges. We show that these nanoribbons exhibit significant and persistent remanent fields which can be employed in ferroelectric heterostructures and neuromorphic circuits.

References [1] M. A. Aslam et al, <https://doi.org/10.48550/arXiv.2304.09738>

O 63.8 Wed 17:00 Poster B

Experimental setup for gas sensing with TMD based field-effect devices — ●AXEL PRINTSCHLER¹, EMAD NAJAFIDEHAGHANI¹, ANTONY GEORGE¹, HAMID REZA RASOULI¹, DAVID KAISER¹, UWE HÜBNER², and ANDREY TURCHANIN¹ — ¹Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena — ²Leibniz Institute of Photonic Technology (IPHT), Jena

Sensing devices based on 2D transition metal dichalcogenides (TMDs) such as MoS₂, WS₂, MoSe₂, WSe₂, *etc.* have attracted significant research interest, as their electronic properties are greatly influenced by variations in the environment, *e.g.*, due to formation of adsorbates. This influence is reflected in changes of the device's electric transport characteristics, which can be precisely measured and used for gas sensing. As toxic gases pose a threat in many fields, there is a high demand in sensitive, selective and flexible gas sensors that also work at low power. Electronic sensors based on TMDs can satisfy this need while being atomically thin and flexible. Here we present an experimental setup and first results on gas sensing with field effect transistors (FETs) fabricated from TMD monolayers grown by chemical vapor deposition (CVD).

O 63.9 Wed 17:00 Poster B

MOCVD synthesis of MoS₂ and WS₂ combination 2D heterostructures — ●NIKOLAS DOMINIK, SEBASTIAN KLENK, FLORIAN HERDL, CORMAC Ó COILEÁIN, TANJA STIMPEL-LINDNER, and GEORG S. DUESBERG — Institute of Physics, University of the Bundeswehr Munich & SENS Research Center, 85577 Neubiberg, Germany

Two-dimensional (2D) materials (such as MoS₂ and WS₂) are materials layered at the atomic scale. This gives them exceptional electrical, mechanical and optical properties, and makes them interesting for electronics, photovoltaics and sensing [1]. Van der Waals heterostructures composed of 2D materials expand on the possible range of properties and so have attracted extensive focus due to factors such as smooth heterostructure interfaces, ultrafast carrier transport, and high bandgap tunability [2].

Here we present the synthesis of MoS₂/WS₂ combination heterostructures via metal-organic chemical vapour deposition (MOCVD) using a high controllable industrial scale multi-precursor system, and show the clearly defined stacked nature of the films produced. We explore the growth parameter space using Raman and X-ray photoemission spectroscopy, and microscopy techniques. We complement our characterisation by examining the influences on the band structure of the layered material.

- [1] Q. H. Wang et al., *Nature Nanotech* 7, 699-712 (2012)
 [2] W. Xia et al., *Nanoscale* 9, 4324-4365 (2017)

O 63.10 Wed 17:00 Poster B

RF-sputtering of Nb and NbN thin films for quantum transport studies — ●PEER HEYDOLPH, VINCENT STRENZKE, ISA MOCH, ANNIKA WEBER, LARS TIEMANN, and ROBERT BLICK — Center for Hybrid Nanostructures (CHyN), Universität Hamburg, Luruper

Chaussee 149, 22761 Hamburg, Germany

Niobium plays a vital role in research and applications, contributing to advancements in superconductivity, quantum computing, and high-performance electronics. Here, we investigate the impact and interdependence of growth parameters on the properties of radio-frequency (RF)-sputtered niobium (Nb) and niobium nitride (NbN) thin films with a high critical temperature for applications in nanostructures and quantum transport studies at 4.2 Kelvin. We demonstrate that high quality superconducting films can be consistently produced even in a basic sputtering setup. We systematically varied the growth parameters such as the power of the RF-plasma and the flow of argon and nitrogen and survey their effects and interdependence on the properties of the thin films. The quality of the resulting films was characterized via X-ray diffraction (XRD), scanning electron microscopy (SEM) and profilometer measurements to gauge the film thickness. For electrical characterization at various temperatures and magnetic fields we employed a PPMS cryostat. We found that lower flow rates or RF powers do not necessarily lead to a higher critical temperature for NbN, which is in agreement with previous publications. Furthermore, it is crucial to finely tune all parameters and take into account their interdependencies.

O 63.11 Wed 17:00 Poster B

Poly(neutral red) as a Possible Electrode Material for Electrochemical Cells — ●LISA ROHOVSKY¹, DANIEL HOLZHACKER¹, TSUKASA YOSHIDA², and DERCK SCHLETTWEIN¹ — ¹Institut für Angewandte Physik, Justus-Liebig-Universität Gießen — ²Department of Organic Materials Science, Graduate School of Organic Materials Science, Yamagata University

Poly(neutral red) (PNR) is used in sensors owing to its redox characteristics and high electrical conductivity. PNR is also easy to prepare and inexpensive. Therefore, it might also be of interest as an electrode material in electrochemical cells like, *e.g.*, electrochromic cells, batteries, or dye-sensitized solar cells (DSSCs). In the latter case, it could even help to replace platinum as an electrode material, which is expensive and not readily available. In this study, thin films of PNR were prepared by an established electrosynthetic procedure by oxidation of neutral red by cyclic voltammetry (CV) in an aqueous solution.[1] Samples were produced for varied number of oxidative cycles and then analysed for their layer thickness and absorbance. As expected, the layer thickness increased linearly with the number of cycles, as did the absorbance. The reversible electrochemical reduction and reoxidation of aqueous solutions of ferro/ferricyanide in contact to the prepared films was studied as a model electrolyte. Results and implications for the applicability of such PNR electrodes will be discussed. [1]. Y. Harada, D. Kono, P. Stadler, T. Yoshida, SPAST Abstracts ,1(01), First International Conference on Technologies for Smart Green Connected Society 2021.

O 63.12 Wed 17:00 Poster B

Growth of Sc(x)Ga(1-x)N on 6H-SiC by plasma assisted molecular beam epitaxy — ●FABIAN ULLMANN^{1,2}, ABDUL QADIR SHAHBAZ^{1,2}, and STEFAN KRISCHOK^{1,2} — ¹TU Ilmenau, Ehrenbergstraße 29, 98693 Ilmenau — ²Zentrum für Mikro- und Nanotechnologie, Gustav-Kirchhoff-Straße 7, 98693 Ilmenau

ScGaN can occur in various crystal orientations. The most important are wurtzite and rock salt formation. Depending on the scandium concentration, a phase transition can be found between these orientations. Plasma-assisted molecular beam epitaxy (PAMBE) in combination with reflective high-energy electron diffraction (RHEED) was performed to create layers with different scandium concentrations in ScGaN. To determine the concentration of the grown layers, X-ray photoelectron spectroscopy was used in the same vacuum chamber. In addition, the surfaces were analyzed using atomic force microscopy (AFM, in-situ) and scanning electron microscopy (SEM) to obtain information on the morphology of the surfaces and to confirm the gained crystal orientations X-ray diffraction (XRD) were performed.

O 63.13 Wed 17:00 Poster B

Optical and morphological properties of thin Nb₂O₅ layers deposited via High Power Impulse Magnetron Sputtering — ●CHRISTOF ZICKENHEINER¹, RAUL RAMOS², VIKTOR UDACHIN¹, WOLFGANG MAUS-FRIEDRICH¹, and JOSÉ R.R. BORTOLETO² — ¹Clausthal University of Technology, Clausthal-Zellerfeld, Germany — ²Instituto de Ciencia e Tecnologia, Sorocaba, Brazil

To address climate challenges and sustainable development, the UN

set ambitious goals. Renewable energy, particularly solar, plays a key role. Emerging technologies like perovskite solar cells (PSC) offer cost-effective production, competing with silicon-based counterparts. This study focuses on the electron transport layer in PSC using Nb₂O₅ thin films deposited on glass substrates via HiPIMS from an Nb-target in an Ar/O₂ atmosphere at 25 °C. Pulse duration and oxygen pressure were varied as experimental parameters. Optical emission spectroscopy (OES) revealed the presence of oxygen species within a plasma and excitation of sputtered metal species for the HiPIMS process. The examination of the morphological properties via profilometry and contact angle analysis showed an influence of the experimental parameters on roughness. That is, shorter pulses as well as lower oxygen pressure result in smoother layer growth with a lower deposition rate. The investigation of optical properties via UV/Vis-Spectroscopy showed no significant impact of pulse duration. It became evident that lower oxygen pressure reduces the incorporation of oxygen into the growing layer. This results in a changed phase composition, with the formation of NbO₂, which in turn affects optical and electrical properties.

O 63.14 Wed 17:00 Poster B

An attempt to predict oligomer sputtering using binary collision approximation simulations — ●HANS HOFSSÄSS, FELIX JUNGE, and PATRICK KIRSCHT — II. Physikalisches Institut, Universität Göttingen, Germany

The binary collision approximation (BCA) program IMINTDYN [1] allows a prediction of ion solid interactions. For sputtering of carbon and SiO₂ experimental sputter yields are significantly higher than yields from BCA simulations. SDTrimSP simulations [2] reproduce experimental sputter yields by adjusting the surface binding energies. For O atoms 1 eV instead of the elemental sublimation energy of 2.58 eV and for carbon 4.5 eV instead of 7.4 eV is used. For sputtering of carbon it was shown [3] that sputtering of oligomers and clusters is relevant. We introduce a model to simulate oligomer sputtering using the IMINTDYN program based solely on thermodynamic formation enthalpies. In particular sputtering of O₂ and SiO dimers and carbon oligomers is energetically favorable. To predict the oligomer sputter fraction, we use Boltzmann factors based on the ratios of oligomer and monomer formation enthalpies. We show that we can quantitatively predict the carbon and SiO₂ experimental sputter yields.

[1] H. Hofssäss, A. Stegmaier, Nucl. Instr. Meth B 517 (2022) 49

[2] A. Mutzke, R. Schneider, W. Eckstein, R. Dohmen, K. Schmid, U. von Toussaint, G. Bandelow, SDTrimSP Version 6.00, MPI Plasma Physics, report IPP 2019-02 (2019)

[3] E.Oyarzabal, R.P. Doerner, M. Shimada, G.R. Tynan, J. Appl. Phys. 104 (2008) 043304

O 63.15 Wed 17:00 Poster B

Growth of Antimony thin films on c-plane Sapphire — ●JONATHAN SPELSBERG, ALEXANDER FUHRICH, and MARTIN SALINGA — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Antimony has been demonstrated to function as a single-element phase change material for electronic memory applications [1]. Confinement into nanostructures is crucial for stabilizing the amorphous phase of this material that is otherwise known for its fast crystallization kinetics. Yet, the exact influence of interfacing dielectrics on the physical properties of Antimony requires a fundamental investigation. To this end, samples with a well-controlled interface are required. Here, we report about the growth of Antimony thin films on c-plane Sapphire by molecular beam epitaxy. Based on characterization with RHEED and AFM, we demonstrate the impact of substrate preparation and process temperatures on the growth of 3 nm to 30 nm thick antimony films. Moreover, we discuss the relevance of Antimony cluster size and the effective use of a cracker effusion cell.

[1] M.Salinga et al., Monatomic phase change memory, Nature Materials 17, p. 681-685 (2018)

O 63.16 Wed 17:00 Poster B

Novel nanofabrication facility for ultra-clean samples — ●ALEXANDER FUHRICH and MARTIN SALINGA — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

We present the capabilities of a novel nanofabrication facility dedicated to the fabrication of nanostructures under ultra-clean conditions. In addition to a UHV cluster for MBE growth, the system comprises a lithography unit in an inert argon atmosphere. Air- and water-sensitive samples, like materials for memristive switches, can be structured using thermal scanning probe lithography with a lateral resolution down to

less than 30 nm. Samples can be analyzed in-situ using RT-STM and RHEED. A self-sufficient UHV suitcase is used to characterize samples in other setups, such as femtosecond-laser pump probe spectroscopy, without ever exposing our samples to air.

O 63.17 Wed 17:00 Poster B

Preparation and Characterization of Mixed Electrodes of WO₃ and MoO₃ as Electrochromic Coatings — ●SMAIL MEKHILEF, THI HAI QUYEN NGUYEN, and DERCK SCHLETTWEIN — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen

Electrochromic coatings can modify the transmittance for ambient light. As smart windows for buildings, relevant contributions can be expected for the energy-efficiency of buildings. Sputter-deposited WO₃ is typically used. Sustainability can be increased if low-temperature processes are established that would, further, allow the use of low-impact and low-weight polymer substrates. For large-scale applications, one may want to avoid W as a critical element and, at least partly, replace it by more abundant Mo. In this study, we extended established wet-chemical methods to prepare porous thin film electrodes of WO₃ [1] towards the processing of mixed oxides of W and Mo. Thin films of different W/Mo were prepared and characterized by scanning electron microscopy, atomic force microscopy and, mainly, by spectroelectrochemical measurements in contact to an inert organic electrolyte at either constant or swept electrode potential and the results will be discussed. [1]. T. H. Q. Nguyen, F. Eberheim, S. Göbel, P. Cop, M. Eckert, T. P. Schneider, L. Gumbel, B. M. Smarsly, D. Schlettwein, Enhancing the Spectroelectrochemical Performance of WO₃ Films by Use of Structure-Directing Agents during Film Growth, Appl. Sci. 2022, 12, 2327.

O 63.18 Wed 17:00 Poster B

Deposition of reduced ceria thin films by reactive magnetron sputtering for the development of a resistive gas sensor — ●PAUL-G. NITSCH¹, MARKUS RATZKE¹, EMILIA POZAROWSKA², JAN I. FLEGE², CARLOS ALVARADO CHAVARIN³, CHRISTIAN WENGER³, and INGA A. FISCHER¹ — ¹Experimentalphysik und funktionale Materialien, BTU-CS, Cottbus, Germany — ²Angewandte Physik und Halbleiterspektroskopie, BTU-CS, Cottbus, Germany — ³IHP - Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany

The use of cerium oxide for hydrogen sensing is limited by the low electrical conductivity of layers deposited from a ceria target. To increase the electrical conductivity, partially reduced cerium oxide layers were obtained from a metallic cerium target by reactive magnetron sputtering. The proportions of the oxidation states Ce³⁺, present in reduced species, and Ce⁴⁺, present in fully oxidized species, were determined by ex-situ XPS. For electrical characterization, films were deposited on planarized tungsten finger electrodes. IV curves were measured over several days to investigate possible influences of oxygen and humidity on electrical conductivity. The morphological stability of the layers under ambient conditions was investigated by microscopical methods. The XPS results show a significant amount of Ce³⁺ in the layers. The electrical conductivity of as-grown samples is several orders of magnitude higher than that of samples grown from a ceria target. However, the conductivity decreases over time, indicating an oxidation of the layers. The surface morphology of the samples was found to be changing drastically within days, leading to partial delamination.

O 63.19 Wed 17:00 Poster B

Modification of the optical and electrical properties of AZO thin films for variety of applications — ●MARIA STEFANOVA¹, DIMITRINA PETROVA^{1,2}, BLAGOVEST NAPOLEONOV¹, STEFANI BOGOEVA¹, VLADIMIRA VIDEVA^{1,3}, VELICHKA STRUKOVA¹, VERA MARINOVA¹, and DIMITRE DIMITROV^{1,4} — ¹Institute of Optical Materials and Technologies-BAS Sofia, Bulgaria — ²South-West University "Neofit Rilski", Blagoevgrad, Bulgaria — ³Sofia University, Sofia, Bulgaria — ⁴Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria

Here we report on the deposition of Aluminium Doped Zinc Oxide (AZO) thin films on sapphire substrates (AZO/Sapphire) by using ALD method and the influence of postdeposition UV-Ozone treatment on the films' properties. XRD revealed a polycrystalline wurtzite structure. The influence of UV-Ozone treatment on surface morphology, electrical and optical properties of AZO/Sapphire was investigated. It was found that UV-Ozone treatment improves the electrical and optical properties while did not cause significant changes to the polycrystalline structure and surface morphology of the AZO films which opens potential for various practical applications.

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O 63.20 Wed 17:00 Poster B

Transient Photoluminescence of Lead Halide Perovskites Beyond Lifetimes: Non-excitonic Geminate Pairs and Carrier Transport — ●HANNES HEMPEL¹, MARTIN STOLTERFOHT², and THOMAS UNOLD¹ — ¹Helmholtz Zentrum Berlin, Germany — ²Chinese University of Hong Kong, China

Transient photoluminescence (trPL) is the standard technique to quantify the lifetimes of photogenerated charge carriers in energy conversion materials. However, trPL decays are sensitive to processes other than only carrier recombination. We show that the initial trPL transients of lead halide perovskite thin films on glass are dominated by charge transport, namely hot carrier transport, spread-out of non-excitonic geminate pairs, and redistribution. Including these processes in the modeling of trPL yields the doping and intrinsic carrier concentration, the mobility and diffusion coefficient, the hot carrier transport length, and the radiative and non-radiative lifetimes. Further, we calibrate trPL to absolute photon numbers, which allows quantifying the transient quasi-Fermi-level splitting and reveals fundamental energy losses in photo absorbers such as the increase of entropy by loss of geminate correlation and redistribution. The presented analysis is crucial for the appropriate interpretation of trPL and yields almost all optoelectronic properties relevant for application as a photo-absorber in solar cells.

O 63.21 Wed 17:00 Poster B

Ultrafast Lattice Dynamics in Epitaxially Grown Bismuth Thin Films — ●TIMO VESLIN¹, FELIX HOFF¹, JONATHAN FRANK¹, ABDUR REHMAN JALIL³, JULIAN MERTENS¹, and MATTHIAS WUTTIG^{1,2,3} — ¹Institute of Physics (IA) RWTH Aachen University — ²Jülich-Aachen Research Alliance (JARA FIT and JARA HPC) — ³PGI 10 (Green IT), Forschungszentrum Jülich GmbH

Femtosecond optical pump probe measurements are carried out in order to detect changes in the reflectivity of the material response of epitaxially grown bismuth thin films on sub-ps timescales. Examination of reflectivity changes due to the coherent phonon response provides insight into the ultrafast lattice dynamics and relaxation of bismuth thin films. The pronounced thickness dependent behavior of bismuth is analysed by coherent phonons within the framework of dispersive and impulsive excitation models. Here, we show how the competition of phonon softening due to different laser fluencies and phonon hardening from confinement effects can be understood. Raman measurements are carried out to help to disentangle both effects. XRD measurements are shown to help to understand the structural change of the lattice structure. These combined measurements will help to understand confinement and fluency effects in a single model and shows how to tune bonding properties in this unconventional class of materials.

O 63.22 Wed 17:00 Poster B

Atomic-Scale Insights Into The Interlayer Characteristics of Thin-Layered Materials Using Ultra-high Vacuum Tip-Enhanced Raman Spectroscopy — ●SOUMYAJIT RAJAK and NAN JIANG — University of Illinois Chicago, Chicago, USA

Optoelectronic properties of molecular thin films are controlled by the local nanostructures of a molecular arrangement. Probing the effect of the local environment of nanostructures is challenging because the spatial resolution of conventional optical spectroscopic techniques is limited by the diffraction limit of light. Coupling light with plasmonic nano-objects creates highly localized surface plasmons (LSPs), which allows us to break the diffraction limit. Herein we present a combined topographical and optical analysis of different surface-sensitive arrangements of molecules and 2D material heterostructures using angstrom-scale resolution scanning tunneling microscopy (STM) and ultra-high vacuum tip-enhanced Raman spectroscopy (UHV-TERS). TERS uses the apex of an STM tip made of a plasmonic metal to couple light to the near field. The Raman modes of the nanostructure underneath this tip are enhanced by the nano-confined surface plasmons which allows us to obtain chemical information with Angstrom scale spatial resolution. STM images combined with localized surface plasmon resonance-enhanced Raman signals reveal different adsorbate configurations of single molecule entities and a fundamental view of interfacial interactions. The atomic scale insights obtained into the local environment enable precise control over the fabrication of nanos-

tructures with tailored optoelectronic properties.

O 63.23 Wed 17:00 Poster B

In-situ Study of Surface Band-Bending in c-ZnO and its Effect on the Excitonic Dielectric Function — ●LUIS ROSILLO OROZCO¹, KURT HINGERL¹, and CHRISTOPH COBET^{1,2} — ¹Zentrum für Oberflächen und Nanoanalytik, Johannes Kepler Universität, Linz, Austria — ²Linz School of Education, Johannes Kepler Universität, Linz, Austria

Semiconductors in air and in vacuum often have a band-bending near the surface caused by surface states capturing bulk charges or simply due to natural polarization in the case of polar materials, as is the case of Zinc Oxide. Nevertheless, when semiconductors are in contact with an electrolyte we can intentionally produce a surface dipole and create a space charge region (SCR) by adding another electrode in the solution and applying a voltage between the two.

Space charge regions have a big impact on the optical and electrical properties of semiconductors and, of course, semiconductor devices. Therefore, it is of high interest to understand the effects caused by them.

We present in-situ spectroscopic ellipsometry (SE) combined with electrochemical techniques to study the response of the discrete excitons and exciton-phonon complexes (EPC) to the inner electric fields produced near the semiconductor surface. Using mono-chromatic transients we are able to identify the flat-band potential. A semi-empirical optical model is developed to study the contribution of the surface band-bending to the total dielectric function for a range between 3.2 e.V. to 3.6 e.V.

O 63.24 Wed 17:00 Poster B

In situ optical tracking of oxidation state changes of NiFe alloys by Reflectance Anisotropy Spectroscopy — ●SANDHYA CHANDOLA¹, KARUPPASAMY DHARMARAJ², JÖRG RAPPICH¹, NORBERT ESSER^{3,4}, and SONYA CALNAN² — ¹Young Investigator Group Nanoscale Solid-Liquid Interfaces (CE-NSLI), Hahn-Meitner-Platz 1, 14109 Berlin, Germany — ²Kompetenzzentrum Photovoltaik Berlin, Schwarzschildstr. 3, 12489 Berlin, Germany — ³Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — ⁴Leibniz-Institut für Analytische Wissenschaften ISAS e.V., Schwarzschildstr. 8, 12489 Berlin, Germany

The oxygen evolution reaction (OER) is a key reaction involved in water splitting and has attracted increasing attention for hydrogen generation for clean energy uses. Nickel/iron (NiFe)-based compounds have been known as active OER catalysts for decades, and there has been increasing interest in developing NiFe-based materials for higher activity and stability.

Reflection Anisotropy Spectroscopy (RAS) in the visible spectral range is a polarisation sensitive optical spectroscopy technique used to study morphological and electronic structure changes of surfaces and thin films in-situ. It achieves high sensitivities in the detection of ultrathin layer structures down to the sub-nanometer scale and can follow the optical changes of the surface during catalytic reactions. By combining in-situ RAS and cyclic voltammetry (CV), the changes in both the redox state and structural phase during OER activity of NiFe alloys can be optically tracked.

O 63.25 Wed 17:00 Poster B

Triptycene as a versatile building block for self-assembled monolayers — TAKANORI FUKUSHIMA¹, MANFRED BUCK², EGBERT ZOJER³, and ●MICHAEL ZHARNIKOV⁴ — ¹Tokyo Institute of Technology, Yokohama 226-8503, Japan — ²EaStCHEM School of Chemistry, University of St Andrews, St Andrews KY16 9ST, UK — ³Institute of Solid State Physics, NAWI Graz, Graz University of Technology, 8010 Graz, Austria — ⁴Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

When employing self-assembled monolayers (SAMs) for tuning surface- and interface-properties, a strong binding to the substrate, structural uniformity, and the ability to align functional groups and to control their density are desirable. To achieve these goals, tripod systems bearing multiple bonding sites have been developed as an alternative to conventional monodentate systems. A bonding of all three sites has, however, hardly been achieved with the consequence that structural uniformity and orientational order in tripodal SAMs are usually quite poor. To resolve that problem, we designed a series of triptycene-based molecules decorated with three anchoring groups, which can be assembled on different substrates. Depending on the character of the anchoring groups, well-defined tripodal SAMs could be prepared

on Au(111), Ag(111), and indium tin oxide. Either unsubstituted or differently substituted triptycene-based molecules were assembled in context of different issues, viz. (i) homogeneous tripodal assembly, (ii) polymorphism and hidden chirality, (iii) on-surface click chemistry, (iv) multiple pathways in charge transfer, and (v) nanofabrication.

O 63.26 Wed 17:00 Poster B

A new design concept for SAMs of N-heterocyclic carbenes — MATEUSZ WRÓBEL¹, DARIA M. CEGIELKA¹, ANDRIKA ASYUDA², KRZYSZTOF KOZIEL³, MICHAEL ZHARNIKOV², and PIOTR CYGANIK¹ — ¹Smoluchowski Institute of Physics, Jagiellonian University, 30-348 Krakow, Poland — ²Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — ³Faculty of Chemistry, Jagiellonian University, 30-387 Krakow, Poland

Self-assembled monolayers (SAMs) of N-heterocyclic carbenes (NHCs) on metal substrates are currently one of the most promising systems in context of molecular engineering of surfaces and interfaces. Interest in these systems is mainly driven by their assumingly higher thermal stability compared to thiolate SAMs most broadly used at the moment. Most of the NHC SAMs utilize imidazolium as an anchoring group for linking molecules to the metal substrate via carbene C atom. It is well established in the literature that upright-oriented and stable NHC SAMs can only be built when using bulky side groups attached to nitrogen heteroatoms in imidazolium moiety, which, however, reduce significantly the packing density. In contrast, combining several complementary experimental techniques, we show that aromatic monolayers exhibiting at least double surface density, upright molecular orientation, and ultra-high thermal stability compared to the NHC SAMs reported before can be readily fabricated on the basis of NHCs with small methyl side groups in combination with simple solution-based preparation procedure. These parameters are crucial for numerous applications, including molecular and organic electronics.

O 63.27 Wed 17:00 Poster B

Interaction study between thin films of polyvinyl acetate and (plasma-treated) aluminum — SASCHA ZIMMERMANN¹, PHILIPP MORITZ¹, OLIVER HÖFFT¹, LIENHARD WEGEWITZ¹, WOLFGANG MAUS-FRIEDRICHS¹, and SEBASTIAN DAHLE² — ¹Clausthal University of Technology, Germany — ²University of Ljubljana, Slovenia

Composite materials made of wood and aluminum are becoming increasingly popular due to the combination of their properties. However, in order to exploit these advantages, the two materials must be bonded with sufficient stability. While the adhesive polyvinyl acetate (PVAc) exhibits high adhesive strength on wood, its bonding capabilities with aluminum are limited. The surface of the aluminum must therefore be modified. In this work, the aluminum surface is treated with a dielectric barrier discharge plasma in air with the aim of enabling molecular interactions. Various analytical techniques, including X-ray photoelectron spectroscopy (XPS), Reflection Absorption Infrared Spectroscopy (RAIRS) and Atomic Force Microscopy (AFM), are employed to analyse the chemical interactions between aluminum and PVAc. This involves producing nm-thin films using spin coating. For untreated aluminum, no interactions were detected. AFM revealed the inability to deposit nanometer-thin films due to the lack of interactions, leading to the formation of PVAc-clusters. Plasma-treated aluminum led to a stronger chemical shift in the XPS spectra indicating hydrogen bonding. This finding was confirmed by RAIRS, which shows bands associated with hydrogen bonding.

O 63.28 Wed 17:00 Poster B

Spectroscopical properties investigation of pyrene based molecules in perspective of singlet fission — SRUTHY ASA RAJAN, SERGEY BAGNICH, and ANNA KÖHLER — Universität Bayreuth, Bayreuth, Germany

Photovoltaics plays a vital role in renewable energy. Theoretically, conventional silicon solar cells' efficiency is limited to 33% known as the Shockley-Queisser limit, which is limited by some practical and fundamental losses like thermalisation loss. Singlet fission (SF) is a carrier multiplication process, which has the potential to overcome Shockley-Queisser limit. In an organic semiconductor, chromophore in its singlet excited state shares its energy with a nearby ground-state chromophore to form two triplet excitons. Recent studies shown that some pyrene derivatives exhibit SF. A study has shown that bridged SF chromophore forms generated triplet pair and hence leading to formation of long-lived triplets.

We are investigating the impact on absorption, photo-luminescence,

lifetime decay, time-resolved spectroscopy and quantum yield of different N-substitution groups on para Diketopyrrolopyrrole (PDPP) based pyrene derivatives, which have a comparable triplet energy to silicon bandgap. We will focus more on the changes in morphology of film of these compounds by varying the conditions of film preparation, such solvents, annealing effect, etc. We hypothesis that certain orientation of these pyrene-base molecules can trigger singlet fission.

O 63.29 Wed 17:00 Poster B

Understanding the disparate interactions of thin polymer films with natively oxidized metal surfaces and metal oxide crystals — FRIEDRICH BÜRGER, PHILIPP MORITZ, LIENHARD WEGEWITZ, and WOLFGANG MAUS-FRIEDRICHS — Clausthal Centre of Material Technology, Clausthal University of Technology, Agricolastr. 2, 38678 Clausthal-Zellerfeld

In the Collaborative Research Centre 1368 "oxygen free production" the molecular interactions between thin films of commonly used polymers, poly(ethyl cyanoacrylate) (PECA) and poly(methyl methacrylate) (PMMA), and different metal oxides have been characterized. In the context of this project, certain interactions became apparent, e. g. hydrogen bonding or ionic interactions that were observed on natively oxidized samples representing very thin oxide films. In contrast, these interactions were absent on a TiO₂ single crystal. To investigate if this effect is reproducible and inherent to metal oxide single crystals, the interactions of PECA and different metal oxide single crystals are determined using X-Ray Photoelectron Spectroscopy (XPS), Ultraviolet Photoelectron Spectroscopy (UPS) and Metastable Induced Electron Spectroscopy (MIES). These results are compared to the interactions of natively oxidized metal samples with thin polymer films. Assuming reproducibility, a root cause for the disparate interactions is proposed.

O 63.30 Wed 17:00 Poster B

Influence of processing atmospheres on curing and bonding of cyanoacrylate adhesives — PHILIPP MORITZ, OLIVER HÖFFT, LIENHARD WEGEWITZ, and WOLFGANG MAUS-FRIEDRICHS — Technical University Clausthal, Clausthal-Zellerfeld, Germany

Cyanoacrylates are fast-curing adhesives that are often used in joining technology to bond components together quickly. The curing and strength of the bond are often improved with numerous additives and surface pre-treatments. However, the surrounding process atmosphere is an aspect that has hardly been used to control curing and adhesive interactions.

To investigate the interactions and curing, thin films of cyanoacrylate are deposited on natively oxidized copper substrates. The surrounding atmosphere is varied between (i) air atmosphere, (ii) argon and (iii) an oxygen-free environment (O₂ partial pressure < 10⁻²⁰ mbar). The curing and underlying molecular interactions at the interface between cyanoacrylate and oxidized copper are investigated using spectroscopic and microscopic methods.

Curing in argon and the O₂-free atmosphere is significantly slower than in air. Nevertheless, strong interactions occur in an oxygen-free atmosphere and air, e.g. hydrogen bonds and ionic interactions. In argon, on the other hand, no molecular interactions are observed.

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O 63.31 Wed 17:00 Poster B

The influence of PDMS residues on the mobility of molecules deposited onto Si/SiO₂ wafers — ERIK VON DER OELSCHNITZ^{1,2}, TIM VÖLZER^{1,2}, JULIAN SCHRÖER¹, TOBIAS KORN^{1,2}, and STEFAN LOCHBRUNNER^{1,2} — ¹Institute of Physics, University of Rostock, Germany — ²Department "Life, Light & Matter", University of Rostock, Germany

The exfoliation and stamping of flakes of 2D materials onto a substrate is one of the most used methods for the preparation of transition metal dichalcogenide (TMDC) monolayers. However, it was found that during the transfer of the flake, impurities and in particular residues of the common stamp material polydimethyl siloxane (PDMS) are transferred to the substrate. This could have a major impact when analyzing TMDCs, especially in TMDC/molecule hybrid structures. In order to examine the effect of these impurities, dye molecules were evaporated onto a Si/SiO₂ wafer and then measured in a fluorescence lifetime microscope (FLIM). Here, in a certain area, the dye coverage is removed by laser-induced photodegradation and the diffusion of the molecules into this depleted area is examined. Three wafers are compared, each representing a specific step of the preparation process. The FLIM measurements showed that the molecules on the bare wafer

diffuse into the depleted area the fastest, while they take significantly longer on the samples that came into contact with PDMS. This shows that the surface properties of exfoliated 2D materials are significantly

influenced by the contact with PDMS, which in turn has a major effect on the mobility and thus the dynamics of deposited molecules.