HL 20: Poster I

The first poster session covers the physics of semiconductor heterostructures, interfaces and surfaces. Moreover, most recent results on oxide semiconductors, as well as perovskite and photovoltaics are presented.

Time: Tuesday 10:00–12:30 Location: P3

HL 20.1 Tue 10:00 P3

Accuracy Requirements for Polarizabilities in MD-based Raman Spectra — •Markus Amaseder[1], Manuel Grumet[1], Tomáš Bučko[2,3], and David A. Egger[1] — [1]TUM School of Natural Sciences, Technical University of Munich — [2]Faculty of Natural Sciences, Comenius University Bratislava — [3]Institute of Inorganic Chemistry, Slovak Academy of Sciences

Raman spectroscopy provides a versatile and accessible method for characterizing atom dynamics in materials. While frozen phonon approaches have proven well for the prediction of Raman spectra in many cases, they do not inherently include anharmonic and temperature-dependent effects. Raman spectra calculated from molecular dynamics (MD) offer an alternative [1] and have received considerable interest. However, they remain computationally challenging as they require many single-point polarizabilities. We have shown previously that machine learning (ML) can aid in the speed-up using a delta learning approach [2]. However, it is still to be fully understood how accurate single-point polarizabilities need to be in order to provide sufficiently correct spectra. We present an evaluation of polarizabilities from density functional theory and ML for MD Raman spectra, investigating the effects of the functional and further parameters. This is relevant both in terms of training data and ML predictions. Since many single-point calculations are needed, the trade-off between accuracy and computational cost is crucial for the practical application of MD-based Raman spectra. [1] Thomas, et al. Phys. Chem. Chem. Phys. 15, 6608-6622 (2013) [2] Grumet, et al. J. Phys. Chem. C 128, 6464-6470 (2024)

HL 20.2 Tue 10:00 P3

low-temperature buffer layer-assisted heteroepitaxial growth of γ-CuI thin films by pulsed laser deposition: tailoring electrical properties — •Yang Chen[1], Michael S. Bar[1], Susanne Selle[2], Daniel Splith[1], Michael Lorenz[1], Marius Grundmann[1], and Holger v. Wenckstern[1] — [1]Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, 04103 Leipzig, Germany — [2]Fraunhofer Institute for Microstructure of Materials and Systems IMWS, 06120 Halle, Germany

As the first discovered p-type transparent conductive material, copper(I) iodide (CuI) is considered to be among the most competitive p-type candidate in the field of transparent electronics. Herein, we introduced a low-temperature buffer-layer-assisted strategy to grow γ-CuI on c-plane sapphire by pulsed laser deposition with unprecedented structural quality and electrical transport properties. By adjusting the growth temperature, we can manipulate the rotation domain structure, control the hole concentration in the range from 10^{14} cm^{-3} to 10^{19} cm^{-3} and achieve mobility $\mu_h = 25$ cm^{2}V^{-1}s^{-1} being similar to that of bulk CuI. Based on the temperature dependent Hall-effect measurement, the ionization energy of shallow acceptors $E_{I,S} = 137 \pm 8$ meV and deeper acceptors $E_{I,D} = 262 \pm 23$ meV were determined. This strategy not only enables high-quality CuI film preparation, but also to tailor their electrical properties for integration with n-type semiconductors in transparent electronic circuits.

HL 20.3 Tue 10:00 P3

Semiconductor membrane transfer for deterministic Circular Bragg Gratings fabrication — •Juan Nicolas Claro Rodriguez, Dennis Deutsch, Leonie Schubert, Dirk Reuter, and Klaus Joens — PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn

Highly indistinguishable single photons and strongly entangled photon-pairs are fundamental for photonic quantum communication [1]. InGaAs quantum dots (QDs) grown on InP substrates using MBE deposition [2] emit in the telecom C-band, making them ideal for long-distance communication, though their brightness is limited. Embedding these QDs in hybrid Circular Bragg Gratings (CBGs) enhances photon collection efficiency and the Purcell factor, supported by a backside mirror and transparent medium configuration [3]. We present a membrane transfer method involving backside mirror growth, press-bonding, and InP substrate removal via HCl etching, enabling emitter localization and CBG integration. PL spectra are used to assess sample quality.

[1] Applied Physics Letters, 118(10), 100502. [2] AIP Advances, 13(5). [3] Journal of the Korean Physical Society, 73(10), 1502*1505.

HL 20.4 Tue 10:00 P3

Comparative Investigations of GaN/p-GaInP and p-GaInP Photocathodes: Stability and Performance in Acidic Electrolytes — •Sahar Shekarabi[1], Mohammad Amin Zare Pour[1], David Osteimer[1], Haoqing Su[2], Wentao Zhang[2], Agnieszka Paszuk[1], Wolfram Jaegermann[3], Shu Hu[2], and Thomas Hannappel[1] — [1]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — [2]Yale University, Department of Chemical and Environmental EngineeringNew Haven, USA — [3]Technische Universität Darmstadt, Department of Materials and Earth Sciences, Darmstadt, Germany

GaInP(100) is a widely used photoabsorber in tandem solar cells and photoelectrochemical (PEC) devices. To enhance stability against photo-induced corrosion, GaN passivation layers have been employed. This study evaluates the stability of p-GaInP/GaN and p-GaInP electrodes for solar-driven hydrogen evolution reactions (HER) in 1.0 M HClO4. Faradaic efficiency was monitored via gas chromatography during PEC, while X-ray photoelectron spectroscopy and atomic absorption spectroscopy were used to investigate surface and dissolution process conditions. The large valence band offset of around 2.0 eV at the GaN/p-GaInP interface acts as a hole barrier, reducing recombination, while conduction band alignment facilitates electron transport. The GaN passivation layer enhances stability and achieves a low onset potential of -0.5 V for HER. Surface and electronic structural changes were analyzed to understand corrosion mechanisms.

HL 20.5 Tue 10:00 P3

Characterization of surfaces of mixed semiconductor crystals — •Marsel Karmo[1] and Martin Brehm[2] — [1]Warburger Str. 100 33098 Paderborn — [2]Warburger Str. 100, 33098 Paderborn

Compositionally disordered crystals, also known as mixed-crystals, play a crucial role in semiconductor engineering. They enable the manipulation of material properties such as the band gap, which is important for opto-electronic devices like solar cells. Additionally, these crystals are used as buffer layers to mitigate strain from lattice constant mismatches between different material layers. However, accurately describing mixed crystals theoretically presents significant challenges. Due to the random occupation of atomic sites it is not possible to introduce a unit cell in other words the crystal as a whole is the unit cell. This prohibits also the use of boundary conditions. A commonly used approach to approximate mixed crystals is the Supercell Method (SCM), which employs a large, unit cell with random atomic site occupations. While this method approximates a mixed crystal, it is limited by computational resources. Another approach is the Virtual Crystal Approximation (VCA), which replaces the mixed crystal with an analytically averaged system. This method reduces the computational effort by using a smaller unit cell but may overlook local atomic environments, potentially limiting its ability to capture certain physical properties. In this work, we compare these two methods, VCA and SCM within the Vienna Ab Initio Simulation Package (VASP) to evaluate their performance in calculating the electronic structure and surface formation energy.

HL 20.6 Tue 10:00 P3

Photoelectrochemical characterisation of InGaN/GaN nanowire arrays — •Genrietta Steingelb[1], Hannah Nell[1], Rudolfo Hötzel[1], Ruben Neelissen[1], Stephan Figge[1], Tim Grieb[1], Florian Krause[1], and Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliotheksstraße 1, 28359 Bremen, Germany

Group III-nitride materials are known for their stability under physiological conditions, making them ideal candidates for use as electro-

chemical biosensors [1]. In this work, we present a detection mechanism that combines simultaneous photoluminescence (PL) and photocurrent measurements of InGaN/GaN nanowire (NW) arrays, allowing sensitive and selective detection of redox-active biomolecules. However, the performance of the NW photoelectrode is limited by non-radiative surface recombination of photogenerated carriers at the semiconductor-electrolyte interface, leading to irreversible photooxidation of the NW surface, mainly caused by unpassivated surface states. The deposition of ultrathin metal oxide films is a possibility to suppress such effects. The influence of surface coatings on sensor properties was analysed through photoelectrochemical characterisation, with and without metal oxide coatings. This analysis highlights how surface modifications affect sensor performance for the detection of redox-active molecules in complex biochemical environments. [1] G. Steinhoff, et al., Appl. Phys. Lett. 83, 177 (2003).

HL 20.7 Tue 10:00 P3

Impact of Surface States on the Performance and Stability of AlGaAs/GaAs HEMT Structures — •Vincent Leon Spreter[1,2], Selma Delic[1,2], Xuelin Jin[1,2], Nils von den Driesch[1], Christoph Krause[1], Detlev Grützmacher[1,2], and Beata Kardynal[1,2] — [1]Peter Grünberg Institut 9, Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Department of Physics, RWTH, 52074 Aachen, Germany

Electrostatic gating is commonly used to define single-electron quantum dots (QDs) in two-dimensional electron gases, such as those in GaAs/AlGaAs heterostructures. It can also be used to tune the electronic states of epitaxial quantum dots. For the use for quantum information processing applications, gated devices must maintain a stable working point over long time.

In our contribution, we investigate the effect of surface preparation of GaAs/AlGaAs heterostructure on the long-term stability of gates on the example of split-gate devices. In addition, we explore the use of passivation layers to mitigate the effects of dangling bonds associated with surface states. We discuss the processing of devices with AlOx passivation and action of electrostatic gates on device performance, offering insights into its potential for optimizing GaAs-based optoelectronic devices.

HL 20.8 Tue 10:00 P3

Low-temperature RAS of MOVPE-prepared Si(100) surfaces — •Kai Daniel Hanke[1], Max Grossmann[2], Chris Y. Bohlemann[1], Mohammad Amin Zare Pour[1], Paszuk Agnieszka[1], Runge Erich[2], and Hannappel Thomas[1] — [1]1Technische Universität Ilmenau, Fundamentals of Energy Materials, Ilmenau, Germany — [2]2Technische Universität Ilmenau, Theoretical Physics I, Ilmenau, Germany

Recent studies have shown that As-modified Si(100)-(2 x 1) surfaces prepared in a MOCVD environment exhibit asymmetric hydrogen-passivated Si-As dimers as dominating surface motif, in contrast to the previously assumed symmetric As dimers. Due to the importance of this surface for subsequent nucleation of III-V materials, such as GaP, for high-efficiency solar cell structures, we have performed low-temperature reflection anisotropy spectroscopy measurements, which are extremely surface sensitive, in combination with density functional theory and many-body perturbation theory calculations. We also performed X-ray photoelectron spectroscopy and low-energy electron diffraction measurements for a detailed understanding of the structure and electronic properties of this surface. Our method seeks to improve knowledge of the spectral properties of semiconductor surfaces by combining theoretical understanding with experimental data to understand the complex variables that influence RAS spectra.

HL 20.9 Tue 10:00 P3

Optimization of GaSb(100) Substrate Preparation for MBE Growth of GaSb Layers — •Peter Zajac[1], Sascha R. Valentin[2], Timo A. Kurschat[2], Rainer Krage[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund, Germany

The preparation of epi-ready substrates for MBE growth typically involves degassing and oxide removal. The latter is often done by thermal processes, resulting in rough interfaces that are associated with pyramidal defects (PDs) in GaSb layers grown on GaSb(100) substrates [1].
This study aims to optimize GaSb substrate preparation and buffer layer growth to reduce PD formation.
We compare standard thermal oxide desorption to methods proposed in the literature, such as Ga-assisted oxide removal [2] and the insertion of an AlAsSb layer into the buffer layer [1].
Using photoluminescence spectroscopy (PL) mapping, we assess quantum well and buffer layer luminescence as indicators of material quality. Additionally, we analyze the surface morphology with atomic force microscopy (AFM), focusing on the properties of pyramidal defects.

[1] Murray, Lee M., et al. *J. Vac. Sci. Technol. B* **31.3** (2013).
[2] Mathews, Sen, et al. *J. Vac. Sci. Technol. B* **35.2** (2017).

HL 20.10 Tue 10:00 P3

Passivation Protection Layers for Highly efficient Multi-Absorber Devices for Photoelectrochemical Solar Fuel Production — •Negin Mogharehabed[1], Mohammad Amin Zare Pour[1,2], Jennifer Velázquez Rojas[3], Christian Höhn[3], Roel van de Krol[3], Thomas Hannappel[2], and Agnieszka Paszuk[1] — [1]Paszuk Group, Technische Universität Ilmenau, Germany — [2]Fundamentals of Energy Materials, Technische Universität Ilmenau, Germany — [3]Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

In photoelectrochemical cells with the highest solar-to-hydrogen conversion efficiencies, the heterointerface between a III-V top layer and a metal oxide protection layer should be optimized to minimize charge carrier losses. Using photoemission spectroscopy, we study the TiO_2/InP(100) heterointerface as a function of InP surface preparation and Ti precursor.

InP(100) substrates were prepared with either a well-ordered, phosphorus-terminated surface in a metal-organic chemical vapor deposition (MOCVD) reactor or with a thin oxide layer. TiO_2 was deposited via atomic layer deposition (ALD) using either titanium tetrachloride ($TiCl_4$) or titanium isopropoxide (TTIP) as the Ti precursor, along with water as the co-reactant.

Depending on the Ti precursor and the InP surface preparation, we observed either a nucleation delay or acceleration and differences in the band alignment. Layers grown with the TTIP precursor showed the presence of Ti^{3+} states, which may act as trap centers.

HL 20.11 Tue 10:00 P3

Characterization of Arsenic- and Antimony Containing Heterostructures Grown by Molecular Beam Epitaxy — •Max H. W. Ziehfreund[1], Peter F. Zajac[1], Sascha R. Valentin[2], Timo A. Kurschat[1,2], Rainer Krage[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik der Ruhr-Universität Bochum, 44801 Bochum, NRW, Germany — [2]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund, NRW, Germany

This study focuses on the investigation of the surface morphology of various arsenic- and antimony-containing semiconductor heterostructures grown by molecular beam epitaxy. The objective is to optimize the growth parameters used in fabrication and to gain a better understanding of the underlying growth process. The characterization methods developed and approved for GaAs-based heterostructures are applied to GaSb-heterostructures. The primary methods employed are photoluminescence spectroscopy and atomic force microscopy. It was possible to examine the influence of various parameters, such as the antimony flux used during growth on the epitaxial quality of the grown layers and collect valuable experience for defect-free growth of arsenic- and antimony-containing heterostructures.

HL 20.12 Tue 10:00 P3

High Resolution Temperature Mapping of GaSb Wafers during MBE Growth — •Timo A. Kurschat[1], Sascha R. Valentin[1], Peter Zajac[2], Rainer Krage[1], and Andreas D. Wieck[2] — [1]Gesellschaft für Gerätebau mbH, Klönnestr. 99, D-44143 Dortmund — [2]Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44801 Bochum

The substrate temperature is one of the most important parameters during MBE growth. Thermocouples and pyrometers, as well as more advanced techniques, measure only a single spot on the wafer at a time. Knowing the temperature distribution allows to optimize the growth parameters from just a single grown sample.

To obtain high-resolution thermal maps we use a commercial SLR camera with its infrared filter removed. The sensor is sensitive up to a wavelength of about 1000 nm and can therefore be used as a high resolution pyrometer. Without substrate rotation and 10 s exposure time, measurements can be made down to $T_S = 400\,^{\circ}\mathrm{C}$. With rotation

enabled and a reduced exposure time of 0.25 s, it is still possible to obtain images at the growth temperature of $T_S = 680\,°C$.

Images of quarter 2-inch GaSb wafers show differences of more than 20 K between the center and the corners. The effect of a washer was investigated with this method, which is a ring placed at the backside of the wafer to improve its temperature uniformity. The temperature differences also effect the photoluminescence intensity of a quantum well grown on the wafer.

HL 20.13 Tue 10:00 P3

Raman spectroscopy on MBE grown III-V semiconductors heterostructures — •Arijit Chakraborty[1], Yiteng Zhang[1], Tom Fandrich[1], Doaa Abdelbarey[1], Tom Rakow[1], Krupali Dobariya[1], Sulabh Shrestha[1], Eddy P. Rugeramigabo[1], Michael Zopf[1,2], and Fei Ding[1,2] — [1]Leibniz Universität Hannover, Institute for Solid State Physics, Hannover, Germany — [2]Leibniz Universität Hannover, Laboratorium for Nano- und Quantum Engineering, Hannover, Germany

We present micro-Raman spectroscopic measurements on molecular beam epitaxy (MBE) grown semiconductors heterostructures, and quantum dots. This technique offers unique insights into the vibrational modes, crystal structure, strain, alloying effects and defects of grown semiconductor structures, making it invaluable for the optimization of MBE processes. The Raman results for the relaxed material have been interpreted in the framework of the modified random element isodisplacement theory considering different vibrational modes of the lattice with changing compositional range. Optical-phonon deformation potentials have been successfully used to fit the different vibrational phonon frequencies in strained layers of semiconductors. Using comparable theoretical models, a substantial compositional dependency with phononic vibrations is found and established. Disordered activated vibrational modes are investigated for layers produced on various substrates. An analogous conclusion with the peak shift in photoluminescence spectra is reached by analyzing the Raman spectra of herostructures grown on InP-based substrates.

HL 20.14 Tue 10:00 P3

Copper tin oxide: an amorphous, bipolar, ternary oxide system with tunable electrical and optical properties — •Arne Jörns, Holger von Wenckstern, and Marius Grundmann — Leipzig University, Felix Bloch Institute for Solid State Physics

Copper oxide (CuO) is one of the most studied p-type semiconducting metal oxides [1]. Tin oxide (SnO_2) features high transparency in the visible range, high n-type electrical conductivity and non-toxicity [2]. Due to mismatching crystal structures of CuO and SnO_2 (and their other oxidation states) an amorphous alloy, copper tin oxide (CTO), can form when combining these materials. Depending on growth pressure and cation composition the material can be p-type [1] or n-type making it a promising candidate for complementary amorphous devices. In this work, we investigated physical properties of CTO thin films, deposited by combinatorial pulsed laser deposition of segmented CuO and SnO_2 targets at room temperature and in oxygen atmosphere, as a function of cation composition and growth pressure. The resulting samples are X-ray amorphous and n-type semiconducting with mobilities up to $11\,cm^2/Vs$ for $Cu/(Cu+Sn) < 0.8$. Optical and electrical properties can be tuned by varying composition ratio and oxygen pressure. A temperature-dependent Hall effect analysis has led to the conclusion that the percolation model provides the most accurate description. For $Cu/(Cu+Sn) > 0.8$, the samples become p-type conducting and feature low mobilities.

[1] Isherwood *et al.*: J. Appl. Phys., 118, 105702, (2015)
[2] Ni *et al.*: Surface and Coating Technology, 206, 4356-4361, (2012)

HL 20.15 Tue 10:00 P3

low-temperature buffer layer-assisted heteroepitaxial growth of γ-CuI thin films by pulsed laser deposition: tailoring electrical properties — •Yang Chen[1], Michael S. Bar[1], Susanne Selle[2], Daniel Splith[1], Michael Lorenz[1], Marius Grundmann[1], and Holger v. Wenckstern[1] — [1]Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, 04103 Leipzig, Germany — [2]Fraunhofer Institute for Microstructure of Materials and Systems IMWS, 06120 Halle, Germany

As the first discovered p-type transparent conductive material, copper(I) iodide (CuI) is considered to be among the most competitive p-type candidate in the field of transparent electronics. Herein, we introduced a low-temperature buffer-layer-assisted strategy to grow γ-CuI on c-plane sapphire by pulsed laser deposition with unprecedented structural quality and electrical transport properties. By adjusting the growth temperature, we can manipulate the rotation domain structure, control the hole concentration in the range from 10^{14} cm^{-3} to 10^{19} cm^{-3} and achieve mobility $\mu_h = 25\ cm^2V^{-1}s^{-1}$ being similar to that of bulk CuI. Based on the temperature dependent Hall-effect measurement, the ionization energy of shallow acceptors $E_{I,S} = 137 \pm 8$ meV and deeper acceptors $E_{I,D} = 262 \pm 23$ meV were determined. This strategy not only enables high-quality CuI film preparation, but also to tailor their electrical properties for integration with n-type semiconductors in transparent electronic circuits.

HL 20.16 Tue 10:00 P3

Mechanical, electronic and optical properties of $LiNbO_2$ and $NaNbO_2$ from first-principles calculations — •Frederik Schmidt and Arno Schindlmayr — Universität Paderborn, Department Physik, 33095 Paderborn, Germany

The layered compound $LiNbO_2$ is of interest as a superconductor and possible battery material, but its electronic and optical properties have not yet been extensively analyzed, especially in theoretical simulations. There are even fewer studies of the closely related $NaNbO_2$. In this work, we perform first-principles calculations to investigate the properties of $LiNbO_2$ and $NaNbO_2$. The elastic constants and related parameters, such as elastic moduli, are determined using density-functional theory. We show that even small biaxial strain up to ±5%, which corresponds to common substrates like $MgAl_2O_4$ or SiC, may lead to significant changes in the electronic band structure and to a qualitative transition from a direct to an indirect band gap. Accurate results for the electronic band structure and the optical absorption spectrum are obtained from the *GW* approximation and the Bethe-Salpeter equation. We find that both the quasiparticle corrections and excitonic effects have a significant influence on the dielectric function. Good quantitative agreement with the experimentally measured absorbance and the absorption edge at 2 eV for $LiNbO_2$ is achieved only by a proper inclusion of both factors.

HL 20.17 Tue 10:00 P3

Bismuth oxyselenide (Bi2O2Se): Insights into chemical bonding and structural properties — •Sumayya Sumayya[1], Yuan Yu[1], Carl Friedrich Schon[1], Kim Dasol[1], Yueyang Yang[2], and Matthias Wuttig[1] — [1]RWTH, Aachen, Germany — [2]Tsinghua University, China

The Bismuth Oxychalcogenides (Bi2O2X, X=S, Se, Te) are potential candidates in various fields such as Thermoelectrics, Ferroelectrics, Piezoelectrics, and photodetectors due to their unique 2D layered structure containing a bismuth oxide layer and a chalcogen layer. In this family, Bi2O2Se is considered the 2D rising star for the semiconductor industry because of its high crystallographic symmetry, tunable band gap, ultra-high electron mobility, strong Shubnikov-des Haas quantum oscillations, unique defects, and excellent stability. The relationship between bonding and material properties offers a versatile platform for tailoring electronic and vibrational properties, potentially leading to improved functional characteristics. Recently, many theoretical and experimental bonding descriptors such as electron transferred and shared values, Born effective charge, electrical conductivity, optical dielectric constant, Grüneisen parameter, and Probability of Multiple events in atom probe tomography have been devised. Our study employs a combination of advanced characterization techniques and theoretical calculations to probe the nature of bonding at different length scales, from local atomic level to extended structural motifs. In the future, this model can be used for other layered materials to understand the structure-property relationship via chemical bonding.

HL 20.18 Tue 10:00 P3

Reactive Sputter Deposition and Nitrogen Modification of $CuBi_2O_4$ as Photocathode — •Dominic Rapf[1,2], Tsedenia A. Zewdie[1,2], Ian D. Sharp[1,2], and Verena Streibel[1,2] — [1]Walter Schottky Institute, Technical University of Munich, D-85748 Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, D-85748 Garching, Germany

Copper bismuthate ($CuBi_2O_4$) is a ternary oxide that is of special interest for photoelectrochemical (PEC) water splitting. Unlike most transition metal oxides, which predominantly exhibit n-type conductivity, copper bismuthate is a native p-type semiconductor. [1] In addition, it has a suitable bandgap for the absorption of visible light, as well as a high photocurrent onset potential > 1 V vs. RHE. [2] These properties make $CuBi_2O_4$ highly desirable as a photocathode. This project focuses on the development of reactive co-sputter recipes

to deposit copper bismuthate thin films and their structural, optical, morphological and opto-electronic analysis. In addition, we explore nitrogen incorporation to narrow the band gap of $CuBi_2O_4$ for more efficient light absorption (N:$CuBi_2O_4$). By modifying the nitrogen content in the reactive gas mixture and applying post-annealing treatments, we can tailor the level of nitrogen incorporation. On a library of N:$CuBi_2O_4$ thin films, we investigate the impact of nitrogen incorporation on optical and structural properties and assess their PEC performance.

[1] J. K. Cooper et al., Chem. Mater. 2021, 33, 3, 934–945 [2] D. Kang et al., Chem. Mater. 2016, 28, 12, 4331–4340

HL 20.19 Tue 10:00 P3

The impact of Bi and Na non-stoichiometry on the electrocaloric effect in (Na0.5Bi0.5)TiO3-BaTiO3 ceramics — •Sobhan M. Fathabad, Mohammadamin H. Kashani, Eva Kröll, Vladimir V. Shvartsman, and Doru C. Lupascu — Institute for Materials Science and Center for Nanointegration Duisubrg-Essen (CENIDE), University of Duisburg Essen, Essen, Germany

The electrocaloric effect (ECE) is the phenomenon where polar crystals experience a change in isothermal entropy or adiabatic temperature in response to the application or removal of an electric field. In this work, we investigate the influence of Bi and Na non-stoichiometry on the depolarization mechanism and electrocaloric effect in BaTiO3 - (Na0.5Bi0.5)TiO3 compounds at the morphotropic phase boundary. Ceramic samples were prepared using the solid-state synthesis method. The polarization hysteresis loops were measured in the temperature range from -20 °C to 200 °C and subsequently the ECE was indirectly estimated in the framework of the thermodynamic approach based on the Maxwell relation. The depolarization temperature was studied using dielectric permittivity, X-ray diffraction, and pyrocurrent analysis. Direct measurements of the ECE were conducted using a quasi-adiabatic calorimeter. It was shown that the introduced defects reduce the depolarization temperature, consequently shifting the maximum ECE towards room temperature.

HL 20.20 Tue 10:00 P3

Structure and lattice distortions of KTaO3(001) studied by LEED I-V and nc-AFM — Dominik Wrana[1,2], Marek Kuzmiak[1], Michele Reticcioli[3], Tomas Dolak[1], Florian Kraushofer[4], Michele Riva[5], Aji Alexander[1], Llorenc Albons[1], Jesus Redondo[1], Cesare Franchini[3], and •Martin Setvin[1] — [1]Charles University, Prague, Czech Republic — [2]Jagiellonian University, Krakow, Poland — [3]University of Vienna, Vienna, Austria — [4]TU Munich, Germany — [5]TU Wien, Vienna, Austria

Perovskites attract attention in many fields, yet understanding their surface structure represents a challenge. Special emphasis is focused on little lattice distortions associated with ferroelectric properties, often present in this broad class of materials. Hydroxylated KTaO3(001)-(2x1) is used here as a test case to extract the precise positions of lattice atoms by means of low energy electron diffraction (LEED) I-V, obtaining a final Pendry R-factor below 0.17. The main challenge lies in the extreme sensitivity of this surface to damage induced by the electron beam; the progressing damage is visualized at the atomic scale by noncontact atomic force microscopy (nc-AFM). Positions of lattice atoms obtained from LEED I-V analysis are used as a benchmark for a comparison with theoretical calculations performed within 30 different setups. The overall trend is that the closest match with the experiment is obtained for setups without the Hubbard U-term and with the SCAN functional

Work supported by GACR 20-21727X and MSMT LL2324.

HL 20.21 Tue 10:00 P3

Photoluminescence and photophysical properties of halide perovskite MAPbBr3 single crystal — •Liangling Wang[1,2], Francesco Vitale[2], Edwin Eobaldt[2], Thomas Alexander Zaunick[2], and Carsten Ronning[2] — [1]School of Physics and Technology, University of Jinan, Jinan 250022, P. R. China — [2]Institute of Solid State Physics, Friedrich-Schiller University Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The remarkable optoelectronic properties of halide perovskite MAPbBr3 (MA=methylammonium), including near-unity photoluminescence quantum yield (PL QY), small full width at half-maximum (FWHM), tunable bandgap by mixing halide and defect tolerance, make it a compelling candidate material in solar cell, light emitting diodes (LED), photodetectors, X-ray imaging, and so on. The PL spectrum of MAPbBr3 at room temperature can be deconvoluted into two emission peaks. The major peak at 545 nm arises from band-to-band transition, while the lower energy peak at 560 nm is associated with recombination in trap states (Br vacancies) below the optical gap. Interestingly, PL enhancement of MAPbBr3 is found under certain laser irradiation, indicating that the surface defects are benefit charge carrier trapping and recombination. In order to verify the origin of the emission centers, power dependent PL, including both power increase and decrease processes, will be analyzed. Furthermore, thermal activation and excitonic effects of PL under different temperature from cryogenic temperature of liquid Helium to room temperature will be investigated.

HL 20.22 Tue 10:00 P3

Resolving temporal signatures of optical excitations in semiconductor nanostructures — •Lion Krüger, Fabian Brütting, Moritz B. Heindl, and Georg Herink — Experimental Physics VIII, University of Bayreuth, Germany

Characteristic ultrafast signatures in the photo-induced response of nanostructured materials encode the class of optical excitations and characterize the performance for opto-electronic applications. Time-resolved visible transient absorption (TA) spectroscopy and optical pump THz probe (OPTP) spectroscopy are well-established methods for contact-free probing of ultrafast dynamics. Here, we present correlated TA-OPTP measurements performed in a setup that combines multiple probing modalities under identical excitation conditions. In particular, we present different strategies to enhance detection speed and sensitivity, enabling the disentanglement of free carrier and excitonic signatures in semiconductor nanostructures of varying dimensionality and quantum-confinement [1].

[1] Motti, Silvia G., et al. "Exciton Formation Dynamics and Band-Like Free Charge-Carrier Transport in 2D Metal Halide Perovskite Semiconductors". Advanced Functional Materials 33 (2023)

HL 20.23 Tue 10:00 P3

Characterization of the electrical properties of Bismuth doped Methylbenzylamine Lead Iodide 2D Perovskites using impedance spectroscopy — •Keito Mizukami[1,2,3], Hannes Hergert[1,3], Tim Schneider[3,4], Jan Heinrich Littmann[1,3], Satoko Fukumori[2], Philip Klement[1,3], Derck Schlettwein[3,4], Hirokazu Tada[2], Sangam Chatterjee[1,3], and Matthias T. Elm[1,3] — [1]Institute of Experimental Physics I, JLU Giessen, Giessen, Germany — [2]Graduate School of Engineering Science, Osaka University, Japan — [3]Center for Materials Research, JLU Giessen, Giessen, Germany — [4]Institute of Applied Physics, JLU Giessen, Giessen, Germany

Low-dimensional organic-inorganic perovskites offer largely tunable materials properties such as the crystal structure or the electronic band gap due to the flexibility of the incorporated building blocks. Perovskites with incorporated chiral organic molecules as the cation attract a lot of attention as they exhibit chiral properties such as chirality-induced spin selectivity or spin-polarized electron current. However, the typically low electrical conductivity hinders applications and requires appropriate doping schemes to improve the device performance. In this study, we investigate the impact of Bi substitution for Pb in methylbenzylamine bismuth lead iodide single crystals and thin films on the electric properties using impedance spectroscopy. Our objective is to get a fundamental understanding of the charge transportation and relaxation mechanism in these mixed conductors.

HL 20.24 Tue 10:00 P3

Hysteretic Piezochromism in a two-dimensional perovskite — •Paul Steeger[1], Mohammad Adnan[1], Thorsten Deilmann[2], Xiang Li[3,4], Susanne Müller[4], Katarzyna Skrzynska[5], Michael Hanfland[4], Efim Kolesnikov[3], Jutta Kösters[6], Theresa Block[6], Robert Schmidt[1], Ilya Kupenko[3,4], Carmen Sanchez-Valle[3], Vijaya Prakash[7], Steffen Michaelis de Vasconcellos[1], and Rudolf Bratschitsch[1] — [1]Physikalisches Institut Universität Münster — [2]Institut für Festkörpertheorie Universität Münster — [3]Institute für Mineralogie Universität Münster — [4]Europäischer Synchrotron ESRF Grenoble — [5]Institute of Earth Sciences University of Silesia — [6]Institut für Anorganische und Analytische Chemie Universität Münster — [7]Department of Physics IIT Dehli

Two-dimensional inorganic-organic hybrid perovskites hold potential for application in the field of optoelectronics. One representative of this class of materials is cyclohexenyl-eythylammonium lead-iodide (CHPI). Here, we present pressure-dependent optical absorption and

emission spectra of CHPI. We find a strong change of the band gap when exerting pressure on the crystal using a diamond anvil cell. In contrast to other 2D perovskites the bandgap of CHPI undergoes a full hysteresis loop under pressure. To reveal the origin of the observed phenomena, we combine our optical experiments with DFT calculations as well as X-ray diffraction measurements under high pressure. Reference: Steeger et al., Hysteretic Piezochromism in a Lead Iodide-Based Two-Dimensional Inorganic-Organic Hybrid Perovskite. JACS 146, 23205 (2024)

HL 20.25 Tue 10:00 P3

Electron and Hole polaron Formation in lead-free CsGeX3 (X=Cl,Br,I) perovskites — •Mehmet Baskurt — Chalmers University of Technology

The unique electronic properties of CsGeX3 (X = Cl, Br, I) perovskites make them promising candidates for nonlinear optical applications. The nature of charge localization must be understood to explain their physical and electronic behaviors. Here, we carry out a theoretical investigation on electron and hole polaron formation in CsGeX3. We carry out density functional theory calculations in the hybrid function level. Our results show that there is a trend in the polaron formation energies, CsGeCl3 > CsGeBr3 > CsGeI3. In particular, single electron polarons form highly favorably in all three materials, whereas single hole polarons can only be formed in CsGeCl3. Moreover, double electron polarons form energetically favorably across the series. These findings constitute a basis for understanding polaronic effects on the electronic properties of CsGeX3 perovskites and open up access to their optimization in nonlinear optical applications.