HL 13: Poster I

Topics:
- Heterostructures, interfaces and surfaces
- Optical properties of semiconductors
- Organic semiconductors
- Oxide semiconductors
- Perovskites and photovoltaics
- Spin phenomena in semiconductors
- THz and MIR physics in semiconductors

Time: Monday 15:00–18:00 Location: Poster E

HL 13.1 Mon 15:00 Poster E

"A Comparative Analysis of Two Different Full-Wafer Photoluminescence Spectroscopy Mappers" — •Elias Kersting, Alexander Schauerte, Hans-Georg Babin, Andreas Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Deutschland

Photoluminescence spectroscopy (PL) is an indispensable method for investigating the optical properties of semiconductor heterostructures. Spectroscopy of a complete wafer is necessary to obtain important growth parameters of samples grown with a molecular beam epitaxy (MBE) system. We present two different approaches for the construction of a fully automated 3-inch PL spectroscopy Mapper. The first setup uses mirrors as optical components and a movable cryostat. In the second setup, the heavy cryostat is fixed and a movable, lightweight optical system of lenses is used instead. The advantages and disadvantages are discussed and measurements on local droplet etched GaAs quantum dots are compared.

HL 13.2 Mon 15:00 Poster E

Quantifying quantum coherence in multi-mode polariton condensates — •Maximilian Nürmberger, Franziska Barkhausen, Xuekai Ma, Jan Sperling, and Stefan Schumacher — Department of Physics, CeOPP, and PhoQS, Paderborn University, Germany

One of the main challenges when engineering future quantum devices based on light-matter interaction is achieving resourceful and long-term coherent quantum states. We theoretically investigate quantum features of a polariton system and quantify the amount of quantum coherence that results from the quantum superposition of Fock states, constituting a measure of the resourcefulness for modern quantum protocols. We use phase-space quasi probability distributions of macroscopic polariton states to quantify changes in the quantum coherence beyond the condensation threshold [1,3] and calculate the time evolution using a regularized Glauber-Sudarshan representation [2,3]. Furthermore, we include the polarization degree of freedom and expand our calculations into orbital angular momentum (OAM) space to investigate the quantum coherence of multi-mode systems. In doing so we can calculate the quantum coherence of different vortex states in polariton condensates. We theoretically study vortices excited nonresonantly in an optically induced ring-shaped potential. By introducing a resonant control pulse in either polarization component, we can switch between different vortex-states [4]. [1] C. Lüders et al., PRX Quantum 2, 030320 (2021). [2] C. Lüders et al., Phys. Rev. Lett. 130, 113601 (2023). [3] C. Lüders et al., Opt. Mater. Express 13, 2997-3035 (2023). [4] M. Pukrop et al., Phys. Rev. B 101, 205301 (2020).

HL 13.3 Mon 15:00 Poster E

Two-photon excitation channels in CuI — •Andreas Müller[1], Leonard Käferstein[1], Lukas Trefflich[1], Steffen Blaurock[2], Harald Krautscheid[2], Marius Grundmann[1], and Chris Sturm[1] — [1]Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany — [2]Institut für Anorganische Chemie, Universität Leipzig, Johannisallee 29, 04103 Leipzig, Germany

Having recently identified strong two-photon absorption (2PA) in CuI [1], we're examining the excitation channels linked to this phenomenon.

We investigate the interferometric autocorrelation (IAC) function of CuI across various excitation energies to discern distinct excitation channels in 2PA-induced photoluminescence (PL). Probing near the 2PA edge (795 nm), the broadening of the IAC function of CuI is similar to the pulse duration of the laser (FWHM $\approx$ 200 fs) suggesting an excitation assisted by a virtual level. In contrast, probing with 460 nm, a different IAC shape emerges with significant broadening (FWHM $\approx$ 475 fs). Given the predicted presence of a defect level at this energy [2] and the alignment with the extension of the DAP band in this excitation range, we attribute these alterations to 2PA process assisted by a real level. Similar variations in the IAC function have been documented in prior literature on GaAs [3], which supports our interpretation. We estimate a real-level lifetime of approximately 220 fs.

[1] A. Müller *et al.*, Appl. Phys. Lett. **123**, 122103 (2023)
[2] S. Koyasu *et al.*, J. Appl. Phys **125**, 115101 (2019)
[3] T. Hattori *et al.*, Jpn. J. Appl. Phys. **39**, 4793 (2000)

HL 13.4 Mon 15:00 Poster E

On-chip lateral Si:Te PIN photodiodes for room-temperature detection in the telecom optical wavelength bands — Mohd Saif Shaikh[1,2], Shuyu Wen[1,3], Mircea-Traian Catuneanu[2], Mao Wang[4], Artur Erbe[1,2], Slawomir Prucnal[1], Lars Rebohle[1], •Shengqiang Zhou[1], Kambiz Jamshidi[2], Manfred Helm[1,2], and Yonder Berencén[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Dresden University of Technology, 01062 Dresden, Germany — [3]Institute of Semiconductors, Chinese Academy of Sciences, Bejing, China — [4]Sichuan Normal University, Chengdu 610101, China

Photonic integrated circuits require photodetectors that operate at room temperature with sensitivity at telecom wavelengths and are suitable for integration with planar complementary-metal-oxide-semiconductor (CMOS) technology. Silicon hyperdoped with deep-level impurities is a promising material for silicon infrared detectors because of its strong room-temperature photoresponse in the short-wavelength infrared region caused by the creation of an impurity band within the silicon band gap. In this work, we present the first experimental demonstration of lateral Te-hyperdoped Si PIN photodetectors operating at room temperature in the optical telecom bands. We provide a detailed description of the fabrication process, working principle, and performance of the photodiodes, including their key figure of merits. Our results are promising for the integration of active and passive photonic elements on a single Si chip, leveraging the advantages of planar CMOS technology.

HL 13.5 Mon 15:00 Poster E

High-reflectivity $Al_2O_3/Al_{0.3}Ga_{0.7}As$ distributed Bragg reflectors and microcavities for photon Bose-Einstein-condensates in GaAs quantum wells — •Lara Schmieder[1,3], Nils von den Driesch[2,3], Yurii Kutovyi[1,3], Siqi Qiao[1,3], Christoph Krause[2], Benjamin Bennemann[2], and Alexander Pawlis[1,2,3] — [1]PGI-9, Forschungszentrum Jülich GmbH — [2]PGI-10, Forschungszentrum Jülich GmbH — [3]JARA-FIT, Jülich Aachen Research Alliance

Significant present research is focused on the realization of Photon-Bose-Einstein-Condensates (P-BECs) for applications in quantum technology. We propose a scalable chip-architectur composed of III-V semiconductor microcavities with GaAs quantum wells. The latter are directly grown between high-reflectivity AlOx based Distributed Bragg Reflectors (DBRs) to form a high-finesse microcavity. In order to reach the thermalization conditions of a semiconductor based P-BEC, extremely high reflectivity of the DBRs is required.

We meet these condition by establishing AlOx based DBRs fabricated via a combined nanostructuring and wet-oxidation process of as-grown $AlAs/Al_{0.3}Ga_{0.7}As$ superlattices. Reflectivity measurements of our AlOx based Bragg reflectors owe much higher reflectivity as standard $AlAs/Al_{0.3}Ga_{0.7}As$ Bragg-mirrors with similar number of periods. Quantitative analysis of microcavities with AlOx based DBRs confirm that 8-fold stacks are already sufficient to achieve high enough

finesse to overcome the above mentioned thermalization limit.

HL 13.6 Mon 15:00 Poster E

Manipulating spectral topology and exceptional points by nonlinearity in non-Hermitian polariton systems — Jan Wingenbach, Stefan Schumacher, and •Xuekai Ma — Physics Department and CeOPP, and PhoQS, Paderborn University, Germany

Exceptional points (EPs) are singularities in parameter space at which two or more eigenstates coalesce. Such singularities occur exclusively in non-Hermitian systems which are subject to gain and loss and exhibit non-orthogonal eigenvectors and complex eigenvalues. Due to their intriguing spectral topology EPs have attracted considerable attention in a broad range of physical systems, with potential sensing applications driving much of the present research in this field [1]. We investigate the EPs in systems with significant nonlinearity, exemplified by a nonequilibrium exciton-polariton condensate. Polaritons are quasiparticles, formed due to the strong coupling of photons and excitons in planar semiconductor microcavities. With the possibility to control loss and gain and nonlinearity by optical means, this system allows for a comprehensive analysis of the interplay of nonlinearities (Kerr-type and saturable gain) and non-Hermiticity [2]. Not only do we find that EPs can be intentionally shifted in parameter space by the saturable gain, we also observe intriguing rotations and intersections of Riemann surfaces and find nonlinearity-enhanced sensing capabilities. These results illustrate the potential of tailoring spectral topology and related phenomena in non-Hermitian systems by nonlinearity. [1] J. Wiersig, et al., Photonics Research 8, 9 (2020). [2] J. Wingenbach, et al., arXiv:2305.04855 (2023).

HL 13.7 Mon 15:00 Poster E

Cathodoluminescence study of point and structural defects in bottom-up GaN nanowires — •Mikel Gómez Ruiz[1], Matt Brubaker[2], Kris Bertness[2], Manfred Ramsteiner[1], Oliver Brandt[1], and Jonas Lähnemann[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Germany — [2]National Institute of Standards and Technology, USA

Luminescence techniques are inherently sensitive to the presence of both radiative and nonradiative defects. In this work, we investigate the prevalence and distribution of both point and structural defects in GaN nanowires (NWs) by low-temperature (10 K) cathodoluminescence (CL) hyperspectral line scans along the NW axis. Ordered arrays of NWs are grown by selective-area molecular beam epitaxy using a Si_3N_4 mask on a N-polar GaN template on Si. The CL intensity of single NWs is observed to vary along the NW axis. During initial NW growth, impinging Ga atoms can react with the Si_3N_4 mask leading to the unintentional incorporation of Si into the NW. The incorporation is gradually reduced once the NW height is approximately equal to their distance, where shadowing prevents the direct impingement of Ga atoms on the mask. The Fermi-level pinning at the NW side facets results in internal electric fields, whose spatial extent depends on the Si concentration and the NW diameter. These fields can dissociate excitons as well as shallow donors and acceptors, thus reducing the corresponding radiative emission intensity. A gradient in Si doping can thus explain the change in emission intensity. This Si doping also causes most of the NWs to have inversion domain boundaries.

HL 13.8 Mon 15:00 Poster E

Topological edge and corner states in coupled wave lattices in nonlinear polariton condensates — •Tobias Schneider[1], Wenlong Gao[2], Thomas Zentgraf[1,3], Stefan Schumacher[1,3,4], and Xuekai Ma[1] — [1]Physics dept. CeOPP, Paderborn University, Germany — [2]EIT Institute for Advanced Study, Ningbo, China — [3]Physics dept. PhoQS, Paderborn University, Germany — [4]Wyant College of Optical Sciences, University of Arizona, Tucson, USA

Topological states are of great interest due to their robustness against perturbations, hence they have been widely investigated in many physical systems including microcavity exciton polaritons[1]. In this work, we explore topological states in exciton polariton condensates in our newly designed double-wave (DW) lattices[2]. Exciton polaritons are quasiparticles composed of excitons and photons in semiconductor microcavities and show strong repulsive nonlinearity. The 1D DW chains we proposed enable multiple types of edge states in both the linear and the nonlinear regime, in which they are shown to be multistable. The strong nonlinearity of polaritons can also lead to the formation of new types of edge states that originate from the bulk eigenstates, i.e. nonlinearity-enhanced edge localization. The 1D lattice can be expanded into a 2D lattice structure, with SSH like structures in the new dimension. The combination of the perpendicularly DW and SSH lattices allows for the formation of additional higher-order topological insulator states (0D corner states). These corner states are also shown to be multistable in the nonlinear regime.[1] S. Klembt et al., Nature 562, 552 (2018).[2] T. Schneider et al., arXiv:2303.12593 (2023).

HL 13.9 Mon 15:00 Poster E

Bulk-Material Supercontinuum Generation for Temporal Compression of Ultrafast Laser Pulses — •Olga Resel, Hana Hampel, Daniel Hipp, Adrian Kirchner, and Martin Schultze — Institute of Experimental Physics, Graz University of Technology, Austria

For the generation of ultrashort laser pulses spectral broadening of the output of commercially available short-pulse laser sources is essential. This can be achieved by nonlinear light - matter interaction. Here we studied self-phase modulation of a commercial Yb:KGW laser system (PHAROS from Light Conversion) in fused silica. In a first step, the spectrum and the interferometric autocorrelation of the unfocused laser beam, propagating through fused silica, were measured and analysed in contrast to measurements without fused silica in the beam path. The obtained spectra were compared to numerical simulations of self-phase modulation with the experimental laser parameters as well as the Fourier transform of the initial spectrum as input. Although dispersion was neglected in the computations, the results and the experimental observations are in excellent agreement. In a second step, limits of self-phase modulation were explored by increasing beam intensities using a focused laser beam. The spectra and further the interferometric autocorrelations of the broadened pulses were measured. At the limit of self-phase modulation, even a white light supercontinuum was observed. Based on these measurements, it could be possible to achieve a 50% reduction of the pulse duration, if proper dispersion compensation can be implemented.

HL 13.10 Mon 15:00 Poster E

Energy-Momentum-Resolved Spectroscopy of Chiral Hybrid Perovskites — •Caroline Aschendorf[1], Jonathan Zerhoch[1,2,3], Shangpu Liu[1,2,3], and Felix Deschler[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg — [2]Walter Schottky Institut, Technische Universität München — [3]Physics Department, TUM School of Natural Sciences, Technische Universität München

Energy-momentum-resolved spectroscopy allows for highly sensitive photoluminescence measurements, revealing the orientation of the emission dipole moment. Different momentum intensity profiles distinguish between in-plane (IP) and out-of-plane (OP) exciton orientations through s- and p-polarized components of the emitted light. Of particular interest is the investigation of the novel chiral 2D hybrid metal-halide perovskite (HMHP) (R/S)-3BrMBA$_2$PbI$_4$, which exhibits a high photoluminescence quantum yield (PLQY) of up to 39% and circularly polarized photoluminescence (CPL) of up to 52%. Energy-momentum spectra were acquired for thin films and facets of single crystals of (R/S)-3BrMBA$_2$PbI$_4$, (R/S)-4BrMBA$_2$PbI$_4$, BA$_2$PbI$_4$, and the inorganic 3D perovskite CsPbBr$_3$. This allowed the modeling of the in-plane (IP) to out-of-plane (OP) exciton ratio, revealing a notable distribution towards OP excitons in certain materials.
The study of CPL in chiral materials aims to investigate the impact of chirality on exciton orientation. This knowledge is crucial for advancing chiral HMHP development with higher CPL and PLQY, holding promise for chiroptical applications and chiral spintronics.

HL 13.11 Mon 15:00 Poster E

Multidimensional Coherent Spectroscopy on naturally grown Cu_2O — •Mariam Harati, Julian Heckötter, Binodbihari Panda, Simon Siegeroth, and Marc-Alexander Assmann — Technische Universität Dortmund, Dortmund, Deutschland

Excitons are elementary excitations in various electronic systems. They play a fundamental role in solid state quantum technology and thus building new optoelectronic devices. Especially the optical prosperities of excitons in Cuprous Oxide (Cu_2O) are of significant interest in the field of precision sensor technologies since Rydberg-Excitons with large quantum numbers n can be created in this material (T. Kazimierczuk et al. Nature 514, 343 (2014)). In this work, we present Multidimensional Coherent Spectroscopy (MDCS) of Rydberg-Excitons of the yellow series in naturally grown Cu_2O. It allows us to measure the third order nonlinear optical response of Cu_2O and to characterize inhomogeneity and coupling. In order to perform MDCS a collinear spectrometer is used. In addition to the spectrometer, the sample is

scanned along the plane perpendicular to the optical axis. This provides us with hyperspectral images of impurities and excitons.

HL 13.12 Mon 15:00 Poster E

In situ time-resolved photoluminescence measurement in the PEC environment — •Peter Kleinschmidt, Elias Hartung, Lucas Krätschmer, David Ostheimer, and Thomas Hannappel — TU Ilmenau, Institute of Physics, Fundamentals of Energy Materials, 98693 Ilmenau

Recombination properties of minority charge carriers are crucial for the optoelectronic performance of a many semiconductor devices. Time-resolved photoluminescence (TRPL) measurement, based on time-correlated single photon counting, provides direct access to the effective minority charge carrier lifetime. Typically, this is carried out separately from preparation and operation of devices. We have developed a flexible TRPL-setup with a remote measuring head which allows measurement in different environments. We demonstrate measurement of charge carrier lifetimes in a photo-electrochemical cell, providing access to device performance and degradation in this environment. The measurement can be performed in correlation with photo-electrochemical operation of the sample and enables observation of different influences on the optoelectronic device properties.

HL 13.13 Mon 15:00 Poster E

Optimization of vertically graded $Mg_xZn_{1-x}O$ layers for the use in wavemeters — •Christoph Brunhuber, Lukas Trefflich, Daniel Splith, Chris Sturm, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, 04103 Leipzig, Germany

To determine the wavelength of monochromatic radiation, a new design for a wavemeter was proposed, that is forward-looking, monolithic and ultra-compact [1]. It consists of two vertically stacked, photosensitive layers, separated by a transparent, insulating layer. The top layer has a vertically graded alloy composition in order to achieve spectral sensitivity. The ratio of the photocurrents generated in the two absorber layers relates to the wavelength of the incident radiation.

We realized such wavemeter devices using a $Mg_xZn_{1-x}O$ alloy system. Within the graded absorber layer the Mg-content increases from $x = 0$ to $x \approx 0.4$. The two absorber layers were deposited on opposite sides of a sapphire substrate by pulsed laser deposition, using a vertical continuous composition spread (VCCS-PLD) technique to obtain the graded layer. Here, we discuss the optimization of the vertically graded $Mg_xZn_{1-x}O$ layer. For structural analysis XRD 2θ–ω-scans were performed. The functionality of the wavemeters was confirmed by spectrally resolved photocurrent measurements under illumination with monochromatic light. The photocurrent-ratio shows a wavelength dependency similar to the theoretically calculated one [1].

[1] M. Grundmann. Phys. Stat. Sol. A **215**, 1800651 (2018)

HL 13.14 Mon 15:00 Poster E

Resonant Raman scattering at split-off band exciton in CuI — •R. Hildebrandt[1], S. Blaurock[2], H. Krautscheid[2], M. Grundmann[1], and C. Sturm[1] — [1]Universität Leipzig, Felix Bloch Institute for Solid State Physics, Germany — [2]Universität Leipzig, Institute of Inorganic Chemistry, Germany

We investigate the resonant Raman spectrum of copper iodide (CuI), and observed up to ten consecutive LO-phonon scattering processes for the split-off band exciton. This exciton is energetically isolated and located above the fundamental bandgap. The resonance condition is varied by using excitation wavelengths of 355 nm, 325 nm and 320 nm, which are located above and below the respective exciton energy of 335nm.

This resonant interaction of excitons and phonons is mediated via the Fröhlich interaction and can give access to fundamental material characteristics such as effective masses, electron-phonon coupling and their wave-vector dependence. Dipole-forbidden transitions can be investigated or localized modes can be used for precise determination of doping concentrations [1]. The observed multiple LO-phonon scattering processes are typical for polar semiconductors[2] and contain information for exciton damping constants, relaxation times as well as acoustic phonon dispersion characteristics [3]. The therewith-derived properties of CuI will be discussed in this work.

[1] Y. Zhang, J. Semicond., **40**, 091102, 2019.
[2] R. Leite, J., Phys. Lett., **22**, 780, 1969.
[3] P. Yu and M. Cardona, Fundamentals of Semiconductors, 2010.

HL 13.15 Mon 15:00 Poster E

Electro-optical phase change devices based on nanocrystalline graphite heaters for integrated photonic circuits — •Niklas Vollmar[1], Anna Ovvyan[2], Wolfram Pernice[2], and Martin Salinga[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Kirchhoff-Institute for Physics, University of Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

In-memory computing with integrated photonic circuits is promising due to high bandwidth and low latency. In such systems, phase change materials (PCMs) can be used as compact and non-volatile modulators: the pronounced contrast in permittivity between their crystalline and amorphous states allow to tune the light transmission through an adjacent photonic waveguide by switching between those configurations. However, mature in-memory computing systems require to tune weights, represented by such transmission states, precisely and reproducibly. To this end, we create electro-optical phase change devices with electrical heaters based on nanometer-thin nanocrystalline graphite, which shows low-loss and can be produced in a simple graphitization process. A PCM is placed directly above stripes of graphite crossing the waveguide. Precise and reproducible tuning of the transmission state is achieved by switching individual, nanoscopic PCM pads fully, avoiding partially crystalline states. Gradual adjustments of the transmission can be achieved by configuring the states of a series of PCM pads with varying size. This way, a limited number of pads can still yield high-resolution weights.

HL 13.16 Mon 15:00 Poster E

Nanoscopic electrical heaters for mixed-mode in-memory computing with phase change materials — •Nishant Saxena[1], Niklas Vollmar[1], Ivonne Bente[2], Frank Brückerhoff-Plückelmann[2], Wolfram Pernice[2,3], and Martin Salinga[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Physical Institute, University of Münster, Heisenbergstraße 11, 48149 Münster, Germany — [3]Kirchhoff Institute for Physics, University of Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

In contrast to von-Neumann processors, in-memory computing systems avoid data movement between the processing unit and memory and are therefore fundamentally more efficient. In particular, matrix-vector multiplications on crossbar arrays of photonic waveguides can be performed with extremely high throughput and low energy consumption. A promising approach uses phase change devices to represent the matrix elements. Depending on the phase of the material, a variable fraction of the incoming light is transmitted. We show the realization of mixed-mode phase change devices for in-memory computing on a silicon-on-insulator platform. Their state is written with heating supplied by electrical PIN diodes, which locally heat up individual pads of phase change material on a waveguide. By switching of separate, nanoscopic phase change pads, this scheme enables a reproducible tuning of transmission states with high resolution. The foundry-fabricated devices allow for large-scale integration in mixed-mode integrated circuits with feedback between the photonic and electronic parts.

HL 13.17 Mon 15:00 Poster E

Theoretical characterization of lead tungstate (PWO-II) crystal structure for improved electromagnetic calorimetry — •Ather Ahmad[1], Kai-Thomas Brinkmann[1], and Simone Sanna[2] — [1]II. Physikalisches Institut, Gießen, Germany — [2]Institut für Theoretische Physik, Gießen, Germany

Fast response, high density and radiation hardness make lead tungstate (PbWO4 or PWO) a well suited scintillator for an electromagnetic calorimeter. Lead tungstate crystals are already used as working material in various experiments, e.g. CMS at LHC in CERN. New generation crystals (PWO-II) with improved properties were developed for the PANDA experiment at FAIR in Darmstadt.

In order to assess the functionality of the calorimeter, we first need to analyse the electronic and optical properties of lead tungstate. To achieve this the determination of the crystal structure of PWO-II is essential. In our work, we calculate Raman spectra for various phases of PWO crystals in the framework of density functional theory (DFT). Subsequently, these calculated spectra can be compared with experimental Raman spectra of our PWO-II crystals, facilitating the identification of its phase.

This project is supported by HFHF and HGS-hire

HL 13.18 Mon 15:00 Poster E

Searching for Effective Temperature Seebeck Voltage in

Nanoscale Organics — •Anton Kompatscher and Martijn Kemerink — IMSEAM Heidelberg University, Im Neuenheimer Feld 225 69120 Heidelberg

In contrast to inorganics, organic semiconductors usually show a high degree of energetic and structural disorder. While we have relatively good insight into organics as an ensemble of many molecules, the regime of small (few nanometer) length scales, at which relatively few molecules are probed, remains hardly explored. A phenomenon we are especially interested in is the concept of effective temperature wherein a high >10^7 V/m electric field is predicted to generate electron distributions that correspond to much higher temperatures than the lattice temperature. As modeled in a recent publication, the effective temperature should be able to generate exceptionally high Seebeck voltages, which gives us a good option for experimental verification of the theory. In order to generate sufficient field strengths, the use of nanoscale structures, which we fabricate via electron beam lithography, is necessary. The main challenge in analyzing the signal is to separate spurious effects in the experimental system from the Seebeck voltage, which we do by measuring the response to AC voltages and comparing to theoretical predictions. In particular, we exploit the fact that the Seebeck signal should have double the frequency and zero phase lag compared to the input signal. First results are consistent with the generation of finite effective temperatures, which would constitute the most direct proof of the concept so far.

HL 13.19 Mon 15:00 Poster E

Theoretical insights into enhanced thermoelectric properties of TTT2I3 and TTT(TCNQ)2 organic nanostructured crystals — •Ionel Sanduleac and Silvia Andronic — Technical University of Moldova, Stefan cel Mare ave. 168, MD-2004, Chisinau, Republic of Moldova

We present a detailed analysis of the thermoelectric properties exhibited by crystals of TTT2I3, which manifests p-type behavior, and TTT(TCNQ)2 being an n -type conductor. These crystals have been shown to exhibit tunable thermoelectric properties through manipulations of the stoichiometry of charge carriers and impurity concentrations [1]. Crystals of TTT2I3, characterized by a layered structure of alternating tetrathiotetracene and iodide layers, demonstrates efficient charge transport along the main crystallographic axis. Similarly, TTT(TCNQ)2 shares the internal structure of TTT2I3, but with electric conductivity provided by electrons along the TCNQ chains. For this study, we developed a theoretical model, considering electron-phonon interactions and impurity scattering, to analyze transport and thermoelectric properties. The kinetic equation is derived using two-particle retarded Green functions. Electrical conductivity, Seebeck coefficient, thermoelectric power factor, and thermoelectric figure-of-merit were calculated numerically, as function of charge carrier concentrations, temperatures, and impurity concentrations. This study contributes to the understanding of organic thermoelectric materials and their potential role in sustainable energy applications.

[1] I. Sanduleac, et.al.: J. Appl. Physics, 126(17), (2019).

HL 13.20 Mon 15:00 Poster E

Quantum-chemical calculations of structure, electronic properties, and spectra of neat PBDB-T:ITIC heterojunctions — Montassar Chaabani[1], Samir Romdhane[1], and •Wichard J. D. Beenken[2] — [1]Advanced Materials and Quantum Phenomena Laboratory, Physics Department, Faculty of Sciences of Tunis, University of Tunis El Manar, Tunis, Tunisia — [2]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

In order to overcome the short-comings of polymer:fullerene heterojunctions in organic solar cells, an exchange of the fullerene by other organic molecules, e.g. ITIC has been proposed. In this context, we simulate the structural, electronic and optical properties of PBDB-T:ITIC interfaces quantum-chemically. We constructed oligomers in various conformations in order to represent a segment of the copolymer PBDB-T as well as three conformers of ITIC. These were combined to dimers in either parallel and T-shaped arrangement, and optimized in DFT calculations utilizing the B3LYP-GD3 functional, which considers the Van der Walls interaction semi-empirically. By comparing the MO-energies of the optimized PBDB-T oligomers, ITIC conformers, and dimers, we classified the resulting heterojunctions. Furthermore, we calculated the excited states of the dimers by TD-DFT in order to determine the exciton binding energies and to distinguish charge transfer from excitonic states. Eventually, we provide some indications, to the influence of the PBDB-T:ITIC interface design on the photovoltaic performance.

HL 13.21 Mon 15:00 Poster E

Effect of trap states on the performance of organic photodetectors — •Anncharlott Kusber, Jakob Wolansky, Karl Leo, and Johannes Benduhn — Institute of Applied Physics, Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany

In recent years, the scientific community has increasingly investigated novel semiconductors for solar energy conversion. Recently, this field has seen rapid development, and, for example, organic solar cells achieve power conversion efficiencies close to 20 %. Additionally, similar systems have been employed in organic photodetectors (OPDs), showing very competitive specific detectivities $D^* > 10^{13}$ Jones. However, these OPDs, operated under reverse bias, are still limited due to the shot noise, which is proportional to the high dark reserve current [1]. Therefore, a complete understanding of the dark reverse current is necessary. Recent research has revealed a negative impact of mid-gap trap states on the reverse dark current in OPDs [1]. To understand this impact, studies investigated the influence of charge-transfer excitons and trap states using ultrasensitive external quantum-efficiency measurements as well as impedance spectroscopy. We use the techniques as mentioned above on a model system where we intentionally introduce trap states within the active layer. We find a clear trend between the device performance and the presence and quantity of trap states.

[1]: Kublitski, Jonas, et al., Nature Communications 12.1 (2021): 551.

HL 13.22 Mon 15:00 Poster E

Shear-coated highly-smooth ion gels as dielectrics in ion-gated organic field effect transistors — Jonathan Perez Andrade[1,2], Angelika Wrzesińska-Lashkova[1,2], Anupam Prasoon[1,3], Felix Talnack[1], •Yulia Krupskaya[2], Xinliang Feng[1,3], Yana Vaynzof[1,2], Mike Hambsch[1], Bernd Büchner[1,2], and Stefan C. B. Mannsfeld[1] — [1]Dresden University of Technology, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden, Germany — [3]Max Planck Institute for Microstructure Physics, Halle (Saale), Germany

We have developed a straightforward method to produce ion gels with surface roughness at the nanometer scale using a shear-coating process and employed these gels as ultra-smooth dielectric substrates in organic field effect transistors (OFET). The exceptional smoothness of the gels allowed us to grow polycrystalline films of C8-BTBT (2,7-Dioctyl[1]benzothieno[3,2-b][1]benzothiophen) and C10-DNTT (2,9-Didecyldinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene) and to evaporate metal contacts on their surface. Besides that, the shear-coating process increased the ion concentration at the gel's surface leading to a remarkably high capacitance up to 10.1 μF/cm^2. The obtained ion-gel-based OFET showed very good characteristics with low hysteresis and maximum charge carrier mobility of 0.54 cm^2/V/s and 0.27 cm^2/V/s for C10-DNTT and C8-BTBT devices, respectively. These results demonstrate the significant potential of using shear-coated ion gels in fabrication of high quality OFET.

HL 13.23 Mon 15:00 Poster E

Study of the metal-insulator transition of Peierls type in quasi-one-dimensional organic crystals. — •Silvia Andronic and Ionel Sanduleac — Technical University of Moldova, Stefan cel Mare ave. 168, MD-2004, Chisinau, Republic of Moldova

The purpose of the current study is to investigate the metal-insulator transition occurring in quasi-one-dimensional organic crystals (Q1D) of TTF-TCNQ, TTT(TCNQ)2 and TTT2I3. The use of these materials brings several advantages, including cost-effectiveness, environmental safety and relatively inexpensive manufacturing processes. Additionally, the growing interest in certain Q1D organic crystals is attributed to their high electrical conductivity. The research employs a 3D approximation method and introduces a physical model that incorporates two significant electron-phonon interaction mechanisms, one akin to the deformation potential and the other exhibiting polaron characteristics. We also account for scattering on defects, a crucial factor in explaining the transition. Using the random phase approximation and Green functions method, we calculate the phonon polarization operator and the renormalized phonon spectrum at different temperatures and various dimensionless Fermi momentum (kF) values. The results suggest that the transition demonstrates Peierls-type characteristics, and the critical temperature linked to the Peierls transition is identified. Furthermore, we observed that the Peierls critical temperature significantly decreases as the carrier concentration increases. The impact of lattice distortion on the dispersion of renormalized acoustic phonons is also considered.

HL 13.24 Mon 15:00 Poster E

Single molecule spectroscopy of emitters in hexagonal boron nitride — •Osama Farooqui and Klas Lindfors — Department of chemistry, University of Cologne, Greinstr.4-6, D-50939, Cologne, Germany

The interaction of light with atoms or molecules is indispensable in the examination of materials for potential use in the development of high-speed communication devices [1]. The primary objective of this project is to observe light emission and absorption within heterostructures comprised of two- and one-dimensional materials, as well as single emitter molecules.

Previously, investigations were conducted on individual triisopropylsilyl pentacene (TIPS-pentacene) molecules on a glass substrate using single molecule spectroscopy. To address the challenge of molecular stability, hexagonal Boron Nitride (hBN) is employed to encapsulate emitter molecules, thereby preventing chemical reactions with the surrounding environment. Initial data from time traces of TIPS-pentacene molecules encapsulated in hBN flakes indicate that these molecules do not undergo photobleaching over a one-hour period at room temperature. However, rapid photoblinking is observed in the time traces of the molecules. The cause of this fast photoblinking is speculated to be the interaction of the molecules with nearby two-level systems, potentially associated with hBN flakes.

Reference

[1] Toninelli, C. et al. Single organic molecules for photonic quantum technologies. Nat. Mater. 1*14 (2021).

HL 13.25 Mon 15:00 Poster E

Optimisation of the surface structure of a Pt/TiOx sensor for low concentrations of hydrogen — •Anastasija Scherer, Marvin Rauhut, Thomas Heinzel, and Mihai Cerchez — Condensed Matter Physics Laboratory, Heinrich-Heine-Universität Düsseldorf

Mesoporous TiOx based hydrogen sensors are highly sensitive also at ppm concentrations [1], however, the results are highly dependent on the parameters of the TiOx internal structure, like defect density or internal surface-to-volume ratio. The sensors are produced by anodisation of industrial grade Ti foil in solution of sulfuric acid [2]. The process leads to the formation of a TiOx thin layer of thickness of the order of micrometers, and surface aspect varying between sandy and spongeous, with a characteristic mesh size of the order of 100 nm. This is controlled by the voltage used during the anodisation process as well as subsequent thermal annealing. Measurements of the sensing capability will be presented. [1] Appl. Phys. Lett. 103, 033522, 2013 [2] Metals 8, 386, 2018

HL 13.26 Mon 15:00 Poster E

Sensing acetaldehyde using Pt/TiOx sensors — •Marvin Rauhut, Anastasija Scherer, Thomas Heinzel, and Mihai Cerchez — Condensed Matter Physics Laboratory, Heinrich-Heine-Universität Düsseldorf

The photocatalytic decomposition has been shown to be the most promising route to air purification for volatile organic compounds, both at TiOx [1] and Pt/TiOx [2] catalyst surfaces. Here, a vertical structure formed by a thin Pt layer on a mesoporous TiOx film with high density of oxygen vacancies is used as a sensor for acetaldehyde. While first results are encouraging, this presentation will show the progress on tuning the surface structure to maximise sensitivity to acetaldehyde, measured as the change of the resistance of the sensor during the exposure to various concentrations of acetaldehyde. [1] Catalysts, 10, 1464, 2020 [2] J. Catal., 179, 171, 1998

HL 13.27 Mon 15:00 Poster E

Heteroepitaxial Growth of Ge-doped γ-Ga_2O_3 Ultrawide Bandgap Semiconductor Thin Films on (100) $MgAl_2O_4$ Substrates by Pulsed Laser Deposition — •Jingjing Yu, Sijun Luo, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth System Sciences, Universität Leipzig, 04103 Leipzig

γ-Ga_2O_3 is a defective cubic spinel metastable phase of ultrawide bandgap gallium oxides. In order to compensate the volatile loss of Ge components, a Ge-rich target with a Ge:Ga atomic ratio of about 17:1 was used to grow (100)-oriented γ-$(Ga_{1.73}Ge_{0.27})O_3$ epitaxial thin films on cubic spinel (100) $MgAl_2O_4$ substrates using pulsed laser deposition. The $(Ga_{1.73}Ge_{0.27})O_3$ epitaxial thin films are fully-strained, and the in-plane orientation relationships are [010] $(Ga_{1.73}Ge_{0.27})O_3$ // [010] $MgAl_2O_4$ and [011] $(Ga_{1.73}Ge_{0.27})O_3$ // [011] $MgAl_2O_4$. The 215 nm thick (100) $(Ga_{1.73}Ge_{0.27})O_3$ epitaxial thin film shows the rocking curve of (400) reflection with a full width at half maximum (FWHM) of about 0.022 degrees (80 arcseconds). The electrical properties of $(Ga_{1.73}Ge_{0.27})O_3$ epitaxial thin film were evaluated by temperature-dependent Hall measurements. The resistivity of film decreases dramatically from about 30000 Ω cm to 6 Ω cm as temperature increases from 125 to 350 K. The electron carrier concentration of thin film increases from 2.1 x 10^{14} cm^{-3} at 125 K to 2.6 x 10^{17} cm^{-3} at 350 K with an estimated activation energy of about 117 meV. While the Hall electron carrier mobility gradually increases from 0.4 to 4.1 cm^2 $V^{-1}s^{-1}$ as the temperature increases from 125 to 350 K.

HL 13.28 Mon 15:00 Poster E

Screening of different p-type materials for pn-heterojunctions on α-Ga_2O_3 — •Paul Bokemeyer, Sofie Vogt, Clemens Petersen, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut, Germany

With a wide band gap of about 5.3 eV [1], the possibility for adjusting the band gap energy by alloying with isostructural aluminum oxide or indium oxide [1], and a high expected breakdown field of up to 10 MV/cm [2], the corundum α-phase of Ga_2O_3 is highly interesting for high power applications. Schottky barrier diodes have been shown to exhibit high rectification ratios [3] and the first isostructural *pn*-diodes using α-Ir_2O_3 as p-type material have been demonstrated [4]. We evaluate the electrical properties of various heterojunction diodes on α-Ga_2O_3:Sn grown by pulsed laser deposition (PLD). Room temperature deposited ZCO (PLD), NiO (PLD) and CuI (sputtering) were used as p^+-type materials. Thereby NiO as well as CuI enable the fabrication of fully transparent devices in the visible spectral range. High current rectification ratios of 6.3 (ZCO), 3.9 (NiO), and 4.6 (CuI) orders of magnitude at ± 3V were achieved.

[1] A. Hassa *et al.*, J. Phys. D: Appl. Phys. 54 223001 (2021)
[2] M. Biswas and H. Nishinaka; APL Materials 10, 060701 (2022)
[3] S. Köpp *et al.*, J. Vac. Sci. Technol. A 41, 043411 (2023)
[4] S. Kan *et al.*; Appl. Phys. Lett. 113, 212104 (2018)

HL 13.29 Mon 15:00 Poster E

Cation segregation in an $(In,Ga)_2O_3$ thin film library beyond the miscibility limit of the bixbyite structure — •Sandra Montag[1], Daniel Splith[1], Max Kneiss[1], Marius Grundmann[1], Javier Garcia Fernandez[2], Øystein Prytz[2], and Holger von Wenckstern[1,2] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Department of Physics/Centre for Materials Science and Nanotechnology, University of Oslo, Norway

The transparent semiconductors In_2O_3 and Ga_2O_3 crystallise in different polymorphs. Hence, a phase change occurs in the alloy system of $(In_{1-x}Ga_x)_2O_3$, grown in bixbyite cubic structure at low x. To observe this change, a material library of thin films with $0.1 \leq x \leq 0.64$ was fabricated by discrete combinatorial synthesis on r-plane sapphire substrates using pulsed laser deposition. The samples crystallize in the bixbyite phase for $x \leq 0.35$, as revealed by X-ray diffraction. However, lattice constant and absorption edge energy systematically decrease and increase, respectively, with increasing Ga content only up to $x = 0.2$. For higher Ga admixtures, both saturate. In addition, a significant change in surface morphology occurs at $x \sim 0.2$. Transmission electron microscopy examinations of selected samples show a homogeneous incorporation of Ga_2O_3 into cubic In_2O_3 for $x = 0.11$, while a segregation of Ga-rich and In-rich regions can be seen for higher x. In a sample with $x = 0.35$, the Ga-rich regions exhibit a preferred orientation, which has been shown to result from a correspondingly faceted In-rich bixbyite layer at the substrate-thin film interface.

HL 13.30 Mon 15:00 Poster E

PLD Deposition of the transistion metal sesquioxides α-Ti_2O_3 and α-Cr_2O_3 — •Lorenz Köhnlein, Sofie Vogt, Clemens Petersen, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut, Deutschland

Corundum phase sesquioxides like Ti_2O_3 and Cr_2O_3 are ideally suited for band gap engineering within α-Ga_2O_3-based ternary alloys to design wavelength-selective optoelectronic devices. It has been shown that rhombohedral Ti_2O_3 has a narrow-bandgap of $\approx$ 0.1 eV [1]. Therefore, Ti could be used as a band gap modifier for α-Ga_2O_3 to tune the bandgap between 0.1 eV and 5.3 eV [2].

We present physical properties of PLD-grown Ti_2O_3 and Cr_2O_3 thin films, deposited on m-, a- and c-plane Al_2O_3 substrates as well as on

α-Ga_2O_3 buffer layers at various growth temperatures, atmospheres and pressures. Hall-effect and XRD measurements were used to investigate the electrical and crystalline properties. A strong dependence of the crystal phase formation on the background gas and pressure was observed. Argon atmosphere faciliated the growth of Ti_2O_3, whereas oxidisation to TiO_2 occured during the deposition in oxygen atmospheres even at low pressures.

HL 13.31 Mon 15:00 Poster E

Reduction of droplet density for pulsed Laser Deposition of functional oxides — •Jonas Elz, Arne Jörns, Holger von Wenckstern, and Marius Grundmann — Leipzig University, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

Pulsed laser deposition is a highly flexible and reproducible technique for epitaxial growth of high quality thin films [1]. Two major problems occurring for certain target materials are the formation of droplets on the substrate and the increasing surface roughness of the target during laser ablation that may cause a change of the expansion direction of the plasma plume towards the direction of the incident laser beam [2, 3]. Thin films containing droplets are undesirable for device applications.

In this work, we present means for a significant reduction of the density of droplets for copper oxide targets using a shadow mask (so-called eclipse) between target and substrate. The effect of the laser fluence incident on target on its surface roughness and the change of plasma plume expansion direction during deposition will be presented in detail.

[1] David P. Norton, in Pulsed Laser Deposition of Thin Films, Wiley, Hoboken (2007)

[2] S. Fahler et al., Appl. Surf. Sci. 109/110 433-436 (1997)

[3] C. Doughty et al., Appl. Phys. Lett. 66, 1276-1278 (1995)

HL 13.32 Mon 15:00 Poster E

The influence of Band bending on valence band offsets determined by Kraut's method: Modeling and experiment for polar-discontinuity doped $LaInO_3/BaSnO_3$ — •Georg Hoffmann[1], Aysha A Riaz[2], Anna Regoutz[2], Oliver Brandt[1], and Oliver Bierwagen[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]Department of Chemistry, University College London , London, UK

Two-dimensional electron gases (2DEGs) in $LaAlO_3/SrTiO_3$ heterostructures due to polar discontinuity have brought huge attention to perovskite oxides [1]. For $LaInO_3/BaSnO_3$ heterostructures, a predicted conduction band offset (CBO) of 1.6 eV confines a charge carrier density of up to 2×10^{14} cm^{-2} in the quantum well at the $BaSnO_3$ side [2], while room temperature mobilities are higher by one order of magnitude compared to $SrTiO_3$ based 2DEGs. To determine the CBO considering interfacial band bending the related valence band offset (VBO) is determined by Kraut's method using x-ray photo electron spectroscopy (XPS) [3].

We developed a model that predicts XPS core-level (CL) shape and shift for given band profiles and thus related VBO correction. Synchrotron-based XPS data are interpreted with this model to determine band bending and VBO at the $LaInO_3/BaSnO_3$ interface.

[1] J. Mannhart, et al., MRS bulletin 33, 1027-1034 (2008). [2] W. Aggoune, and Claudia Draxl, npj Computational Materials 7, 174 (2021). [3] E. A. Kraut, et al., Phys. Rev. Lett. 44, 1620 (1980).

HL 13.33 Mon 15:00 Poster E

Investigating the iodoplumbate complex evolution of perovskite solution during spin coating via UV-VIS in-situ spectroscopy — •Maximilian Spies, Simon Biberger, and Anna Köhler — University of Bayreuth, Bayreuth, Germany

We investigated the precursor solution for the fabrication of $MAPbI_3$ perovskite thin films via UV-VIS absorption spectroscopy during the spin coating process (in-situ). The iodoplumbate complexes present in this precursor solution absorbe light in the UV range, providing insights into the precursor chemistry that is crucial for the formation of the final perovskite film. Since these iodoplumbate complexes are very sensitive to their environment and can alter their coordination considerably when changing parameters like the solvent or concentration, we conducted an in-situ study during the critical phase before the nucleation in order to get a deeper insight into the formation dynamics of neat perovskite thin films. We find that an absorption peak, commonly stated to originate from the PbI_3^- complex, shifts to lower energies with respect to time during spin coating, indicating a growth of the electronic system. The amount of this red shift depends on the precursor concentration and the composition of the solvent in use.

HL 13.34 Mon 15:00 Poster E

Mask and Plate Metallization for High-Efficiency Solar Cells — •Maral Ghanbari[1,2], Jörg Schube[1], Tadeo Schweigstill[1], Gabriele Mikolasch[1], Roman Keding[1], and Andreas W. Bett[1,2] — [1]Fraunhofer Institute for Solar Energy Systems ISE, Heidenhofstraße 2, 79110 Freiburg — [2]University of Freiburg, Institute of Physics, Hermann-Herder-Straße 3, 79104 Freiburg

The pursuit of higher conversion efficiency in solar cells is a central objective in photovoltaic manufacturing. Narrowing fingers is one option due to a significant decrease in shading losses. Through precise control of finger dimensions, we aim to enhance solar cell conversion efficiency, specifically for perovskite-silicon tandem solar cells. This study introduces a potential remedy, involving mask and plate metallization technology for perovskite-silicon tandem solar cells. The technique, detailed here, comprises three stages: masking, electroplating, and mask stripping. In the masking phase, hotmelt ink is applied to the substrate via inkjet printing, creating a wax-based phase-change mask with open areas. In the electroplating phase, metal contacts are precisely positioned on these areas, enabling silver-free metallization. In the final stage, the mask can be easily removed using isopropyl alcohol. The primary aim of this study is to develop and understand the inkjet printing process for producing a mask with the narrowest openings, aiming to reduce shading-related losses with metal contacts achieving a width of less than 20 micrometres.

HL 13.35 Mon 15:00 Poster E

Strain effects on the electronic structure of Cs-based metal halide perovskites — •Freerk Schütt[1], Ana M. Valencia[1,2], and Caterina Cocchi[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Oldenburg — [2]Humboldt-Universität zu Berlin und IRIS Adlershof, Berlin

Metal-halide perovskites (MHPs) are promising materials for photovoltaics, but fundamental studies on their structure-property relationships are still needed to exploit their full potential. Using density-functional theory, we analyze the effects of compressive and tensile strain between -3% and 3% in $CsXI_3$ with X = Sn, Pb, in order to provide fundamental insight into the influence of lattice deformation on the structural and electronic properties of these materials, particularly related to the modulation of the band gap. These underlying structural changes, notably the significant distortion of the characteristic octahedra, are larger with Sn than with Pb, likely due to the larger flexibility of Sn-based MHPs over their Pb-based counterparts. Our results provide useful insight for tuning electronic properties and improving stability through strain-engineering of MHPs.

HL 13.36 Mon 15:00 Poster E

Temperature-induced limitation of charge carrier mobility in perovskite absorbers and its influence on recombination — •Patrick Dörflinger, Philipp Rieder, and Vladimir Dyakonov — Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

The charge carrier mobility μ is a crucial parameter in semiconductors. Together with the lifetime, it quantifies the diffusion length of the charge carriers. Moreover, its temperature-dependent power-law $\mu \propto T^{-\gamma}$ provides information about the predominant scattering mechanism that limits mobility at a certain temperature. For lead-halide perovskites γ values of $\approx 1.5-3$ are observed at room temperature, which are related to pronounced displacements of the lead-halogen bonds due to the rather mechanically soft lattice.[1] More importantly, this scattering mechanism dominates at elevated temperatures and severely restrics charge carrier mobility, an effect relevant for photovoltaic applications.

For this reason, we systematically investigated the charge carrier decay, mobility, and power-law behavior between 80K and 360K using time-resolved microwave conductivity (TRMC). We find a correlation between the scattering mechanism and the recombination behavior of the charge carriers in methylammonium lead triiodide. Furthermore, by substitution of the A-site cation and halide anion we quantify the predominant scattering mechanism of different organic/inorganic lead halide perovskites, which exhibit different temperature dependencies.

[1] Dörflinger et al., *Adv. Sci.* **2023**, 2304502.

HL 13.37 Mon 15:00 Poster E

Circular Dichroism and Polarized Emission in Bismuth doped

Pyridyl-ethylamine Lead Iodide 2D Perovskites — •Henrik Spielvogel[1], Jan-Heinrich Littmann[1], Philip Klement[1], Lukas Gümbel[1], Satoko Fukumori[2], Hirokazu Tada[2], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I, JLU Gießen, Germany — [2]Graduate School of Engineering Science, Osaka University, Japan

The incorporation of chiral organic cations into lead halide perovskites enables the resulting 2D system to exhibit properties such as chiroptical activity and chirality-induced spin selectivity allowing the generation and detection of circularly polarized light. Doping and alloying serve to modify and enhance the properties and performance of such materials. When doping with cations of differing charge to the constituting Pb^{2+} ions, defect creation is inevitable and the effects on chiroptical activity are not yet known due to complex structure-property relationships and experimental limitations.

Here, we present Bi^{2+}-doped pyridyl-ethylamine lead iodide as a model compound for doped chiral lead iodide perovskites. Through polarization-resolved spectroscopy, we characterize the relationship between circular dichroism and structural factors. This analysis offers valuable insights for designing new materials with high chiroptical activity.

HL 13.38 Mon 15:00 Poster E

Circular Dichroism and Polarized Emission in Bismuth doped Methylbenzylamine Lead Iodide 2D Perovskites — •Jan-Heinrich Littmann[1], Henrik Spielvogel[1], Philip Klement[1], Lukas Gümbel[1], Satoko Fukumori[2], Hirokazu Tada[2], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I, JLU Gießen, Germany — [2]Graduate School of Engineering Science, Osaka University, Japan

Organic-inorganic metal-halide perovskites are intriguing research materials due to their remarkable semiconductor properties and the potential applications ranging from photovoltaics to solid-state lighting and detectors. The incorporation of chiral organic cations into lead halide perovskites showcased chiroptical activity as well as chirality-induced spin selectivity. These characteristics hold promise for applications in emitters and detectors of circularly polarized light. Performance can be further boosted via doping and alloying. However, heterovalent doping using Bi^{3+} is currently not fully understood due to intricate structure-property relationship. We investigate a Bi^{3+}-doped methylbenzylamine lead iodide model compound specifically on circular dichroism and emission polarization. Additionally, the substitution of Pb^{2+} by Bi^{3+} introduces free charges that lead to additional defects and dopants. Our objective is to uncover how structural factors impact circular dichroism, aiming to provide insights for designing materials with elevated chiroptical activity.

HL 13.39 Mon 15:00 Poster E

Exploring anharmonicity in metal halide double perovskites using machine-learned ACE potentials — •Mattis Gossler and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

Metal halide perovskites (MHPs) have gained much attention for their exceptional photo-electrical properties, making them ideal for photovoltaic applications. Seeking eco-friendly alternatives to traditionally lead-based MHPs, double-cation perovskites $A^{I}_{2}M^{I}M^{III}X_6$ offer fine-tuned photo-electrical properties through their variable composition.

MPHs are softer compared to other inorganic semiconductors, displaying significant structural fluctuations at room temperature. Understanding their electronic and structural properties involves anharmonic vibrational modes, best explored through *ab initio* molecular dynamics (AIMD). To overcome the severe simulation limitations of AIMD, we employ an on-the-fly active-learning workflow to train an atomic cluster expansion (ACE) machine-learned interatomic potential with minimal human intervention. The capabilities of the generated ACE potential are then tested to investigate structural and dynamic properties of the double perovskite $Cs_2AgBiCl_6$ from the CANBIC family at elevated temperatures, which are still ambiguous from experimental data.

HL 13.40 Mon 15:00 Poster E

Excitonic and optical properties of a novel halide-based double perovskite from ab-initio many body techniques — •Manaswita Kar, Maria Hellgren, Michele Casula, and Benjamin Lenz — Sorbonne Univesité, Paris, France

Halide perovskites have proved to be promising candidates for next-generation photonics applications, including both classical and quantum emission. The exceptional excitonic and optical properties of this class of materials are in particular in focus in their quantum-confined regime. In this study, we investigate the optical and excitonic properties of a novel halide-based double perovskite, which was first predicted by machine learning and subsequently validated by synthesis and characterization of quantum dots. Here, we characterize the optical properties of the bulk phase through theoretical simulations. We employ many-body perturbation theory (GW) and Bethe-Salpeter equation techniques to study its excitonic properties, which are not captured within standard density functional theory.

HL 13.41 Mon 15:00 Poster E

Understanding the Methylammonium Chloride-Assisted Crystallization for Improved Performance of Lead-Free Tin Perovskite Solar Cells — •Daniele Cuzzupè — University of Konstanz, Konstanz, Germany

In the quest for perovskite materials with reduced toxicity, Sn perovskites are emerging. However, they suffer from material instability and rapid crystallization, leading to high defect densities in the films. In this work, the methylammonium chloride (MACl)-assisted crystallization as a route to improve stability and optoelectronic quality of quasi 2D/3D PEA0.08FA0.92SnI3 perovskite is demonstrated. For an optimal additive amount (10 mol%), a 37% increase in power conversion efficiency is found. Notably, MACl enhances the films' stability, evidenced by temporal PL tracking. Understanding the effect of MACl addition in this system is interesting for the pursuit of efficient and stable tin-based devices. The investigations show that MACl addition causes a shift in the optical bandgap and improves morphology, indicating effects in the bulk crystal structure. X-ray photoelectron spectroscopy confirms the presence of Cl on the surface, but no indication of MA+ is found. Intriguingly, UV photoelectron spectroscopy shows pronounced changes in the density of states. For the first time, it is shown that MACl promotes the formation of a two-dimensional layer via the surface accumulation of PEA+. The MACl additive lowers the absorber's ionization energy, possibly facilitating hole extraction. Overall, this work highlights a facile route to control the crystallization of Sn perovskites.

HL 13.42 Mon 15:00 Poster E

Photoelectron spectroscopy and in-situ time-resolved photoluminescence for the characterization of thin film solar cells — •Philine Stötzner, Alexander Stauffenberg, Torsten Hölscher, Roland Scheer, and Stefan Förster — Martin-Luther Universität Halle-Wittenberg, Institute of Physics, 06120 Halle, Germany

Alkaline doping plays an important role in improving the efficiency of chalcogenide solar cells based on $Cu(In,Ga)(Se,S)_2$ (CIGS). By X-ray photoelectron spectroscopy (XPS) performed in ultrahigh vacuum (UHV), we identified the segregation of sodium towards the absorber surface after a controlled exposure to light and various gases. It leads to a degradation of uncoated absorbers that persists even after completion of the whole solar cell [1]. The reduction of the charge carrier lifetime has been confirmed by ex-situ time-resolved photoluminescence (TRPL). Here, we present a setup that combines XPS and in-situ TRPL in UHV accompanied by UPS to study the valence band electronic structure. The experimental setup contains a high-pressure gas cell for exposure to ultra-pure gases or air, a controlled illumination, and alkali dispensers. This setup is perfectly suited to trace back chemical surface modifications and changes in the charge carrier mobilities and electronic properties to a distinct environmental stimulus. Thus, it is not limited to CIGS but also for other absorber materials like organo-metal halide perovskites.

[1] T. Hölscher et al., Progress in Photovoltaics 26 (11), (2018)

HL 13.43 Mon 15:00 Poster E

Low temperature photoexcitation dynamics in triple cation lead halide perovskites — •Alexander Schauerte[1], Isabel Allegro[2], Anton Krüger[1], Ian Howard[2], Uli Lemmer[2], and Marina Gerhard[1] — [1]Department of Physics and Material Sciences Center, Philipps-Universität Marburg, Germany — [2]Light Technology Institute, Karlsruhe Institute of Technology, Germany

Hybrid perovskites are a promising class of materials not only for cheap and efficient solar cells, but they also show a huge potential for lasing applications. In both cases, the charge carrier dynamics is of great interest.
Here, we study the recombination dynamics of the triple cation lead

halide perovskite $Cs_{0.1}(MA_{0.17}FA_{0.83})_{0.9}Pb(I_{0.84}Br_{0.16})_3$ using time-resolved photoluminescence spectroscopy. The combination of spectrally and spatially resolved measurements allows us to explore the relaxation pathways of carriers and their spatial diffusion on the picosecond time scale.
At low temperatures, the diffusion at early times is enhanced compared to higher temperatures, but saturates within a nanosecond. Moreover, the low-temperature spectra reveal a red-shift over time, particularly below approximately 70 K, indicating the population of energetically relaxed and more localized states. We attribute the dispersive dynamics at low temperatures to the absence of dynamic disorder, which mitigates self-trapping effects at early times, but leads to the population of localized emissive tail states at later times, unraveling the underlying static disorder.

HL 13.44 Mon 15:00 Poster E

Nanoparticle and polymer based optical coating for stability and thermal management of perovskite solar cells — •Steffen Richter, Sema Sarisözen, Sercan Özen, Frank Jaiser, Thomas Hultzsch, and Felix Lang — Radiation-Tolerant Electronics with Soft Semiconductors , University of Potsdam, Germany

Photons with energies outside the band gap are not only not utilized, but often decrease performance and stability of perovskite solar cells. Harsh UV light can trigger various degradation mechanisms, while IR light leads to excessive heating.

Commercial protections are usually quite expensive. To increase the stability, reduce heat and improve performance with an affordable and simple approach we aim at introducing an optical coating containing various nanoparticles embedded into an encapsulating polymer.

Our first results show that indium tin oxide nanoparticles absorb and reflect near infrared light, while (aluminum doped) zinc oxide nanoparticles absorb ultraviolet radiation and downshift the latter to an emission in the visual spectrum. Further, PDMS as an embedding polymer acts like a natural anti reflection layer. Bioinspired structuring of the surface with rose petals decreases reflectance and increases transmittance additionally. In literature PDMS is used for radiative cooling because of its conversion of heat to emission in higher infrared wavelengths which could reduce the cell temperature even further.

In this poster we will present detailed transmission and reflection spectra as well as evidence of downshifting. Further, we will show how the optical coating will affect device performances.

HL 13.45 Mon 15:00 Poster E

Ultra-thin subwavelength detection of polymer layers using highly-doped n-Ge plasmonic antenna in the THz range — •Elena Hardt[1], Carlos Alvarado Chavarin[1], Julia Flesch[2], Oliver Skibitzki[1], Romualdo Varricchio[3], Alessandra di Masi[3], and Giovanni Capellini[1,3] — [1]IHP - Leibniz Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]University of Osnabrueck, Barbarastrasse 11, 49076 Osnabrueck, Germany — [3]Department of Sciences, Università Roma Tre, Viale G. Marconi 446, 00156, Roma, Italy

The advatanges of THz instrumentation for biosensing is based on the high sensitivity to polar substances and on very low energy photons of the THz range. Thus, recent improvements in THz sources and detectors allow label-free, reliable measurements of biomolecules. LSPR is an ideal concept to enhance the spectroscopy signal and to improve the sensitivity. In this work, we investigate the sensitivity of highly n-doped Ge plasmonic THz antennas realized on Si and SOI substrates in presence of ultra-thin subwavelength polymer layers. The antenna response to the well-known electrostatic layer-by-layer deposition is investigated by observing the shift of the LSPR in the THz spectra. 5, 15 and 22 layers of poly-(allylamine)PAN/poly-(acrylic acid)PAA show a linear response. By using an optimized antenna design relying on low losses SOI substrates, we detect resonance spectral shifts as large as 14.5 GHz in response to 22 PAN/PAA layers of a few nm-thickness. We believe that this result could pave the way to a low-cost CMOS compatible biosensing platform.

HL 13.46 Mon 15:00 Poster E

THz Spectroscopy on Bi_2Se_3 — •Debankit Priyadarshi[1,2], Amit Haldar[1], Sunil S. Kushvaha[3], Manfred Fiebig[2], and Shovon Pal[1] — [1]School of Physical Sciences, National Institute of Science Education and Research, HBNI, Jatni, India. — [2]Department of Materials, ETH Zurich, Zurich, Switzerland. — [3]CSIR-National Physical Laboratory, New Delhi, India.

Topological insulators (TI) have come up as an important condensed matter system showing exotic metallic surface states protected by their topology and time reversal symmetry. The investigation of the conductivity of these surface states is difficult with traditional electrical techniques due to contributions from the free carriers in the bulk and the quantum well states to the total conduction. Terahertz (THz) spectroscopy is an emergent field in probing the conduction properties of these surface states due to the low photon energies (meV) of the THz radiation. Our measurements show contributions from Drude-like charge carriers and two Lorentz oscillator-like resonances to the conductivity of the Bi_2Se_3. The oscillator responses are attributed to the bulk-phonon resonance and inter-sub-band transitions in the quantum well states. The Drude response is expected to have contributions from the surface state carriers, 2D electron gas present on the quantum well states and free carrier states of the bulk. Going into the relaxation dynamics of these carriers by doing pump-probe measurements would reveal the exact contribution of the surface state carriers to the conductivity.

HL 13.47 Mon 15:00 Poster E

Ultrafast THz Engineering of Semiconductor Photoluminescence — •Maximilian Frenzel, Joanna M. Urban, Michael S. Spencer, Martin Wolf, and Sebastian F. Maehrlein — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Exploring the interaction between THz radiation and semiconductor photoluminescence (PL) presents a potential avenue for developing future optoelectronic devices and gaining novel insights into ultrafast semiconductor physics. In this work, we employ single-cycle THz pulses (0.5-4 THz) with peak fields exceeding 1 MV/cm to control the PL of a bulk ZnTe semiconductor. We find that THz pulses can quench the total emitted PL by more than 50% at room temperature. In addition to reducing the emission magnitude, the THz pulses also affect the PL's spectral weight, thus allowing the PL to be tailored by the THz fluence. Moreover, we study THz-induced quenching as a function of time delay with respect to the photo carrier injection, which provides a further control knob to tune the emission, whilst also constituting an ultrafast probe for studying the interplay of lattice and carrier dynamics. Our work serves as a systematic study to control the emission and carrier dynamics using THz light and establishes a testbed for future investigations of electron-phonon interactions in emerging semiconductors.

HL 13.48 Mon 15:00 Poster E

Investigating the stability and electronic properties of CuI (111) polar surfaces — •Preeti Sharma[1], Silvana Botti[1,2], and Tomáš Rauch[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Germany — [2]Research Center Future Energy Materials and Systems of the Research Alliance Ruhr, Faculty of Physics and ICAMS, Ruhr University Bochum, Germany

In recent years, CuI has drawn the attention of many researchers as a most suitable p-type transparent conducting material (TCM) due to its large band gap (3.1 eV), large exciton binding energy (62 meV), and high carrier mobility. Because of these properties, CuI thin films are proposed as prominent candidates for optoelectronics devices such as solar cells, light-emitting diodes, etc. It is crucial to understand the surface properties, like, surface reconstruction, surface energy, and band structure for the development of CuI-based devices. Here, we investigated the stability and electronic properties of Cu-terminated and I-terminated (111) polar surfaces using first principles. A standard slab method cannot be used to calculate the surface energies for polar surfaces. Therefore, we used the wedge structure model and evaluated surface energy for one polar surface without involving its associated surfaces.

HL 13.49 Mon 15:00 Poster E

Optimisation of pulsed-laser-deposition-grown CuI polariton microcavities — Kirsty E. McGhee, Lukas Trefflich, Aaron Giess, Marius Grundmann, and •Chris Sturm — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany

Exciton-polaritons are light-matter quasiparticles that possess properties of both excitons and photons, making them of great interest for ultra-low threshold lasers, all-optical circuits, and quantum simulators. Because excitons and photons are both bosons, polaritons are also bosons and, under certain conditions, can undergo a non-equilibrium Bose-Einstein-like condensation. In this work, we discuss our efforts to realise polariton condensation in a microcavity containing copper iodide (CuI), a transparent semiconductor currently of great interest due to its inherent p-type behaviour. We discuss the optimisation of the

growth of the CuI layer and of the distributed Bragg reflectors (DBRs), the highly-reflective mirrors used to confine the cavity mode, using pulsed laser deposition. In particular, we have found adhesion problems between CuI and the low-refractive-index dielectrics Al_2O_3 and MgO ($n\sim1.7$). These adhesion problems disappear when we instead grow the CuI between layers of yttria-stabilised zirconia (YSZ, $n\sim2.1$). However, while we demonstrate the presence of exciton-polaritons, we do not see any evidence of polariton condensation at room temperature or cryogenic temperatures, likely due to the low cavity quality factor. In order to enhance this quality factor, further optimisation is required, which will be presented here.

HL 13.50 Mon 15:00 Poster E

State of the art S/TEM-based strain measurement techniques — •Laura Niermann[1], Tore Niermann[1], Frederik Otto[1], Rahel Spect[1], Paul Schmiedeke[2], Gregor Koblmüller[2], and Michael Lehmann[1] — [1]Technische Universität Berlin, Berlin — [2]Technische Universität München, München

Strain fields influence the electronic and optical properties of semiconductor materials. (Scanning-) transmission electron microscopy (S/TEM) enables the measurement of strain fields on the nanometer scale. We present results from current S/TEM-based strain measurement techniques on several semiconductor hetero-structures: Dark-field electron holography excels at strain measurements over extended regions within semiconductor devices by analyzing the phase of a single diffracted beam. Alternatively, nano beam electron diffraction enables strain mapping through the acquisition of entire electron diffraction patterns at each scan position. The precision of the latter technique can be further improved upon by means of precession electron diffraction. However, so far these approaches required the strain to be constant along the electron beam. We present new methodologies for evaluating three-dimensional strain variations from a single projection. This is achieved by combining scanning convergent beam electron diffraction (SCBED) patterns or dark field electron holographic tilt series with numerically efficient multi-beam calculations. Additionally, we demonstrate how such combined measurement and modeling approaches even enables a classification of quantum dot shapes.

HL 13.51 Mon 15:00 Poster E

Heterostructure diodes based on reactively co-sputtered $Ag_xCu_{1-x}I$ thin films — •Jorrit Marius Bredow, Sofie Vogt, Christiane Dethloff, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Germany

A wide band gap of 3 eV at room temperature and its intrinsic p-type conductivity[1] render copper iodide (CuI) a promising candidate for the fabrication of transparent heterostructure diodes. However, the often degenerate hole concentration of up to $10^{20}\,cm^{-3}$[1] of binary CuI impedes the realization of rectifying heterostructures where the depletion layer is located in the CuI. By alloying CuI with Ag, a reduction of conductivity and carrier density was demonstrated for an increasing silver fraction x[2]. Additionally, a switch from p- to n-type conductivity was reported, which enables the fabrication of heterostructure pn-diodes based on silver copper iodide ($Ag_xCu_{1-x}I$)[3].

We present transparent heterostructure diodes based on the ternary alloy $Ag_xCu_{1-x}I$ on different n-type back contact layers. $Ag_xCu_{1-x}I$ is deposited by means of reactive co-sputtering of metallic Cu and Ag in an argon and iodide atmosphere. The influence of the back contact layers on the functionality and the rectifying behaviour of the pn-junctions is compared and presented.

[1] C. Yang *et al.*, PNAS, 113, 12929-12933, 2016.
[2] A. Annadi *et al.*, Appl. Mater. Today, 20, 100703, 2020.
[3] J.-H. Cha and D.-Y. Jung, ACS Appl. Mater. Interfaces, 9, 43807-43813, 2017.

HL 13.52 Mon 15:00 Poster E

Combined Optical and Atomic Force Microscopic Investigation of Type-I CdSe/CdS Dot-in-Rod Particles with Metal Tips — •Nicklas Giese, Mareike Dittmar, Moritz Wehrmeister, Alf Mews, and Tobias Kipp — Institute of Physical Chemistry, University of Hamburg, 20146 Hamburg, Germany

Semiconductor-metal-hybrid nanostructures can split water and produce hydrogen by illumination, such as dot-in-a-rod particles with a charged metal tip. The understanding and control of the charge transfer processes of these particles is crucial for their further development. We investigate hybrid nanostructures consisting of a CdSe-core/CdS-shell with a metal tip attached. Optical characterization is performed by time-resolved single-particle photoluminescence (PL) spectroscopy. Thereby, the attachment of the metal tip can be correlated with the decrease in quantum yield (QY) and PL lifetime of the semiconductor, giving detailed information on charge-carrier separation. We present an all-in-one setup that combines PL spectroscopy to Kelvin probe force microscopy (KPFM) with simultaneous local illumination of the nanostructure. KPFM is based on an atomic force microscope (AFM) with a conductive cantilever and provides information about the local surface potential by measuring the contact potential difference (CPD) between the sample and the AFM tip. This requires a transparent substrate with a back-gate on which markers can be generated using electron beam- or optical-lithography. The combination of optical and KPFM techniques allows the study of energy-band profiles and the generation of charge-carriers and their concentrations.

HL 13.53 Mon 15:00 Poster E

Trench-etched In-Plane-Gate Transistors: Fabrication, Characterization, Logical Gates and Simulation — •Lennart Anderson[1], Phil Badura[1], Matthias Kroll[2], Benjamin Feldern[1], Arne Ludwig[1], and Andreas Wieck[1] — [1]Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]Experimental Physics IV - Solid State Physics, Ruhr-Universität Bochum

In contrast to conventional field effects transistors (FETs), in which the channel is modulated by a perpendicular electric field, in the In-Plane-Gate transistor (IPGT) gate and channel (and hence source and drain) are in the same plane, leading to a lateral field effect and hence to a two-dimensional system.

In $GaAs/Al_xGa_{1-x}As$ high electron mobility structures conducting channels were defined in a two-stage wet chemical etching process. Current-voltage measurements show characteristic transistor behaviour. A NAND gate is realized based on a single IPGT, showing clear input-output characteristics. Interconnecting several NAND gates, all further basic logical gates, i.e. AND, OR, NOR, XOR and NOT, are realized. The IPGT structure is modelled in *nextnano++*, and its band structure is obtained by solving the self consistent Schrödinger-Poisson equation numerically. The effect of geometric parameters, i.e. trench width and channel width, as well as the applied gate voltages on the band structure and hence the transistor behaviour is studied. We find that surface states have a significant influence and provide a simple electrostatic model.

HL 13.54 Mon 15:00 Poster E

Investigating Performance Limiting Recombination of Perovskite/C60 Interfaces using First Principle Calculations — •Richard Gundermann[1], Felix Lang[1], Christopher Penschke[2], Peter Saalfrank[2], Filippo De Angelis[3], and Dieter Neher[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Germany — [2]Institute of Chemistry, University of Potsdam, Germany — [3]Department of Chemistry, Biology and Biotechnology, University of Perugia, Italy

Perovskite semiconductors became an interesting field to overcome the limitations of standard silicon based photovoltaic (PV) technologies. However, it is shown that performance-limitations are largely caused by significant nonradiative recombination at the perovskite/organic electron transport layer junctions. Especially the extensively used perovskite/C_{60} junctions appear to have a reduction in PLQY within the first 1nm of C_{60}, which indicates nonradiative across-interface recombinations [1]. In this work, we investigate for the origin of these recombinations, e.g., packing faults in the first C_{60} layer or inhomogeneous electrostatics. Also, electron-transfer-rates are discussed. Therefore, we use DFT calculations, including structure optimization of a perovskite/C_{60} supercell. For reduced computational effort we also investigate for empirical Tight-Binding-Models to access heterostructure-modeling and features as transport properties.

[1] Warby, J. et al., Understanding Performance Limiting Interfacial Recombination in pin Perovskite Solar Cells. Adv. Energy Mater. 2022, 12, 2103567. https://doi.org/10.1002/aenm.202103567

HL 13.55 Mon 15:00 Poster E

Characterization of Arsenic- and Antimony-Containing Layers Grown in a Source-Material Transformed MBE — •Peter 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 Festkörperpysik, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund, Germany

The results of the growth of arsenic- and antimony-containing layers

are presented. These layers were grown in a MBE system which underwent a transformation from II-VI (HgCdTe) to III-V (AlGaIn-AsSb) materials growth.

RHEED is utilized to determine surface reconstructions and growth rates *in situ*. Post-growth atomic force microscopy is employed to study the surface properties, such as roughness, step density and terrace width of the grown layers. With photoluminescence spectroscopy mapping of quantum well samples the radiative recombination yield on a whole wafer is compared between different samples. As a measure of epitaxial layer quality Hall-effect measurements on high electron mobility structures are performed.

These works represent the early steps after the commissioning of a used MBE system towards the growth of mid-IR emitters.

HL 13.56 Mon 15:00 Poster E

Photoemission study and band alignment of GaN passivation layers on GaInP(100) heterointerfaces — •Sahar Shekarabi[1], Mohammad Amin Zare Pour[1], Haoqing Su[2], Wentao Zhang[2], Chengxing He[2], Oleksandr Romanyuk[3], Agnieszka Paszuk[1], Shu Hu[2], and Thomas Hannappel[1] — [1]Grundlagen von Energiematerialien, Institut fur Physik, Technische Universit at Ilmenau, 98693 Ilmenau, Germany — [2]Department of Chemical and Environmental Engineering, Yale University, New Haven, CT 06520, USA — [3]FZU Institute of Physics of the Czech Academy of Sciences, Cukrovarnicka 10, Prague 16200, Czech Republic

GaInP(100) is commonly used as a top photoabsorber in tandem devices and photoelectrochemical (PEC) cells. Since the photo corrosion degrades the cell stability and efficiency, GaN is used as a promising passivation layer. Therefore, studying the band alignment at this heterointerface is crucial for efficient charge transfer and minimizing photovoltage losses. Here, we study the band alignment of the multijunction heterostructure by X-ray photoelectron spectroscopy and ultraviolet photoelectron spectroscopy. GaInP(100) layers were grown by metalorganic chemical vapor deposition on top of GaAs(100), with a P-rich surface reconstruction. GaN passivation layers were grown by atomic layer deposition on oxidized GaInP(100) surfaces. On the P-rich n-GaInP(100) we found upward surface BB of 0.44 eV. Oxidation partly passivates surface states, lowering BB to 0.16 eV. Between the GaInP(100) and GaN passivation layer, we found a VBO of 1.9 eV, suggesting efficient electron transport but impeding hole transport.

HL 13.57 Mon 15:00 Poster E

Comparison of multiple methods to determine the growth rate of MBE-grown layers — •Timo A. Kurschat[1,2], Sascha R. Valentin[1], Peter Zajac[2], Arne Ludwig[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

This work compares multiple methods to determine the growth rate and thickness of thin layers grown by MBE.

The first method used is RHEED, which is the standard method to determine the growth rate in-situ. In contrast, the other measurements can only be carried out post-growth. One of these is photoluminescence (PL) spectroscopy. By measuring a sample containing multiple quantum wells and comparing it with the calculated emission energies, the widths of the quantum wells were calculated. Because our PL setup is capable of mapping entire wafers, deviations of the thickness can be seen. By stopping the rotation of the wafer during the growth of a quantum well, a thickness gradient is visible via an energy shift of the corresponding PL peak. The resulting growth rate can be used to derive the beam profile of the effusion cell. Three further methods make use of a sample with a distributed bragg reflector. Firstly, its reflectivity was measured and compared to simulations using the matrix-transfer method. Secondly, the thickness of the grown layers were measured using interference microscopy. Thirdly, AFM measurements were performed on the cleaved edge of the sample and the material contrast is utilized to obtain the layer thickness.

HL 13.58 Mon 15:00 Poster E

Spherical harmonics expansion method for a semi-classical matrix transport equation describing spin dynamics in semiconductors — •Felix Willert and Franz Xaver Bronold — Institut für Physik, Universität Greifswald, 17489 Greifswald, Germany

We discuss the transport of hot electrons, originating from a magnetized ferromagnet, in a semiconductor and the spin dynamics governed by the D'yakonov-Perel (DP) mechanism, which is the dominant spin relaxation process in semiconductors without inversion symmetry in the unit cell. For that we use a semi-classical model, where charge transport and scattering processes are described classically, but the spin-processes follow a quantum mechanical description. Due to the fact, that the DP mechanism changes the orientation of the spin and not directly its magnitude, it is not sufficient to describe the dynamics by two coupled equations for spin-up- and spin-down-electrons. Therefore we derive a Boltzmann equation for 2x2-density matrices in spin space with an additional term governing the DP process. To solve this equation, the H-Transformation and a spherical harmonics expansion is used.

Preliminary numerical results are presented, showing energy relaxation and partial thermal equilibration of the electron distribution as well as the spin relaxation throughout the system, which is strongly dependent on the energy, due to the DP mechanism depending on the third power of the electron momentum.

HL 13.59 Mon 15:00 Poster E

Strongly driven germanium quantum dot — •Bashab Dey and John Schliemann — University of Regensburg, Regensburg, Germany

Hole qubits in germanium quantum dots are promising candidates for coherent control and manipulation of the spin degree of freedom. The suppression of contact hyperfine interaction due to p-character of the holes, isotopic purification and absence of valley degeneracies are favourable for sustaining longer spin coherence and relaxation times in these systems. Furthermore, stronger spin-orbit interaction in germanium hole states facilitates faster qubit operations in these dots as compared to silicon or III-V semiconductors. Quantum NOT gates can be realized using these qubits through electric dipole spin resonance (EDSR) where Rabi oscillations are induced between the spin-up and -down states using ac-gate voltages. In this work, we theoretically study the time dynamics of a single hole qubit in a laser-driven planar germanium quantum dot confined laterally by a parabolic potential in presence of Rashba spin-orbit coupling(s) and a perpendicular magnetic field. We employ different methods such as Floquet theory and unitary transformations to study the time evolution of the qubit under the laser field. We obtain approximate analytical formula for the Rabi oscillations using a Schrieffer-Wolff transformation and establish a connection of our model with the ESDR results obtained for this system.

HL 13.60 Mon 15:00 Poster E

Characterizing time resolved random laser and cavity exciton polariton supported random laser action in disordered ensembles of the hybrid perovskite CH3 NH 3 PbBr 3 (MAPB) — •Regine Frank[1,2], Paul Bouteyre[3], Hai Son Nguyen[4,5], Christian Seassal[4,5], Emmanuelle Deleporte[3], and Bart A. van Tiggelen[6] — [1]College of Biomedical Sciences, Larkin University, Miami, Florida, USA — [2]Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain — [3]Université Paris-Saclay, ENS Paris-Saclay, CNRS, CentraleSupélec, LuMIn, Gif-sur-Yvette, France — [4]Université de Lyon, Institut des Nanotechnologies de Lyon, INL/CNRS, Ecole Centrale de Lyon, Ecully, France — [5]Institut Universitaire de France (IUF), Paris, Franceb — [6]Universite Grenoble Alpes, Centre National de la Recherche Scientifique, LPMMC, Grenoble, France

We present semi analytical as well as numerical results (WENO) for photonic transport and Anderson localization of light in active disordered ensembles of the hybrid perovskite CH3 NH 3 PbBr 3 (MAPB) capped by PMMA. We compare experiments of two dimensional and three dimensional transport to time ans space resolved numerical results in the sense of finding the mechanism of coherent feedback for directed random laser emission and exciton-polariton supported random laser emission. This includes the analysis of the interplay of light-matter interaction in the sense of dynamics within the pumped microstructure with the mesoscopic physics of photonic transport in disordered and quasi ordered ensembles.