

HL 30: Poster 2

Topics:

- Materials and devices for quantum technology
- Nitrides: Devices
- Nitrides: Preparation and characterization
- Oxide semiconductors
- Perovskite and photovoltaics
- Ultra-fast phenomena

Time: Thursday 11:00–13:00

Location: P3

HL 30.1 Thu 11:00 P3

NV⁻ center in the vicinity of linear defects in diamond — ●REYHANEH GHASSEMIZADEH¹, WOLFGANG KRÖRNER¹, DANIEL URBAN¹, and CHRISTIAN ELSÄSSER^{1,2} — ¹Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany — ²University of Freiburg, Freiburg Materials Research Center (FMF), Stefan-Meier-Straße 21, 79104 Freiburg, Germany

The NV⁻ center is a point-defect complex in the diamond crystal with an excellent potential for implementing qubits in future quantum computing hardware. However, the structuring of point defects on the atomic scale remains an experimental challenge. Here we study theoretically the interaction between dislocations and the NV⁻ center. We evaluate to which extent dislocation lines that are naturally present in the diamond crystal may be used for structuring NV⁻ center as a first step towards a NV-based quantum register. Using density functional theory (DFT) we model NV⁻ centers in the vicinity of the most common dislocations in diamond and calculate the defect formation energy, structural geometry, defect levels and zero-field (ZFS) parameters. Our simulations reveal that dislocations potentially trap the NV⁻ with an energy release of up to 3 eV. Although the analysis of geometry, defect levels and ZFS parameters of NV⁻ centers being close to dislocations in general show strong deviations from their values in the perfect bulk structure, the lowest energy configuration of a NV⁻ center at the reconstructed dislocation cores have ZFS values with less than 5% deviation from their NV⁻ bulk values. Our results opens new insights for the design of NV-based quantum computing devices.

HL 30.2 Thu 11:00 P3

Quantifying Quantum Coherence in Polariton Condensates — ●CAROLIN LÜDERS¹, MATTHIAS PUKROP², ELENA ROZAS¹, CHRISTIAN SCHNEIDER³, SVEN HÖFLING⁴, JAN SPERLING⁵, STEFAN SCHUMACHER^{2,6}, and MARC ASSMANN¹ — ¹Experimentelle Physik 2, TU Dortmund, Germany — ²Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Universität Paderborn, Germany — ³Institute of Physics, University of Oldenburg, Germany — ⁴Technische Physik, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany — ⁵Integrated Quantum Optics Group, Institute for Photonic Quantum Systems (PhoQS), Paderborn University, Germany — ⁶Wyant College of Optical Sciences, University of Arizona, USA

We theoretically and experimentally investigate quantum features of an interacting light-matter system from a multidisciplinary perspective, unifying approaches from semiconductor physics, quantum optics, and quantum information science. As an example of a hybrid light-matter interface, we drive a polariton microcavity across the condensation threshold and observe the transition from an incoherent thermal state to a coherent state in the emission. By analyzing the phase-space distributions of the emitted light, we quantify the amount of quantum coherence that results from the quantum superposition of Fock states, constituting a measure of the resourcefulness of the produced state for modern quantum protocols.[1]

[1] C. Lüders et al., PRX Quantum 2, 030320 (2021)

HL 30.3 Thu 11:00 P3

Machine Learning enhanced in-situ electron beam lithography of photonic nano-structures — ●JAN DONGES, MARVIN SCHLISCHKA, CHING-WEN SHIH, MONICA PENDERLA, IMAD LIMAME, JOHANNES SCHALL, LUCAS RICKERT, SVEN RODT, and STEPHAN REITZENSTEIN — Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The unique in-situ electron beam lithography (iEBL) nanotechnology concept enables us to embed single quantum emitters into photonic nano-structures with a 34nm precision. To obtain the fitted position of the quantum emitter with high accuracy, the signal-to-noise ratio of their cathodoluminescence (CL) needs to be well above unity even for ms integration times. Here we show that for samples with dark quantum emitters, such as telecom quantum dots or low planar photon-extraction efficiency, machine learning (ML) is very well suited to drastically improve the performance of iEBL at low CL intensities. The machine learning software utilizes computer algorithms, which were trained through data samples to denoise data with a barely visible quantum dot emission. We present experimental results for In-GaAs quantum dots, which could be successfully embedded into circular Bragg grating structures with the assistance of machine learning. Our experimental results yield that by using ML, the CL sensitivity and the alignment accuracy could be increased by more than an order of magnitude compared to standard iEBL.

HL 30.4 Thu 11:00 P3

Photon propagation between quasinormal mode cavities — ●ROBERT FUCHS, SEBASTIAN FRANKE, ANDREAS KNORR, and MARTEN RICHTER — Technische Universität Berlin, Berlin, Germany

Quasinormal modes (QNMs) provide a useful and intuitive way to define modes for open cavities. They have been utilized for a variety of problems both in classical electrodynamics, and recently used in a fully quantized description for three dimensional geometries.

We show that a multi-cavity extension of the QNM quantization is possible if the cavities are far away from each other so that retardation effects are important. However, this quantization approach leads to a set of non-bosonic operators with a continuous spectrum. In the multi-cavity theory, this continuum serves as a bath which can be used to describe photon propagation between the separately quantized cavities.

Using a fourth-order Nakajima-Zwanzig equation, we point out how to get equations of motion for the system density matrix that include dissipation as well as inter-cavity transfer terms with significant retardation delays described by microscopic QNM parameters.

HL 30.5 Thu 11:00 P3

Sionludi - A table-top dilution refrigerator — ●VIKTOR ADAM, ALEXANDER ZILZ, and WOLFGANG WERNSDORFER — KIT, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe

Dilution cryostats are the only technology that provides continuous cooling performance from room temperature down to several mK. These devices utilize the endothermic process of diluting liquid He³ into liquid He⁴, which occurs even at 0 K. By evaporating He³ from this mixture and returning it to the mixing chamber, the refrigerator can be operated continuously.

The Sionludi dilution refrigerator is a unique platform for low-temperature research. The table-top design combined with its small dimensions of approximately 25 cm in diameter and 50 cm in height allow for comfortable mounting of experiments and periphery to the cryostat. The key advancement of this cryostat is the fast injection line, which allows direct cooling of the dilution stage of the cryostat by the circulation of 4 K cold mixture during precooling without affecting the operation at lowest temperatures. As a result, the Sionludi features fast cool-down and warm-up times of less than 3 and 1.5 hours, respectively, while providing cooling powers of up to 200 μW at 100 mK as well as base temperatures of below 20 mK. The fast turnaround time can accelerate sample throughput and thus progress in many research applications such as quantum sensing or quantum computing.

HL 30.6 Thu 11:00 P3

Telecom-band single photons from functionalized carbon nanotubes coupled to an open cavity — ●LUKAS HUSEL¹, JULIAN TRAPP¹, XIAOJIAN WU², MANUEL NUTZ³, THOMAS HÜMMER³, YUHUANG WANG², DAVID HUNGER⁴, and ALEXANDER HÖGELE^{1,5} — ¹Ludwig-Maximilians-Universität, 80539 München — ²University of Maryland, 20742 Maryland, USA — ³Qlibri GmbH, 80337 München — ⁴Karlsruher Institut für Technologie, 76131 Karlsruhe — ⁵Munich Center for Quantum Science and Technology, 80799 München

Quantum light at telecom wavelengths is of fundamental relevance in science and technology. A promising room temperature source of telecom single photons are functionalized carbon nanotubes (CNTs). In this system, dephasing and spectral diffusion limit spectral purity and indistinguishability of the generated photons, which can in principle be overcome by coupling the emitters to a cavity. Here, we demonstrate spectrally narrow single photon emission at wavelengths around 1460 nm from single CNT defects coupled to a fiber-based Fabry-Pérot resonator. We operate the cavity at ambient conditions and in the regime of low Purcell enhancement. By changing the cavity length, we tune the emission wavelength over a range of tens of nm, and the power spectral density by a factor of six. The coherence time of the generated photons matches the cavity linewidth, which constitutes an increase compared to the expected dephasing-limited free-space linewidth. Our results represent a step towards CNT-based sources of telecom-band single photons with high purity and indistinguishability.

HL 30.7 Thu 11:00 P3

Bright Electrically Controllable Quantum-Dot-Molecule Devices Fabricated by In Situ Electron-Beam Lithography — ●JOHANNES SCHALL¹, MARIELLE DECONINCK¹, NIKOLAI BART², MATTHIAS FLORIAN³, MARTIN VON HELVERSEN¹, CHRISTIAN DANGEL⁴, RONNY SCHMIDT¹, LUCAS BREMER¹, FREDERIK BOPP⁴, ISABELL HÜLLEN³, CHRISTOPHER GIES³, DIRK REUTER⁵, ANDREAS D. WIECK², SVEN RODT¹, JONATHAN J. FINLEY⁴, FRANK JAHNKE³, ARNE LUDWIG², and STEPHAN REITZENSTEIN¹ — ¹IFKP, TU Berlin, Germany — ²LS AFP, Ruhr-Universität Bochum, Germany — ³ITP, University of Bremen, Germany — ⁴WSI, TU München, Germany — ⁵Department Physik, Universität Paderborn, Germany

In quantum repeater networks it is of central importance to temporarily store and retrieve quantum information. Concepts based on quantum dot molecules (QDMs) promise storage times in excess of 1 ms. To make use of QDM based quantum memories, efficient coupling to flying qubits needs to be realized while maintaining precise electrical control. We report on the development of electrically tunable single-QDM devices with strongly enhanced broadband photon extraction efficiency. The quantum devices are based on stacked quantum dots in a pin-diode structure underneath a deterministically defined circular Bragg grating using in situ electron beam lithography. We determine the photon extraction efficiency, demonstrate bias voltage dependent spectroscopy and measure excellent single-photon emission properties. The metrics make the developed QDM device an attractive building block for use in future photonic quantum networks.

HL 30.8 Thu 11:00 P3

Machine Learning-Based Optimization of Chiral Photonic Nanostructures: Evolution- and Neural Network-Based Designs — OLIVER MEY¹, ●MANAN SHAH², and ARASH RAHIMI-IMAN² — ¹Fraunhofer IIS/EAS, Fraunhofer Institute for Integrated Circuits, Division Engineering of Adaptive Systems, Dresden — ²I. Physikalisches Institut und Zentrum für Materialwissenschaften, Justus-Liebig Universität Gießen, D-35392, Germany

Machine learning (ML) techniques such as deep learning (DL) and evolutionary algorithms (EA) exhibit unprecedented capabilities in the scientific ML realm. DL uses artificial neural networks to infer unintuitive solutions for complicated design requirements and specific functionalities. Likewise, the EA attempts to find the optimized solution by utilizing principles such as mutation of parameters and extinction of less promising solutions. These approaches are faster and more effective in the inference of nanostructure design parameters for desired properties, such as wavelength coverage and peculiar response functions, compared to conventional numeric simulations.

We present a nano-patterned GaP dielectric substrate that favors single-handed circularly polarized light (CPL) in reflection or transmission [1]. The optimization in chiral dichroism (CD) by neural networks is compared with the evolutionary algorithm. The increased CD in simulated spectra for designs with stronger reflectivity of right CPL

and lower transmissivity of left CPL makes the ML techniques effective to optimize a myriad of properties for metamaterials and photonic nanostructures. [1] Phys. Status Solidi RRL 2022, 16, 2100571.

HL 30.9 Thu 11:00 P3

Strain-tunable GaAs quantum dot-based circular Bragg gratings towards entangled photon pairs with high indistinguishability — ●CHENXI MA¹, JINGZHONG YANG¹, CONSTANTIN SCHMIDT¹, XIN CAO¹, YITENG ZHANG¹, MAXIMILIAN HELLER¹, JÜRGEN BECKER², EDDY P. RUGERAMIGABO¹, MICHAEL ZOPP¹, and FEI DING^{1,3} — ¹Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — ²Institut für Mikroproduktionstechnik, Leibniz Universität Hannover, Garbsen, Germany — ³Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, Hannover, Germany

The on-demand generation of bright entangled photon pairs is an attractive goal for the realization of quantum communication networks. Epitaxial GaAs quantum dots (QDs), grown via local droplet etching and nanohole infilling, are promising candidates because they are symmetric and strain-free. This leads to small exciton fine structures and high entanglement fidelities of photons emitted from the biexciton-exciton cascade. However, the photon indistinguishability is intrinsically limited in this scheme. GaAs QDs also suffer from inefficient photon extraction, which was addressed by embedding QDs in circular Bragg gratings. Here, we propose to engineer the cavity mode to match the biexciton transition with the assistance of strain-tuning techniques. The resulting asymmetric Purcell enhancement will increase the decay rate of the biexciton transition and consequently improve the photon indistinguishability. This heterogeneous photonic nanostructure can serve as a blueprint for future quantum communication devices.

HL 30.10 Thu 11:00 P3

GaAs heterostructures for coupling of spin qubits to self-assembled quantum dots — ●SELMA DELIĆ^{1,2}, PRIYABRATA MUDI^{1,2}, SEBASTIAN KINDEL², PAOLA ATKINSON³, DETLEV GRÜTZMACHER¹, and BEATA KARDYNAL^{1,2} — ¹Peter Grünberg Institute 9, Forschungszentrum Jülich, 52425 Jülich, Germany — ²Department of Physics, RWTH Aachen University, 52074 Aachen, Germany — ³Institut des Nano Sciences de Paris, CNRS UMR 7588, Sorbonne Université, 75005 Paris, France

Operation of quantum networks relies on encoding qubits on photons. These photons can be converted into spin qubits in many material systems. Yet, in order to take full advantage of the electrons with information encoded in their spins, the spin qubits should be scalable or the spin should be transferred to spin qubits that can be scaled into quantum processors. Here, we use singlet-triplet (S-T) qubits defined in a GaAs/AlGaAs gate-defined quantum (double-) dot (GDQD) as a scalable qubit. While GaAs is suitable for a qubit exchange with photons due to its direct bandgap, the GDQD does not confine holes. Therefore, we use a GaAs droplet dot (QD) to achieve a coherent transfer of information between a photon and a spin of an electron before the electron is transferred to the S-T qubit. In this contribution, we show the design of heterostructure that can be used to fabricate S-T qubit coupled to epitaxial GaAs QD. We further report on the progress in optical and electrical characterisation of the device in gated structures aligned to the GaAs QD.

HL 30.11 Thu 11:00 P3

GaN/AlGaIn/GaN solution gate field effects transistors as pH- and enzymatic sensors — ●GENRIETTA STEINGELB, ALEXANDER HINZ, STEPHAN FIGGE, and MARTIN EICKHOFF — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

A GaN/AlGaIn/AlGaIn-heterostructure solution gate field effect transistors (SGFETs) as pH-sensors will be presented. We discuss the performance of differential sensors realized by one SGFET with passivated gate and one with a bare GaN cap layer as a gate on one chip. The compensation of drift-effects such as like persistent photocurrent and temperature dependence will be discussed.

We have used such devices to study the time-dependent response of covalently immobilized enzymes on the gate surface towards the presence of their specific substrate molecules with acetylcholinesterase and penicillinase as examples.

HL 30.12 Thu 11:00 P3

Impact of GaN barrier thickness on indium incorporation in GaInN/GaN multiple quantum wells grown via MBE —

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The internal quantum efficiency (IQE) of optical devices based on GaInN is highly sensitive to the thickness of GaInN quantum well. The main way to increase the emission wavelength of GaInN quantum wells is to increase the indium content in the quantum well by enhancing the incorporation rate of indium. We grew fivefold GaInN MQWs at a substrate temperature of 580°C and the GaN barrier layer was grown in two steps. The first step is at the same growth temperature of GaInN quantum wells (580°C), called the low-temperature GaN (LT-GaN) layer and the second step is the high-temperature GaN (HT-GaN), which was grown after the ramping of the substrate temperature up to 725°C. From high-resolution XRD and high-resolution TEM measurements, we found that the thickness of the GaInN wells increased significantly with the increase of the growth time of the LT-GaN layer. The effects of changing the growth time of the LT-GaN layer include changing the indium content of the GaInN well and the thickness of the barrier layer. The analysis of GaInN/GaN MQWs samples using different characterization methods such as HR-XRD, HR-TEM, AFM, and PL provides a detailed understanding of the role of the indium adlayer and its impact on the growth mechanism at low temperatures.

HL 30.13 Thu 11:00 P3

Aging of GaN-based laser diodes investigated by micro-EL and micro-PL spectroscopy — •LUKAS UHLIG¹, CONNY BECHT¹, ERIK FREIER², JI-HYE KANG², VEIT HOFFMANN², CHRISTOPH STÖLMACKER², SVEN EINFELDT², and ULRICH T. SCHWARZ¹ — ¹Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany — ²Ferdinand-Braun-Institut gGmbH, Leibniz-Institut für Höchstfrequenztechnik, 12489 Berlin, Germany

For the work towards long-time reliable GaN-based ridge waveguide laser diodes it is essential to understand the specific degradation effects that occur after some time of operation. Among the reported aging mechanisms are the generation of point defects in the active layer and a decrease in p-side conductivity.

To clarify this, we compare a previously stressed device with a similar but unstressed laser diode using micro-electroluminescence (EL) and confocal micro-photoluminescence (PL) spectroscopy. The devices are mounted p-side-down and the metal layer on the n-side is polished away to allow optical characterization in the plane of the quantum wells.

In contrast to the homogeneous EL-emission from the non-stressed device, the stressed laser diode exhibits bright and dark areas along the ridge on the scale of few 10 μm . The systematic correlation of high intensity with a spectral blue-shift and vice versa indicates local changes in the charge carrier density that we attribute to inhomogeneous electrical pumping. The micro-PL-measurements show an increased defect density in the active region.

HL 30.14 Thu 11:00 P3

Spectral and temporal behavior of the near field of 10 μm broad area blue laser diodes — •DOMINIC J. KUNZMANN¹, LUKAS UHLIG¹, JANNINA J. TEPASS¹, ANNA KAFAR^{2,3}, SZYMON STANCZYK^{2,3}, PIOTR PERLIN^{2,3}, and ULRICH T. SCHWARZ¹ — ¹University of Technology Chemnitz, 09126 Chemnitz, Germany — ²Institute of High Pressure Physics PAS, Warsaw, Poland — ³TOP-GAN Ltd., Warsaw, Poland

We investigate the near field for the laser diodes driven in pulsed conditions with pulse lengths in the range of a few 10 ns up to 100 ns and currents from 1.5 I_{th} to 4 I_{th} . A streak camera image and a high resolved longitudinal mode spectrum are taken at each point of a near field scan for blue laser diodes with a 10 μm broad ridge.

The combination of the streak camera setup and the high resolution spectrometer allows us to investigate: the spectral-lateral-temporal behavior with complex dynamics due to lateral-longitudinal mode competition, the wavelength shift at the lasing onset and on the other hand to get the longitudinal mode spectrum. Different mode combs are interacting in this longitudinal mode spectrum and the predominating mode comb changes for different parts of the spectrum.

An increasing laser current leads to a broadening of the spectrum as well as to the filling of the gain volume, while for higher currents the lateral distribution seems to be similar across the whole spectrum. Comparing these results to previously measured devices with a 40 μm broad ridge, we observe a less homogeneous near field distribution with a slight systematic asymmetry.

HL 30.15 Thu 11:00 P3

Molecular beam epitaxy of ScGaN on 6H-SiC — •AARON GIESS, FABIAN ULLMANN and STEFAN KRISCHOK — Institut für Mikro und Nanotechnologien, Institut für Physik, TU Ilmenau

Group III-nitrides are well-suited semiconductors for optoelectronic and sensor devices. Among them, Sc-containing nitrides are of recent interest as well. In this contribution we report on our present progress in ScGaN PAMBE growth. We grow ScGaN using plasma-assisted molecular beam epitaxy on Si-faced 6H-SiC. Prior growth the SiC-surface is cleaned by a HF-Dip and a gallium anneal. Compared to GaN growth the implementation of scandium poses significant challenges: (i) ScN inclines to cubic growth and (ii) Gallium tends to form liquid droplets. In order to find optimal growth conditions, parameters such as substrate-temperature and nitrogen as well as Sc and Ga flux have been systematically varied. During growth, reflection high-energy electron diffraction (RHEED) diffraction patterns have been monitored. Further characterization has been performed by X-Ray photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM). In future we plan systematic studies on the electronic properties of high quality epitaxial ScGaN thin films as well as their interaction with molecules.

HL 30.16 Thu 11:00 P3

MOVPE-grown optoelectronic devices with GaN:Mg/GaN:Ge tunnel junctions — •CHRISTOPH BERGER, ARMIN DADGAR, JÜRGEN BLÄSING, GORDON SCHMIDT, HANNES SCHÜRMAN, PETER VEIT, FRANK BERTRAM, JÜRGEN CHRISTEN, and ANDRÉ STRITTMATTER — Otto-von-Guericke-Universität Magdeburg, Deutschland

We report on low resistive GaN-based tunnel junctions (TJ) and TJ optoelectronic devices grown by metalorganic vapor phase epitaxy. Very high donor concentrations, which are mandatory for low-resistive TJs, are achieved by using germanium instead of commonly used silicon. For efficient activation of GaN:Mg, a growth process was developed that includes an in-situ activation step and overgrowth of the p-type GaN with GaN:Ge in nitrogen ambient to prevent the repassivation of the buried p-type layer. Electrical and optical characterization of the fabricated LEDs shows that GaN:Mg is efficiently activated and additional ex-situ activation is expendable. Tunnel-junction LEDs show an improved light output by approximately 20 % in comparison to conventional LEDs with semitransparent contacts and exhibit a comparable differential resistance of $1.2 \times 10^{-2} \Omega\text{cm}^2$ at a current density of 100 Acm^{-2} without voltage penalty. Such tunnel-junctions were implemented in laser diode structures and were used to realize cascaded LEDs with up to three pn-junctions stacked on top of each other. We will present our latest results on the growth, the challenges and the characteristics of these sophisticated optoelectronic devices.

HL 30.17 Thu 11:00 P3

object detection of patterned GaN using convolutional neural networks and synthetic data — •MAHDI KHALILI HEZARJARIBI, UWE ROSSOW, MARKUS ETZKORN, HEIKO BREMERS, and ANDREAS HANGLEITER — Institut für Angewandte Physik, Technische Universität Braunschweig

Employing a practical object detection algorithm, we have developed a process to detect GaN pyramid structures, extracted from SEM images. A procedure has been developed to generate synthetic images for training the algorithm instead of the drudgery of multiple imaging of samples. These synthetic data include noise, blurring, and other contributing factors in order to realize images that are accurate enough to train an object detection algorithm. A MobileNet algorithm has been employed for the Object detection process. The synthetic database proved pragmatic leading to a promising confidence value of 75% for detecting real objects.

HL 30.18 Thu 11:00 P3

Nominally identical GaInN/GaN single quantum wells : variations of optical and structural properties — •RODRIGO DE VASCONCELLOS LOURENCO^{1,2}, MALTE SCHRADER^{1,2}, UWE ROSSOW¹, HEIKO BREMERS^{1,2}, and ANDREAS HANGLEITER^{1,2} — ¹Institute of Applied Physics, Technische Universität Braunschweig, Germany — ²Laboratory for Emerging Nanometrology, Braunschweig, Germany

We have unexpectedly observed differences in luminescence and structural properties in GaInN/GaN single quantum wells (SQW), grown under nominally identical conditions. This may be related to specific growth condition such as variation in substrate temperature or doping level; or substrate characteristics, e.g. bowing and offset; as well

as the status of the growth system. The samples were grown in low-pressure metalorganic vapour-phase epitaxy (MOVPE) on c-plane sapphire substrate. The differences in emission wavelength of the SQWs suggest that either there is a discrepancy in In content or in doping level. From the reference multiple quantum wells samples, a variation of 5 % in In concentration was observed. This fluctuation in In content may explain variations in the lattice constants of the SQWs measured by high-resolution X-ray diffraction (HRXRD). We aim to understand how the In content and among other attributes could influence the internal quantum efficiency at room temperature of GaInN/GaN SQWs ranging from 0.6 to 47%.

HL 30.19 Thu 11:00 P3

Skull-melting technique for the crystal growth of high-melting oxides — ●DEMIAN RANFTL, KLAUS-DIETER LUTHER, and CORNELIUS KRELLNER — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt/Main, Germany

For growing high melting oxide single crystals a quasi crucible-free induction melting technique can be used. Within a so-called skull-oven a high frequency electric field is applied to a powdered sample. A metallic part in the center of the powder will absorb the field and increase in temperature while also increasing the temperature of the oxides surrounding it. By cooling the outer sections of the sample it is possible to create a melt of a semiconductor in a crucible made out of its own sintered material, thus avoiding integration of unwanted crucible elements and enabling melts even at temperatures where no crucible material exist. This method was developed for the growth of, for example, ZrO₂ crystals with a melting temperature of 2700°C [1]. In this contribution we will present the working principles of the skull-oven built at the Physikalisches Institut (Goethe Universität, Frankfurt) together with a brief introduction to skull-melting and its features. Additionally, we will present first attempts of the single crystal growth of pure titanium(IV) oxide using this skull-melting technique. [1] Assmus, W. and Whippey, N. Ueber das Skull-Schmelzen. Chem.-Ing.-Tech. 55, 716-717 (1983).

HL 30.20 Thu 11:00 P3

Investigation into the electric properties of α -Ga₂O₃ based Schottky diodes with various Schottky metals — ●S. KÖPP, C. PETERSEN, H. VON WENCKSTERN, and M. GRUNDMANN — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

We present current-voltage measurements of α -Ga₂O₃:Sn based Schottky diodes with various Schottky metals and show on/off current ratios of up to 8 orders of magnitude. We thereby evaluate the effective Schottky barrier height by temperature dependent measurements in the range of 40K up to 400K.

Due to its possible applications in high-power electronics, a great deal of attention has been drawn to the wide bandgap semiconductor Ga₂O₃. In recent years, in addition to the well-researched thermodynamically stable monoclinic polymorph β -Ga₂O₃ the metastable corundum-structured α -phase of Ga₂O₃ has shown to have promising physical properties. With a bandgap of 5.0-5.3 eV [1] and a predicted breakdown field of 8 MV/cm [2] it surpasses the theoretical limits of β -Ga₂O₃ in terms of Baliga's figure of merit [1]. Further, α -Ga₂O₃ is isostructural to α -Al₂O₃ and hence epitaxial growth on cost-efficient sapphire substrates is possible.

[1] Yang, D. *et al.*, El. Mat. Letters 18.2 p. 113-118 (2022)

[2] Higashiwaki, M. *et al.*, Semicond. Sci. Technol, 034001, (2016)

HL 30.21 Thu 11:00 P3

Copper tin oxide: An amorphous ternary oxide with tunable optical and electrical properties — ●ARNE JÖRNS, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — University of Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group

Due to the mismatching crystal structures of copper oxide (CuO) and stannic oxide (SnO₂) an amorphous alloy can form when these materials are combined. Few reports show that the resulting alloy exhibits *p*-type behavior, but low hole mobility results in unreliable Hall measurements [1]. Nevertheless, optical and electrical properties can be tuned by the alloy composition.

In this work we investigated copper tin oxide thin films deposited by pulsed laser deposition of ceramic CuO and SnO₂ targets at room temperature and in oxygen atmosphere. The resulting samples are

highly disordered and *n*-type semiconducting with room temperature mobilities up to 11 cm²V⁻¹s⁻¹. Optical and electrical properties can be tuned in a wide range by varying composition ratio and chamber pressure. Temperature dependent Hall-measurement for different cation contents and a first approach on Schottky diodes will be reported.

[1] P. J. M. Isherwood *et al.*, J. Appl. Phys., 118, 105702, 2015

HL 30.22 Thu 11:00 P3

Indium oxide metal-semiconductor field-effect transistors — ●FABIAN SCHÖPPACH, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Felix Bloch Institute for Solid State Physics, Universität Leipzig, Germany

Indium oxide (In₂O₃) combines promising physical properties such as high carrier mobility and transparency in the visible. However, In₂O₃ is generally challenging to use in active devices. This is mainly due to its tendency to form an electron accumulation layer on its surface (SEAL) which is reported to be caused by surface near oxygen vacancies [1]. Both, compensating Mg doping and oxygen plasma treatment can be used to suppress the SEAL formation [2,3]. Moreover, as a sesquioxide, In₂O₃ is a very robust material that resists classical patterning processes and cannot be patterned by wet chemical processes.

In this work, In₂O₃ films grown by pulsed laser deposition are structured via dry-etching techniques. With that field-effect transistors were fabricated for the first time, reaching on-off ratios of over 5 orders of magnitude and low sub-threshold swings of about 110 mV/dec. For the source and drain contacts, gold was deposited by inert ambient sputtering. Schottky gate diodes were fabricated in a reactive sputtering process, which is a prerequisite for obtaining electrically rectifying contacts to In₂O₃ [4].

[1] KING, et al. Physical Review B 80.8, 081201 (2009)

[2] SCHMIDT, et al. physica status solidi (b) 252.10, 2304-2308 (2015)

[3] MICHEL, et al. ACS Appl. Mater. Interf. 11, 27073-27087 (2019)

[4] VON WENCKSTERN, et al. APL Materials 2.4, 046104 (2014)

HL 30.23 Thu 11:00 P3

Electrical transport properties of Sn, Si and Ge doped α -Ga₂O₃ — ●THORBEN SLOTSCH, CLEMENS PETERSEN, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

We present Schottky barrier diodes based on PLD-grown α -Ga₂O₃ thin films, doped with the effective mass donors Sn, Si and Ge. By employing temperature dependent current-voltage measurements, Hall-effect measurements and thermal admittance spectroscopy of the space charge region we investigate the electric transport properties of α -Ga₂O₃ in relation to the doping levels provided by the combinatorial PLD method.

Materials with large bandgaps (> 3.4 eV) have attracted scientist's interest more and recently. With its high bandgap of 4.6-5.3 eV Ga₂O₃ is well suited for applications in high-power devices [1]. Numerous studies have already reported on the thermodynamically stable monoclinic β -phase of gallium oxide. However the metastable α -polymorph has gained scientist's attention. Its corundum structure allows α -Ga₂O₃ to form alloys with other corundum-structured materials like α -Al₂O₃ over the whole composition range to tune the bandgap energy up to 8.75 eV [2]. In order to grow α -Ga₂O₃ combinatorial pulsed laser deposition can be employed, which offers the advantage of a precise dopant incorporation and lateral continuous doping gradients [3].

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HL 30.24 Thu 11:00 P3

Characterization and optimization of MgZnO thin films with steep lateral composition gradient — ●LAURENZ THYEN, MAX KNEISS, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnestraße 5, 04103 Leipzig, Germany

The materials magnesium- and zinc-oxide have been widely investigated in the past. Corresponding step graded ternary alloy thin films of Mg_xZn_{1-x}O have been of great interest [1]. Pulsed laser deposition (PLD) has been used to grow laterally and vertically graded thin films [2]. The precise control of its chemical composition is of great importance for possible applications. Additionally, in the course of miniaturization of electrical devices like wavelength-selective multi-channel UV photodetectors, a well-defined steep slope of the material

gradient will be beneficial [3,4].

In this contribution the properties of $\text{Mg}_x\text{Zn}_{1-x}\text{O}$ thin films with lateral compositional gradient grown by pulsed laser deposition will be discussed. In order to obtain information about the material composition of the thin films, energy-dispersed X-ray spectroscopy, spatially resolved ellipsometry and micro-photoluminescence spectroscopy measurements have been conducted. Moreover, steep lateral gradients with a slope of up to 20% Mg content per millimeter were realised.

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HL 30.25 Thu 11:00 P3

Characterization of Schottky barrier contacts on a (Mg,Zn)O thin film with lateral composition gradient — ●MAURICIO BAS-SALLO, LAURENZ THYEN, MAX KNEISS, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstraße 5, 04103 Leipzig, Germany

A lateral chemical gradient composition structure based on (Mg,Zn)O is a promising material that allows a spectrally resolved detection of UV photons due to a systematic shift of the absorption edge with the position. In that sense, N different photodetectors, fabricated at different positions of the gradient, would be sensitive to specific photon energies [1]. Due to the challenges of stable p-type (Mg,Zn)O fabrication with high conductivity and mobility, metal-semiconductor-metal (MSM) structures are preferentially chosen for (Mg,Zn)O-based photodetectors [2]. These consist of two small interdigitated coplanar Schottky contacts, which are $10\mu\text{m}$ wide and $10\mu\text{m}$ apart and whose simplicity in fabrication makes the MSM structure promising for photodetection. In this contribution the electrical properties of the Schottky contacts in such MSM structures are discussed using the current-voltage measurements. Additionally, the influence of the surface characteristics on the contacts are discussed using Atomic Force Microscopy measurements.

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HL 30.26 Thu 11:00 P3

Porosity Analysis of Mesoporous Silicon by SEM Images of Polished Cross Sections — ●STEFANIE LAWUNDY^{1,2}, WALDEMAR SCHREIBER¹, and STEFAN JANZ¹ — ¹Fraunhofer ISE, Freiburg i. Br., Germany — ²University of Freiburg, Germany

Porous silicon fabricated by electrochemical etching is a material known for decades with a wide field of applications ranging from photovoltaics to medicine. Nevertheless, the determination of its key property porosity is still an issue that is to be refined.

Especially, the spatially resolved porosity analysis of layered mesoporous silicon stacks are challenging due to the small structures of only about 10 nm. Current measurement techniques as gas adsorption are not appropriate for such structures since they cannot fully penetrate the pores, cannot resolve the porosity profile over layer depth and lead to no information about the pore morphology.

In order to account for these challenges a new approach has been developed. It is based on the analysis of SEM cross section images where contrast and homogeneity are enhanced by a preceding polishing procedure. Pores are defined by using an image processing software and porosity profiles are calculated.

Results of this procedure are assumed to be an important step towards an accurate description of the etching process.

HL 30.27 Thu 11:00 P3

Temperature dependent light beam induced current (LBIC) investigation of PCMO-STNO interfaces — ●SOPHIE SCHAIBLE¹, TOBIAS WESTPHAL¹, FELIX MÜLLER¹, STEPHAN MELLES², CHRISTIAN JOOSS², and MICHAEL SEIBT¹ — ¹IV. Physical Institute, University of Goettingen, Göttingen, Germany — ²Institute for Materials Physics, University of Goettingen, Göttingen, Germany

Pn-heterojunctions of calcium doped praseodymium manganite $\text{Pr}_{0.66}\text{Ca}_{0.34}\text{MnO}_3$ and niobium doped strontium titanate $\text{SrTi}_{0.998}\text{Nb}_{0.002}\text{O}_3$ (PCMO-STNO) are used as a model system to investigate next generation solar cells going beyond the Shockley-Queisser limit by harvesting hot polaron-type charge carriers. In order to study the photovoltaic response in combination with the temperature and wavelength dependent generation of charge carriers, LBIC

is used on a specially grown wedge-shaped PCMO thin film. A position dependent signal is obtained, which translates into the variation of the absorber thickness. PCMO has a perovskite structure and exhibits strong electron-phonon coupling leading to stable polarons. At the charge ordering temperature ($T_{CO} \approx 230\text{K}$) PCMO undergoes a phase transition from the semiconducting paramagnetic to the charge ordered phase [1]. Liquid nitrogen cooling of the LBIC setup enables temperature dependent LBIC measurements below room temperature and thus gives insights into this transition. Comparison with temperature dependent electron beam induced current (EBIC) measurements highlights differences between photon and electron excitation. [1] L. Wu *et al.*, Phys. Rev. B 76, 174210 (2007)

HL 30.28 Thu 11:00 P3

Mapping Excitonic and Ionic Dynamics in Lead Halide Perovskite Thin Films — ●YENAL YALCINKAYA¹, PASCAL ROHRBECK¹, EMILIA SCHÜTZ², LUKAS SCHMIDT-MENDE², and STEFAN A.L. WEBER¹ — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — ²Department of Physics, University of Konstanz, Universitätsstr. 10, 78464, Germany

Understanding the dynamics of excitons and ions is crucial for improving the lead halide perovskites and related devices. In this study, we fabricated triple cation lead halide perovskite half cells (ITO/SnO₂/Perovskite) with small and large grain sizes. We obtained nearly $100\mu\text{m}$ large grains by heat treating perovskite films under methylamine gas atmosphere. Since the grain boundaries are known to be the main source of defects and ion migration in lead halide perovskites, a certain change between charge carrier and defect behaviour between these two types of films is expected. Therefore, we utilized Time-resolved Kelvin Probe Force Microscopy (Tr-KPFM) for mapping the recombination of free charge carriers and ion migration in triple cation lead halide perovskite films with varying grain sizes. Mapping these excitonic and ionic components of photovoltage allowed us to map the defects within the perovskite films. Our results showed a significant increase in free electron-hole lifetimes in large grained perovskite films. Furthermore, we demonstrate the ion migration was suppressed by having fewer grain boundaries within the film. Our study shows how grain sizes affect the free charge carrier movements and how we can track these changes on nanoscale via KPFM.

HL 30.29 Thu 11:00 P3

The Effects of Residual Lead Iodide on the Stability of Perovskite Solar Cells — ●XIONGZHUO JIANG and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, 85748 Garching, Deutschland

Over the past few years, hybrid organic-inorganic lead halide perovskite materials have attracted tremendous interest as its excellent photovoltaic properties in perovskite solar cells (PSCs) with record power conversion efficiency. The residual lead iodide is easy to form during the fabrication of perovskite layer, especially for the two-step deposition method. In addition, residual lead iodide has been universally used in the state-of-the-art devices to boost the device performance. However, the effects of residual lead iodide on the stability of PSCs has not been fully understood and, therefore, needs to be deeply investigated for further improvement of device performance. Herein, it is shown that residual lead iodide exhibits insufficient stability under continuous light radiation and heating. The photodecomposition products (lead and iodine) of lead iodide pose a threat to the efficiency and stability of devices. Thus, unstable lead iodide under light radiation and heating is one of the main reasons for the degradation of perovskite device. Therefore, carefully controlling or eliminating the residual lead iodide in perovskite film is one of the critical methods to improve the long-term stability of PSCs.

HL 30.30 Thu 11:00 P3

Multi-photon induced ultrafast absorption dynamics of optical excitons in 2D inorganic-organic hybrid semiconductor — ●MOHAMMAD ADNAN^{1,2}, RUDOLF BRATSCHITSCH², and GADDAM VIJAYA PRAKASH¹ — ¹Nanophotonics Lab, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016 India — ²Institute of Physics, University of Münster, Wilhelm-Klemm-Straße 10 48149 Münster, Germany

Two-dimensional inorganic-organic (IO) hybrid semiconductors have attracted prodigious attentions due to unique crystal structural packing and tunable exciton characteristics and exhibit strong optical exciton features at room temperature due to their large exciton binding energies (200-250 meV) [1]. These optical excitons are highly sensitive

to the layer thickness and demonstrate distinct excitonic behaviors from surface and bulk regions. Multi-photon absorption spectroscopy is a novel probing tool which can monitor excitons from the deeper energy levels [1]. Nonlinear one-photon (3.54 eV), two-photon (1.55 eV) and three-photon (1.21 eV) transient absorption studies have been carried out to have better understanding of hot-carrier relaxations from different lower lying exciton energy levels. Fluence-dependent studies clearly demonstrate various nonlinear effects such as hot phonon bottleneck effect, exciton-exciton annihilation and Auger processes at higher fluences [2]. The results presented here may find interesting applications in developing advanced optoelectronic devices.

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2. Adnan et al., *J. Phys. Chem. C.*, 2021, 125, 12166.

HL 30.31 Thu 11:00 P3

Electron Beam Induced Current (EBIC) Investigations of Femtosecond Laser Sulfur Hyperdoped Silicon — •MENG RU SUN¹, TOBIAS WESTPHAL¹, SIMON PAULUS², SÖREN SCHÄFER², STEFAN KONTERMANN², and MICHAEL SEIBT¹ — ¹University of Goettingen, IV. Physical Institute, Göttingen, Germany — ²Institute for Microtechnologies (IMtech), University of Applied Sciences Rhein- Main, Rüsselsheim, Germany

S hyperdoped Si formed by fs-laser irradiation improves the absorption of the Si-based optoelectronic devices to infrared wavelengths. A p-n junction is created between the B doped p-type Si wafer and the S hyperdoped n-type region produced as a result of fs-laser pulse irradiation of the Si wafer surface under SF₆ atmosphere. The structural and electronic properties of the fs-laser hyperdoped S depend strongly on the laser-processing parameters such as the number of pulses per spot and laser fluence. In this contribution, we focus on S hyperdoped Si fabricated via fs-laser irradiation at 800nm wavelength and various laser processing parameters. Electron Beam Induced Current (EBIC) performed in plan-view and cross-section geometry is used for characterizing the electronic properties of the sample like excess minority carrier diffusion length. Combining EBIC with SEM images, the correlations between electronic properties and the surface textures can be observed. The results of this work show the important role of processing parameters on the surface macro- and microstructure. EBIC data further indicates the different behaviors of the excess carriers within the ridges and the valleys at the surface.

HL 30.32 Thu 11:00 P3

Spin Polarization Dynamics of Photo-excited Carriers in CsPbX₃ Nanocrystals — •AHMET TOSUN, SIMONE STROHMAYER, ANJA BARFÜSSER, QUINTEN AKKERMAN, TUSHAR DEBNATH, AMRITA DEY, and JOCHEN FELDMANN — Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany

We present results on spin relaxation dynamics of photoexcited carriers in CsPbX₃ nanocrystals by employing time-resolved differential transmission spectroscopy. After photoexcitation with circularly polarized light we observe a pronounced spin polarization in CsPbI₃ nanocrystals. This spin-polarization is caused by selectively exciting spin-allowed transitions and is lost during thermalization and cooling of the photoexcited charge carriers. From temperature-dependent experiments we conclude that carrier-spin relaxation in CsPbI₃ nanocrystals is predominantly caused by carrier-LO phonon scattering and can be described by the Elliot-Yafet mechanism.

HL 30.33 Thu 11:00 P3

Characterizing the conductive channels of 2D perovskite field-effect transistors with Kelvin probe force microscopy — •KONSTANTINOS BIDINAKIS, SHUANGLONG WANG, PAUL W.M. BLOM, WOJCIECH PISULA, TOMASZ MARSZALEK, and STEFAN A.L. WEBER — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Perovskite-based field-effect transistors (FETs) are a promising class of electronic materials, which also provide a basis for understanding the lateral charge transport within perovskites. Specifically, FETs of 2D perovskite materials exhibit diminished ion migration and improved stability against moisture compared to their 3D counterparts, due to their specific structure. The performance of the transistors is strongly influenced by the nanoscale morphology of the perovskite film. We used Kelvin probe force microscopy (KPFM) to correlate the local morphology and crystallinity with the potential distribution across a bottom-gate top-contact perovskite FET channel under operating con-

ditions. The measured potential distribution from source to drain can indicate unwanted losses, e.g. at grain boundaries or at the electrodes.

In order to increase the crystalline quality of a Sn-based perovskite film, an additive with high Lewis alkalinity is used in the precursor solution, which coordinates with the Sn cation and retards crystallization. Using KPFM, we examined devices with and without such an additive and correlated the measured potential profiles with the charge transport characteristics, as well as ion migration and behavior at the perovskite grain boundaries.

HL 30.34 Thu 11:00 P3

Cross linkable hole transport materials for p-i-n perovskite solar cells — •MOHSEN HOSSEINI FARD, MANUEL NEUBAUER, ERVIN ALJIC, SIMON EWERTOWSKI, SELINA OLTHOF, DIRK HERTEL, and KLAUS MEERHOLZ — Department of Chemistry, University of Cologne, Germany

The use of hole transport materials (HTMs) in perovskite solar cells (PSCs) is indispensable. Many reports illustrate the importance of layer thickness, energy level alignment, doping and mobility of HTMs on PSCs performance. However, there are ambiguities regarding the properties of HTMs, which invoke further fundamental studies. Here, we investigate a series of cross-linkable hole transport materials (x-HTMs), TPD and TAPC derivatives, with different HOMO and LUMO energy positions. The advantage of HOMO and LUMO tunability of the above-mentioned compounds by exchanging molecular substituents is applied to investigate their hole extraction and electron blocking abilities. J-V characterization was used to investigate changes in the device characteristics. Major improvement in fill factor and Voc of MAPbI₃ based solar cells was demonstrated by adjusting the thickness of x-HTMs. As a result, large improvements were observed in power conversion efficiency (PCE). A thin layer application of x-HTMs showed competitive results in PCE performance compared to the commonly used, commercially available materials like PTAA. Nevertheless, the application of a thin layer of QUPD (less than 5 nm) leads to high-efficient PSCs with a shown record PCE up of 19.56% using MAPbI₃ as absorber, similar to the performance of a PTAA-based device.

HL 30.35 Thu 11:00 P3

Effect on Surface Morphology on 1.7eV-GaInAsP-layers on GaAs by surfactant-assisted MOVPE growth — •IVO RAHLFF, PATRICK SCHYGULLA, JENS OHLMANN, and DAVID LACKNER — Fraunhofer ISE, Freiburg i. B., Germany

III-V-compound multi junction solar cells hold record efficiencies since many decades. Recently, we have demonstrated a GaInP(1.9eV)/AlGaAs(1.44eV)/GaInAsP(1.09eV)/GaInAs(0.74eV) 4-junction wafer bonded solar cell that reaches 47.6% under a concentration of 665 suns (AM1.5d). All subcells are epitaxially deposited by MOVPE. To further increase the realistic efficiency potential above 50% a 6-junction device with the following bandgaps (1.94eV/1.71eV/1.42eV//1.19eV/0.98eV/0.74eV) is suggested. One promising candidate for the 1.71eV junction is GaInAsP. The challenge for this material system lies in the compositional regime between 1.60eV and 1.75eV, where phase separation has been reported.

In this work we investigate the effect of surfactant-assisted growth of GaInAsP alloys on the surface morphology during MOVPE growth. It is found that the GaInAsP growth without surfactant leads to severe surface roughening which is believed to be due to the onset of phase separation. XRD measurements revealed further decreasing tensile strain with increasing TMSb/III ratios which is expected, since the surfactant alters the atomic incorporation. Further investigations on the effect of the opto-electrical quality of the surfactant on the GaInAsP 1.7eV material is currently in progress.

HL 30.36 Thu 11:00 P3

Getting started in Perovskite Solar Cells - The little complications that are unmentioned — •MAXIMILIAN SPIES, SIMON BIBERGER, and FABIAN PANZER — University of Bayreuth, Bayreuth, Germany

Due to the current interest in highly efficient perovskite solar cells (PSCs), many groups are attempting to produce such PSCs based on published recipes. Since these recipes often assume a lot of prior knowledge or do not consider environmental conditions in sufficient detail, resulting efficiencies are low. This work shows some of the complications one faces when attempting to build a PSC in n-i-p-structure, considering especially the transport layers. Starting from low single digit power conversion efficiency (PCE), we exceeded PCEs of 12% due to modifications of the production process. We tested different variations

of the hole transport layer "on device", including a relatively new approach of solution-based CO₂-doping. With the detrimental factor of humidity to perovskite being known, we show systematically the impact of in-glovebox-processing on PCE and V_{OC}. Further, we found that surface properties of the bottom electrode critically influence the fillfactor.

HL 30.37 Thu 11:00 P3

First-principles study of perovskite/halide interfaces — ●SAMUELE SPREAFICO and BERND MEYER — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

Lead halide perovskites are a promising new class of semiconductors, which are easy and cheap to process and show high efficiency in optoelectronic applications. Photovoltaic engineering requires a controlled integration of the photo-active perovskite into a multi-layer heterostructure or quantum dot composite [1]. However, the interfaces in these devices unavoidably affect their optical response, for example the photoluminescence quantum yield. Here we present a density-functional theory investigation on the properties of the interfaces in a composite of CsPbBr₃ quantum dots embedded in a CsBr or NaBr matrix. First we performed a systematic screening of the structure and chemical composition of the interfaces. For the most stable configurations we determined the band alignments and we show how the band offsets at these interfaces depend on the interface structure, which can be tuned by changing synthesis conditions.

[1] B. Chaudhary, Y.K. Kshetri, H.S. Kim, S.W. Lee, T.H. Kim, *Nanotechnology* **32** (2021) 502007

HL 30.38 Thu 11:00 P3

Energy Transfer in Stability-Optimized Perovskite Nanocrystals — ●MICHÈLE G. GREINER, ANDREAS SINGLDINGER, NINA HENKE, CAROLA LAMPE, ULRICH LEO, MORITZ GRAMLICH, and ALEXANDER S. URBAN — Nanospectroscopy Group and Center for Nanoscience (CeNS), Nano-Institute Munich, Department of Physics, Ludwig Maximilians University Munich, Koeniginstr. 10, 80539 Munich, Germany

Halide perovskites nanocrystals (NCs) are auspicious materials for low-cost, high efficient photovoltaic and light-emitting devices. Nevertheless, the fast degradation in contact with moisture is one critical issue. Another problem constitutes the inefficient charge transfer between different layers. To counteract both problems, we employ micelles made of diblock copolymers filled with methylammonium lead bromide (MAPbBr₃) NCs. With this approach, we bypass the charge transfer issue by exploiting energy transfer (ET) between CsPbBr₃ nanoplatelets and the MAPbBr₃ micelles. We chose micelles with different diameters to find the best balance between protection and ET efficiency. As a result, we found an increase in stability by around 56% from the smallest to the thickest shell and a transfer efficiency up to 73.6% for the smallest micelle. These findings could help improve different optoelectronic devices, such as perovskite-based solar cells or light-emitting devices.

HL 30.39 Thu 11:00 P3

Probing structural dynamics in optically excited 2D heterostructures by Ultrafast Electron Diffraction — ●MASHOOD TARIQ MIR, ARNE UNGEHEUER, AHMED HASSANIEN, LUKAS NÖDING, ARNE SENFTLEBEN, and THOMAS BAUMERT — University of Kassel, 34132 Kassel, Germany

Layered transition metal dichalcogenides (TMDs) host a rich collection of physical properties, opening many different applications with atomically thin films such as sensors, electronic switching, or energy storage. Among those materials, 1T-TaS₂ exhibits a complex phase diagram depending on temperature encompassing charge density waves (CDW) with diverse commensurabilities. New phenomena have been observed and are further expected from combining different materials to 2D heterojunctions. We aim to use femtosecond laser pulses to induce rapid structural changes and probe them with ultrafast electron diffraction (UED). In this work, free-standing single-crystalline heterostructure samples were prepared down to a few nanometre thicknesses to allow electron diffraction in transmission mode. The preparation method was optimized using atomic force microscopy and optical microscopy to isolate atomically thin flakes. In addition, we present an initial UED study of CDW heterostructure (1T-TaS₂ / Graphite). Upon lattice heating, the CDW material undergoes several phase transitions. We focus on the reversible phase transition of 1T-TaS₂ from the nearly

commensurate to the incommensurate phase and study the effect of interlayer coupling of stacked 1T-TaS₂ / Graphite heterostructures.

HL 30.40 Thu 11:00 P3

Theory of non-integer high-harmonic generation in a topological surface state — ●MAXIMILIAN GRAML¹, MAXIMILIAN NITSCH^{1,2}, ADRIAN SEITH¹, FERDINAND EVERS¹, and JAN WILHELM¹ — ¹Institute of Theoretical Physics, University of Regensburg — ²NanoLund and Solid State Physics, Lund University, Sweden

High-harmonic emission from a topological insulator has been observed recently [1] opening a platform to explore topology and relativistic quantum physics using strong laser fields. Strikingly, the higher order resonance frequencies can be continuously shifted to non-integer multiples of the driving frequency by varying the carrier-envelope phase (CEP) of the driving field. Based on a semiclassical model we explain this finding as a characteristic property of the Dirac dispersion. We complement analytical results with numerical simulations based on the semiconductor Bloch equations.[2]

[1] C.P. Schmid, et al.: Tunable non-integer high-harmonic generation in a topological insulator, *Nature* **593**, 385-390 (2021).

[2] M. Graml, et al.: Theory of non-integer high-harmonic generation in a topological surface state, arXiv:2205.02631 (2022)

HL 30.41 Thu 11:00 P3

Ultrafast spectroscopy of single quantum dots utilizing synchronized GHz-Oscillators — ●VALENTIN DICHTL, MICHAEL SEIDEL, GERHARD SCHÄFER, and MARKUS LIPPITZ — Experimental Physics III, University of Bayreuth, Germany

Ultrafast transient absorption or reflection spectroscopy of single semiconductor quantum dots is a well established technique, typically based on laser oscillators with about 80 MHz repetition rate. The excited state lifetime of the emitter is however much shorter than the pulse separation in these experiments. Most of the time one thus waits for the next laser pulse.

Here we present a modified setup based on two synchronized Ti:Sa lasers operating at 1 GHz repetition rate and a line camera with a spectral rate of 127 kHz. Noise suppression is accomplished via double modulation using a field programmable gate array (FPGA) for synchronizing AOMs with the line camera.

We demonstrate the perturbed free induction decay of single AlGaAs quantum dots at temperatures below 20 K. The total integration time is less than three minutes – currently software limited.

HL 30.42 Thu 11:00 P3

Non-linear optimization and error estimation for the dynamical modelling of photoluminescence spectra — ●SEBASTIAN BOHM¹, MAX GROSSMANN¹, STEFAN HEYDER¹, KLAUS SCHWARZBURG², PETER KLEINSCHMIDT¹, ERICH RUNGE¹, and THOMAS HANNAPPEL¹ — ¹Fakultät für Mathematik und Naturwissenschaften, Technische Universität Ilmenau, Ehrenbergstraße 29, 98693 Ilmenau — ²Institut Solare Brennstoffe, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

Modern compute power and improved algorithms allow to determine, e.g., the parameters of a kinetic model of time-resolved photoluminescence spectroscopy (TRPL) via the simultaneous fit of many excitation-dependent TRPL spectra. Since our method is based on a maximum likelihood estimator, we obtain information on the reliability of the derived values as well. As example, we use a TRPL model of M. W. Gerber and R. N. Kleiman [*J. Appl. Phys.* **122**, 095705 (2017), URL 10.1063/1.5001128].

HL 30.43 Thu 11:00 P3

Pulse-driven non-adiabatic tunneling in nanocontacts: quasi-classical approach — SANGWON KIM¹, TOBIAS SCHMUDE², GUIDO BURKARD², and ●ANDREY S. MOSKALENKO¹ — ¹KAIST, Daejeon, Korea — ²University of Konstanz, Konstanz, Germany

We develop a general quasiclassical theory for the description of the tunneling through time-dependent barriers induced by ultrashort light pulses and apply it to the tunneling induced by such pulses in nanocontacts [1]. In particular, we analyze the situation when the tunneling is driven by ideal half-cycle pulses. Among the numerous solutions that contribute to the tunneling probability, we choose two main solution branches with the largest contributions: The 1st solution exhibits the "tunneling" behavior of a wave packet whereas the 2nd solution exhibits the "evanescent-wave" behavior. For a large enough intercontact

distance, the 1st solution dominates in terms of the tunneling probability. However, for minute distances and small field strengths, when the electron does not manage to escape from the classically forbidden region, the 2nd solution starts to dominate. Finally, we study a situation when the tunneling is driven by realistic few-cycle pulses. We see that the direction of the electron transport in the nanocontacts may be altered in dependence on the carrier-envelope phase of the driving pulse. We also find that the time when the electron effectively emerges from under the barrier does not necessarily exactly coincide with one of the peaks of the driving electric field.

[1] Sangwon Kim et al., *New J. Phys.* 23, 083006 (2021).

HL 30.44 Thu 11:00 P3

Time-resolved broadband transient reflectivity studies in ultrathin bismuth films — ●ALEXANDER KASSEN¹, FABIAN THIEHMANN¹, GERMÁN SCIANT², and MICHAEL HORN-VON HOEGEN¹ — ¹University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — ²University of Waterloo, 200 University Avenue West, ON N2L 3G1, Canada

Bismuth, through its Peierls-Jones distorted lattice, offers the possibility to excite coherent phonon modes upon irradiation with ultra-short laserpulses. The optical A_{1g} mode at ≈ 3 THz is triggered by the dispersive excitation mechanism due to transient changes of the atomic potential energy surface. These changes arise from optical excitation of the electron system and thus lead to a strong coupling between the phonons and charge carriers. The density of excited charge carriers, which depends on the incident fluence and film thickness, alters the equilibrium position of the atoms and softens the potential energy surface, leading to a redshift of the A_{1g} mode. Conversely, in an all optical pump-probe experiment with a measurement of the relative change of reflectivity $\Delta R/R_0$, we utilized the redshift of the A_{1g} mode to determine the level of excitation of the electron system. In the next step, this allowed us to compare the relaxation behavior and transient optical properties of films with different thicknesses leading to a broader insight in the phonon and carrier excitation mechanisms.

HL 30.45 Thu 11:00 P3

Dimensionality Reduction Techniques in Femtosecond Time-Resolved Ellipsometry Data Analysis and Theory — ●NOAH STIEHM¹, YIXUAN ZHANG², ERICH RUNGE³, STEFAN KRISCHOK¹, HONGBIN ZHANG², and RÜDIGER SCHMIDT-GRUND¹ — ¹Technische Universität Ilmenau, Fachgebiet Technische Physik I, Weimarer Straße 32, 98693 Ilmenau, Germany — ²Technische Universität Darmstadt, Research Group Theory of Magnetic Materials, Otto-Berndt-Straße 3, 64287 Darmstadt — ³Technische Universität Ilmenau, Fachgebiet Theoretische Physik I, Weimarer Straße 32, 98693 Ilmenau, Germany

Physical modeling and interpretation of the transient dielectric function obtained from femtosecond time-resolved spectroscopic ellipsometry [1] poses a significant challenge, as it consists of many temporally and spectrally overlapping processes that need to be reliably separated to obtain stable and physically meaningful fit results. Ab-initio theory can help to separate these processes, but is not available for the whole time scale (≈ 100 fs to several ns) of the experiment, due to the associated computational costs.

To help overcome these challenges we investigate the use of dimensionality reduction techniques like dynamic mode decomposition and manifold learning methods like locally-linear embeddings and autoencoders to be applied I) in model approximation of the experimental data and II) on ab-initio results from time-dependent density functional theory to cover larger time scales. By this we identify strategies for a reliable modeling pipeline with minimal human intervention.

[1] S. Richter *et al.*, *Rev. Sci. Instrum.* 92, 033104 (2021).

HL 30.46 Thu 11:00 P3

Numerically exact simulations of quantum devices coupled to arbitrary environments using tensor networks — ●MORITZ CYGOREK¹, VOLLRATH MARTIN AXT², BRENDON W. LOVETT³, JONATHAN KEELING³, and ERIK M. GAUGER¹ — ¹Heriot-Watt University, Edinburgh, UK — ²Universität Bayreuth, Germany — ³University of St Andrews, UK

Reliable predictions of the dynamics in nanoscale quantum devices with applications in photonics, transport, quantum information and communication require a careful consideration of environment effects. Here, we present the novel numerical method Automated Compression of Environments (ACE): The open quantum systems dynamics is expressed in terms of a tensor network, where the influence of the environment is incorporated into a matrix product operator in time, the

so-called process tensor. ACE provides a direct way to calculate this process tensor numerically exactly with numerical errors originating only from time discretization and matrix product operator compression. As the numerical procedure starts directly from the microscopic Hamiltonian, no problem-specific derivations are required. Thus, as we show on a series of examples, one and the same computer code can be used to simulate the dynamics of open quantum systems with environments as diverse as photons, phonons, electrons, and spins, as well as combinations of multiple environments. This proof of principle demonstrates the tremendous potential of tensor network approaches as one-size-fits-all solutions to open quantum systems dynamics.

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Transient negative thermal expansion in HgTe/CdTe heterostructures by heating of transverse phonons — ●MATTHIAS RÖSSLE¹, MARC HERZOG², JAN PUDELL^{1,3}, WOLFRAM LEITENBERGER², MAXIMILIAN MATTERN², LUKAS LUNCZER⁴, CLAUD SCHUMACHER⁴, HARTMUT BUHMANN⁴, LAURENS MOLENKAMP⁴, and MATIAS BARGHEER^{1,2} — ¹Helmholtz-Zentrum Berlin, Germany — ²Institut für Physik und Astronomie, Universität Potsdam, Germany — ³European XFEL Facility GmbH, Schenefeld, Germany — ⁴Physikalisches Institut EP3, Universität Würzburg, Germany

We investigate the transient negative thermal expansion of semimetallic HgTe and semiconducting CdTe by using synchrotron-based time-resolved X-ray diffraction. At $T = 20$ K, far below the Debye temperature of both materials, the selective optical excitation of the HgTe top layer with an ultrashort near-infrared laser pulse leads to a rapid expansion of HgTe that is followed by a long lasting contraction. The CdTe substrate is compressed by the HgTe thin film expansion, and subsequently CdTe contracts due to thermally excited transverse phonon modes. This shows that negative thermal expansion is manifest on ultrafast timescales, consistent with the negative Grüneisen coefficient for transverse phonons in semiconducting materials with sphalerite crystal structure. At $T = 200$ K, far above the Debye temperature of both materials, the expansion driven by longitudinal acoustic phonons is prevalent. We simulate the lattice dynamics in an elastic model where transient thermal stresses are calculated via heat diffusion based on equilibrium thermoacoustic properties.

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Resonant and phonon-assisted ultrafast coherent control of a single hBN color center — ●DANIEL GROLL¹, JOHANN A. PREUSS², ROBERT SCHMIDT², THILO HAHN¹, PAWEŁ MACHNIKOWSKI³, RUDOLF BRATSCHITSCH², TILMANN KUHN¹, STEFFEN MICHAELIS DE VASCONCELLOS², and DANIEL WIGGER^{3,4} — ¹Institute of Solid State Theory, University of Münster, Germany — ²Institute of Physics, University of Münster, Germany — ³Department of Theoretical Physics, Wrocław University of Science and Technology, Poland — ⁴School of Physics, Trinity College Dublin, Ireland

For the development of scalable quantum technologies, reliable single-photon emitters in solid state systems are required. In this context, promising candidates are the recently discovered color centers in the van der Waals insulator hBN. These single photon emitters are attracting increasing attention due to their quantum performance at room temperature and wide range of transition energies. Here we report on our recent results on the ultrafast optical coherent state manipulation of a single hBN color center [1]. By combining experiment and theory we achieve a sound understanding of the impact of environment noise and the coupling to phonons on the emitter's coherence. Specifically, we detect the decoherence of optical phonon-assisted transitions, stemming in part from the finite lifetime of these phonons. The creation of acoustic phonons manifests in a rapid decrease of the emitter coherence during their emission and can lead to an ultrafast beat of the coherent control signal.

[1] J. Preuss, D. Groll, et al., *Optica* 9, 522-531 (2022)

HL 30.49 Thu 11:00 P3

Coherent acoustic phonons in a Graphite-hBN heterostructure observed by ultrafast electron diffraction — ●ARNE UNGEHEUER¹, NORA BACH², AHMED HASSANIEN¹, MASHOOD MIR¹, LUKAS NÖDING¹, SASCHA SCHÄFER², THOMAS BAUMERT¹, and ARNE SENFTLEBEN¹ — ¹University of Kassel, Institute of Physics, Kassel, Germany — ²University of Oldenburg, Institute of Physics, Oldenburg, Germany

We investigate the dynamics of photoexcited coherent acoustic phonon modes in a graphite- hexagonal boron nitride (hBN) heterostructure. Since the hBN layer is transparent at our excitation central wavelength

of 785 nm we assume that the optically induced stress pulse occurs mainly in the graphite layer. Subsequent lattice coupling to the hBN layer depends on the coupling strength at the bilayer interface and determines the nanomechanical resonance frequencies of the system. Observation of specific coherent acoustic phonon modes in the individual layers is interpreted within the framework of ultrafast electron diffraction [1] and experimental results are compared with numerical simulations based on a discrete numerical linear chain model [2].

[1] Gerbig, C., et al. *New Journal of Physics* 17.4 (2015): 043050.
 [2] Bach, N., and S. Schäfer, *Structural Dynamics* 8.3 (2021): 035101.

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Unraveling electron-phonon and exciton-phonon couplings in transition metal dichalcogenides. — ●AHMED HASSANIEN, ARNE UNGEHEUER, MASHOOD TARIQ MIR, LUKAS NÖDING, ARNE SENFTLEBEN, and THOMAS BAUMERT — University of Kassel, Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), D - 34132 Kassel, Germany

The observation of coherent phonons following resonant electronic excitation is a clear sign of the coupling between the electronic and the lattice degrees of freedom [1]. Using a highly compact femtosecond electron diffractometer developed in our group [2], we were able to differentiate between the electron-phonon and exciton-phonon couplings in mechanically exfoliated few-layers WSe₂. Based on our results, both free and bound charge carriers couple to the interlayer vibrational modes. Further analysis of our results unveiled the specific modes coupled to either type of charge carrier.

[1] Jeong, Tae Young, et al. *ACS Nano* 10.5 (2016): 5560-5566
 [2] Gerbig, C., et al. *New J. Phys.* 17.4 (2015):043050.

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Measuring ultrashort electron pulse durations by streaking with free electrons — ●LUKAS NÖDING, ARNE UNGEHEUER, AHMED HASSANIEN, MASHOOD TARIQ MIR, ARNE SENFTLEBEN, and THOMAS BAUMERT — Institute of Physics; Experimental Physics III, Kassel University

Ultrafast electron diffraction is a well-known method for time-resolved measurements on molecules and condensed matter. The duration of the electron pulse directly determines the temporal resolution of the UED setup as it works like the shutter speed of a camera. A streaking setup utilizing free electrons is implemented to measure the duration of the electron pulse. For this, a new measurement device was designed. It consists of an aperture and a metal surface behind the aperture, parallel to the path of the electron pulse. A femtosecond laser pulse is focused onto the metal surface. As the beam incides, electrons are released from the metal surface. Because of their momentum at first, they separate from the surface, create an electric field perpendicular to the surface and then recombine. This short-lived electric field is used to streak the electron pulse. The electron pulse at the front of the pulse should experience a different field strength than the electrons at the end. By that the duration of the pulse is mapped into a spatial extension of the pulse. The spatial and temporal overlap for the electron pulse and the laser beam had to be set exactly. The results are shown with their evaluation and compared to simulations.