# HL 7: Poster I

Topics:
- Functional semiconductors for renewable energy solutions
- Heterostructures, interfaces and surfaces
- Optical properties
- Organic semiconductors
- Perovskite and photovoltaics
- Quantum dots and wires

Time: Monday 13:00–15:00 Location: P2/EG

HL 7.1 Mon 13:00 P2/EG

**Investigation of the P-line in indium doped silicon with low temperature photoluminescence by applying an illumination and annealing cycle** — •Dominik Bratek, Katharina Peh, Kevin Lauer, Dirk Schulze, Stefan Krischok, Aaron Flötotto, and Robin Müller — Institut für Physik, Technische Universität Ilmenau, Weimarer Str. 32, 98693 Ilmenau, Germany

In recent years a photoluminescent feature called P-line is of rising interest for the current research [1,2,3] and, in combination with the so called ASiSii-defect model, may lead to an explanation of the infamous light induced degradation (LID) process in indium doped silicon [2,3]. In this contribution we show studies of indium implanted silicon by using low temperature photoluminescence (LTPL) spectroscopy. We investigate the LID cycle and it*s influence on the P-line and show a possibility to explained the observed behavior by the proposed energy diagram of the ASiSii-defect. In addition we present activation energies, determined during these investigations, which can be associated to ASiSii-defect transitions. [1] K. Terashima und T. Matsuda, Japanese Journal of Applied Physics 41 Part 1, No. 3A (2002). [2] K. Lauer, C. Möller, D. Schulze, and C. Ahrens, AIP Advances 5, 017101 (2015). [3] K. Lauer, C. Möller, C. Teßmann, D. Schulze and N. V. Abrosimov, physica status solidi, c 14.5 (2017).

HL 7.2 Mon 13:00 P2/EG

**Investigation of the influence of light-induced degradation on boron-doped silicon** — •Robin Lars Benedikt Müller, Katharina Peh, Kevin Lauer, Dirk Schulze, Stefan Krischok, Dominik Bratek, and Aaron Flötotto — TU Ilmenau

For Si-based devices like solar cells or radiation detectors, the light-induced-degradation (LID) in doped Czochralski Si is a profound issue. A reasonable explanation for the appearing LID process is the so-called ASi-Sii defect model [1,2], whose possible defect configuration manifests itself in indium-doped silicon by the appearance of the so-called P-line in the spectrum of low-temperature photoluminescence (LTPL) [3]. Comparatively, boron-doped Si does not exhibit a equivalent line, instead showing near the associated energy only the well-known electron-hole liquid (EHL) luminescence [4]. Therefore we investigate the influence of various treatments such as illumination, annealing or quenching on the LTPL spectrum of different boron-doped Si samples with emphasis on the behavior of the EHL. Additionally we present EPR studies on the impact of these treatments. [1]: Möller, C. et.al, (2013), Light-induced degradation in indium-doped silicon. Phys. Status Solidi RRL, 7: 461-464 [2]: Möller, C. et.al. , ASi-Sii-defect Model of Light-induced Degradation in Silicon, Energy Procedia, Volume 55, 2014, Pages 559-563 [3]: Lauer, K. et.al., "Identification of photoluminescence P line in indium doped silicon as InSi-Sii defect", AIP Advances 5, 017101 (2015) [4]: Peh, K. et.al., Low-Temperature Photoluminescence Investigation of Light-Induced Degradation in Boron-Doped CZ Silicon. Phys. Status Solidi A, 219: 2200180.

HL 7.3 Mon 13:00 P2/EG

**Atomic layer deposition of iron titanate for use as a photoanode** — •Nina Miller[1,2], Ryan Kisslinger[1,2], and Ian Sharp[1,2] — [1]Walter Schottky Institut Technical University of Munich — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany

$TiO_2$ is of significant importance in the field of energy research. However, to develop it for artificial photosynthesis, the band gap of $TiO_2$, which is 3.2 eV and consequently absorbs only ultraviolet light, must be paired with a material capable of absorbing visible light. Here, we experimentally explore the effect of depositing thin films of hematite ($\alpha$ - $Fe_2O_3$) on nanostructured $TiO_2$ using atomic layer deposition, with a further high-temperature annealing step to produce visible-light absorbing iron titanate ($Fe_2TiO_5$). Iron titanate may allow enhance charge transfer at the photoanode surface, and serve as a visible light absorbing layer. Furthermore, the $TiO_2$ nanotube arrays used as the substrate during atomic layer deposition can orthogonalize light absorption with respect to charge separation, leading to enhanced photocatalytic conversion during solar water splitting.

HL 7.4 Mon 13:00 P2/EG

**Polaron Transport in $BiVO_4$** — •Sven Doll, Tim Rieth, David Vogl, Viktoria F. Kunzelmann, Ian D. Sharp, and Martin S. Brandt — Walter Schottky Institut and School of Natural Sciences, Technische Universität München, 85748 Garching

Bismuth vanadate ($BiVO_4$) is a promising photoelectrode material for solar-to-fuel conversion. This semiconductor is particularly interesting considering its strong visible light absorption, efficient charge carrier separation, and favorable quasi-Fermi-level alignment with relevant redox potentials. However, temperature-dependent photoconductivity measurements indicate thermally-activated hopping transport of small polarons, with transport barriers of several hundred meV. To gain further insight into charge carrier transport and the nature of these polaronic states, we explore whether the hopping of the small polarons in $BiVO_4$ is spin-dependent using electrically detected magnetic resonance. Since such spin-dependent signals are known (e.g., from similar experiments on doped crystalline silicon) to critically depend on the charge carrier density, we evaluate the possibility to use the persistent photoconductivity of $BiVO_4$ to tune the polaron density. This technique may provide valuable insights into the microscopic transport processes in modern photoelectrodes used for energy conversion. This work was supported by the DFG under Germany's Excellence Strategy - EXC 2089/1 - 390776260.

HL 7.5 Mon 13:00 P2/EG

**In silico tuning the properties of inorganic-organic hybrid systems** — •Mohammed El Amine Miloudi and Oliver Kühn — Institute of Physics, Rostock University, Albert-Einstein-Str. 23-24 18059 Rostock

Two-dimensional (2D) materials are expanding the range of processes that can be studied in two dimensions as well as in van der Waals (vdW) heterostructures. Integrating organic molecules into these systems has enormous potential because nature offers a finite number of 2D materials. Still, an almost unlimited range of molecules can be tailored and synthesized with predictable properties. Organic compounds are widely known for their high absorption with low mobility and charge stability, whereas inorganic compounds have comparatively low absorption with excellent charge transport properties. Thus, the formation of vdW heterostructures that combines an inorganic compound with organic molecules potentially offers the advantages of both. Molybdenum disulfide (MoS2), one of the transition-metal dichalcogenides (TMDs), is one of the most exciting 2D semiconductors holding promises for potential applications in transistors, optoelectronics, and catalysis. Perylenes are widely used dyes whose optical properties can be tuned by chemical modification of the perylene core. Here we report on a systematic study of the structural, electronic, and optical properties of MoS2/perylene hybrid systems by means of density functional theory. Using different perylenes (perylene orange, perylene diimide, and perylene red) highlights the extent to which property tuning can be achieved in the hybrid system.

HL 7.6 Mon 13:00 P2/EG

**Epitaxial growth of GaN buffer layers on Si(111) by reactive**

**magnetron sputtering** — •Ralf Borgmann, Florian Hörich, Jürgen Bläsing, Anja Dempewolf, Frank Bertram, Jürgen Christen, Gordon Schmidt, Peter Veit, André Strittmatter, and Armin Dadgar — Otto-von-Guericke-Universität Magdeburg, FNW-IfP, Universitätsplatz 2, 39106 Magdeburg

GaN is a key material typically grown by MOVPE for high-voltage electronic devices. Reactive sputter epitaxy is an alternative to MOVPE, potentially offering much lower growth cost. Recently, we achieved high quality AlN layers on Si(111) [1] on which (Al,Ga)N layers can be grown. We present study on the effects of ammonia flow and growth temperature on GaN layer quality using MOVPE-grown GaN templates, high purity gases and targets. At Tgrowth ~705 °C and an ammonia flow of ~20 sccm, GaN shows a smooth surface and XRD (0002) $\omega$-FWHMs around 340 arcsec. AlGaN layers can be grown in a large composition range by Al- and Ga- co-sputtering resulting in very smooth surfaces. A sputtered 1.4 mum thick AlN/AlGaN/GaN layer stack on Si(111) shows high resistivity and a vertical breakdown field strength >2.5 MV/cm, ideal as buffer for transistor devices. [1] F. Hörich et al., Journal of Crystal Growth 571, 126250 (2021)

HL 7.7 Mon 13:00 P2/EG

**Molybdenum disulfide/diselenide deposition by radio frequency sputtering towards facile integration as heterojunction** — •Oscar Alberto Lopez Galan[1,2], Manuel Ramos[3], and Torben Boll[1] — [1]Institute of Applied Materials (IAM-WK), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopolshafen, Germany — [2]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopolshafen, Germany — [3]Instituto de Ingenieria y Tecnologia, Universidad Autonoma de Ciudad Juarez (UACJ), Ciudad Juarez, Mexico

The fabrication of heterojunctions using transition metal dichalcogenides remains a fundamental challenge in solid-state technology. In this work, we studied vertical MoS2/MoSe2 heterojunctions deposited by radio frequency sputtering at 3 thicknesses, 300 nm, 500 nm, and 600 nm. We found a dependency between thickness and crystal structure; the sample with a total thickness of 500 nm presents a crystal size of 64 nm while the thinner and thicker samples appear amorphous. Scanning electron microscopy and Raman spectroscopy reveal the presence of MoS2 and MoSe2 distinctly. Measurements by atom probe tomography indicate that MoS2 and MoSe2 are not having a sharp interface. This may influence the electrical performance of the device since dangling bonds and lattice mismatch between MoS2 and MoSe2 limit the charge carriers flow. Density functional calculations reveal a type-I heterojunction, with a reduced band gap of ~1.0 eV and a potential alignment of 0.5 eV.

HL 7.8 Mon 13:00 P2/EG

**Atomic structure of As-modified Si(100) surfaces prepared in CVD ambience** — Manali Nandy[1], Agnieszka Paszuk[1], Oleksandr Romanyuk[2], •Chris Yannic Bohlemann[1], Aaron Flötotto[3], Aaron Giess[1], Peter Kleinschmidt[1], Ivan Gordeev[2], Jana Houdkova[2], Erich Runge[3], and Thomas Hannappel[1] — [1]Fundamentals of Energy Materials, Institute of Physics, Ilmenau University of Technology, Ilmenau, Germany — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [3]Theoretical Physics 1, Institute of Physics, Ilmenau University of Technology, Ilmenau, Germany

For highly efficient III-V-on-Si devices, a low-defect III-V nucleation and a sharp interface are prerequisites. Stabilization of Si surfaces by arsenic is a promising technological step allowing to grow As-based III-V epitaxial layers in consecutive process steps. Here, we study the atomic structure of Si(100) surfaces prepared in As-rich ambiance utilizing MOCVD. Arsenic was supplied either directly via the precursor (TBAs) or indirectly as background $As_4$. The Si(100):As surfaces were analysed with a multitude of techniques such as STM, LEED, AR-XPS and FTIR after contamination-free transfer to ultra-high vacuum. The experimental results are supported by *ab initio* density functional theory (DFT) calculations. STM scans provide atomic-scale details of As-stabilized Si(100) surface structure consisting of rows of predominately asymmetric dimers. DFT simulations revealed a new stable structure with asymmetric As-Si-H dimers. The presence of hydrogen on the surface was confirmed by FTIR.

HL 7.9 Mon 13:00 P2/EG

**Preparation of P- and III-rich GaInP (100) with subsequential water & oxygen exposure** — •David Ostheimer, Mohammad Amin Zare Pour, Sahar Shekerabi, Agnieszka Paszuk, and Thomas Hannappel — Technische Universität Ilmenau, Ilmenau, Deutschland

III/V semiconductor multi-junction photoelectrochemical cells enable, either direct or indirect solar-to-fuel conversion with highest efficiencies to date, as their tunable bandgap enables optimal use of the solar spectrum. In tandem devices, GaInP has an appropriate bandgap for a top photoabsorber or a transparent, charge selective contact (window layer). A detailed understanding of the reactions at the semiconductor/electrolyte heterointerface is crucial to tailor the semiconductor surface appropriately to avoid trapping of the photogenerated charge carriers and reduce corrosion. Here, we study interaction of oxygen and water with the mixed-dimer, group-III-rich and phosphorus-rich GaInP (100) surface by combining in situ optical spectroscopy and in system photoelectron spectroscopy. The GaInP(100) surfaces were prepared by metal-organic chemical vapor deposition. The surface reconstruction of the as-prepared samples and after exposure was investigated by low energy electron diffraction. We find that the surface reconstruction of the GaInP(100) significantly affects its interaction with water. P-rich GaInP(100) surface shows much higher stability compared to the group-III-rich.

HL 7.10 Mon 13:00 P2/EG

**Band energy diagrams of n-GaInP/n-AlInP(100) surfaces and heterointerfaces** — •Mohammad Amin Zare Pour[1], Oleksandr Romanyuk[2], Dominik C. Moritz[3], Agnieszka Paszuk[1], Clément Maheu[3], Sahar Shekarabi[1], Kai Daniel Hanke[1], David Ostheimer[1], Thomas Mayer[3], Jan P. Hofmann[3], Wolfram Jaegermann[3], and Thomas Hannappel[1] — [1]Technische Universität Ilmenau, Ilmenau, Germany — [2]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [3]Technical University of Darmstadt, Darmstadt, Germany

n-AlInP(100) charge selective contacts are commonly grown on n-p GaInP(100) top absorbers in high-efficiency III-V multijunction solar or photoelectrochemical cells. Understanding the atomic and electronic properties of the GaInP/AlInP heterointerface is crucial for the reduction of photocurrent losses in multijunction devices. We investigated chemical composition and electronic properties of n-GaInP/n-AlInP heterostructures by X-ray photoelectron spectroscopy (XPS). 1-50 nm thick n-AlInP(100) epitaxial layers were grown on n-GaInP(100) buffer layer on n-GaAs(100) substrates by metal organic vapor phase epitaxy. We observed (2x2)/c(4x2) low-energy electron diffraction patterns on both AlInP(100) and GaInP(100) as-prepared surfaces. An upward surface band bending probably caused by localized mid-gap electronic states was observed. Pinning of the Fermi level by localized electronic states remained in n-GaInP/n-AlInP heterostructures. A valence band offset of +0.2 eV was derived by XPS and band diagram models for the n-n junctions were suggested.

HL 7.11 Mon 13:00 P2/EG

**GaAs/PEDOT:PSS Hybrid Solar Cell Improvement by the Incorporation of Ternary Quantum Dots** — •Alexander Ehm[1], Oleksandr Selyshchev[1], Serhiy Kondratenko[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, TU Chemnitz, Chemnitz D-09107, Germany — [2]Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine

Colloidal quantum dots (QD) have gained much interest over recent years due to their absorption and photoluminescence properties, which can be tuned by varying the particle size. Among these, ternary In-based chalcogenide QDs possess the advantage of low toxicity, making them more environmentally friendly candidates for the application in solar harvesting devices for green energy production.

As a prove of concept, colloidal AgInS and CuInS QDs [1] are deposited on n-GaAs(100) substrates in order to incorporate them in hybrid GaAs/PEDOT:PSS solar cells. The deposition is verified and analysed by X-ray photoemission and optical spectroscopy methods as well as atomic force microscopy. A significantly enhanced power conversion efficiency of such solar cells modified by colloidal QDs compared to the devices without QDs is shown by current density-voltage measurements under AM1.5 equivalent illumination.

[1] A. Raevskaya et al., J. Phys. Chem. C 2017, 121, 9032

HL 7.12 Mon 13:00 P2/EG

**One-dimensional topological interface states: a novel approach for optical pressure sensors** — •Jakob Lindenthal[1,2], Anton Widulla[1], Johannes Benduhn[1], and Karl Leo[1,2] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden — [2]ct.qmat - Würzburg-Dresden

Cluster of Excellence

The research field of nano-optics in connection with topological photonics has quickly evolved over the past decade. Topological considerations in the design of photonic systems open a wide range of possibilities for disorder protection and electric field alignment optimisation. Different material systems and topological setups are discussed in the context of pressure-sensitive nano-optical resonators, demonstrating a novel, highly versatile pressure sensor concept. The demonstrated system combines a compressible optical microcavity with an organic absorber material, which allows highly sensitive pressure-dependent tuning of the mode intensity. The contribution features modelling and characterisation results for systems with different topologies, showing pathways to significant topology-induced sensitivity enhancement. The use of coupled cavities is shown to provide additional sensing information with potential for industrial implementation.

HL 7.13 Mon 13:00 P2/EG

**Electric-field-induced second harmonic generation in amorphous materials for hybrid photonic structures** — •Laurids Wardenberg, Benito Bunk, and Jörg Schilling — Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

We investigate electric-field-induced second harmonic generation (EFISH) on different amorphous materials, e.g a-Si and $As_2S_3$ films. These materials have sizeable $\chi^{(3)}$ values but a vanishing $\chi^{(2)}$ due to their amorphous structure. Applying a dc-voltage we gain the ability to create a quasi-$\chi^{(2)}$ and perform second order nonlinear optical processes. The possibility to manipulate value and polarity of the created quasi-$\chi^{(2)}$ allows an unprecedented control over these second order wavelength conversion processes. Introducing a way to electrically modulate and switch this nonlinearity, is of high practical interest for the realization of nonlinear active hybrid photonic structures.

Since EFISH is strongly associated with the $\chi^{(3)}$, we use the z-scan technique to determine the real and the imaginary parts of the $\chi^{(3)}$ of the investigated films. Subsequently chromium contacts were deposited on the films and electric fields up to $10^5$ V/m were applied. Our voltage and intensity dependent SHG measurements show a quadratic dependence on input intensity and applied DC field, which is a clear indicator for EFISH. The nonlinear optical measurements are mainly performed at a wavelength of 1030 nm using a femtosecond laser system supplying 200 fs pulses at a repetition rate of 1 kHz. Additional measurements at wavelengths above 1200 nm, which are of interest for silicon photonics, will be demonstrated as well.

HL 7.14 Mon 13:00 P2/EG

**Excitons in lithium niobate and their impact on non-linear optical properties** — •Agnieszka Kozub, Wolf Gero Schmidt, and Uwe Gerstmann — Universität Paderborn, Department Physik, 33095 Paderborn, Germany

The influence of self-trapped and vacancy-trapped excitons on the lithium niobate ($LiNbO_3$, LN) dielectric function and nonlinear susceptibility is calculated based on density-functional theory. The PBE0 hybrid functional is used for the description of electron exchange and correlation. The dielectric function it obtained by solving the Bethe-Salpeter equation. This yields an absorption peak at 2.6 eV, in perfect agreement with experiment [1]. The second- and third order- nonlinear susceptibility tensors are obtained from a Berry-phase formulation of the dynamical polarization. A strong enhancement of the susceptibilities for photon energies in the band gap region is noted to arise from localized excitons.

[1] L.E. HALLIBURTON, K.L. SWEENEY and C.Y. CHEN, Nuclear Instruments and Methods in Physics Research Bl 344-347 (1984)

HL 7.15 Mon 13:00 P2/EG

**Structured Gradient Index Silicon (Oxy)Nitride Layers for Antireflection in Silicon Solar Cells** — •Florian Damerau[1], Maria Gaudig[1], Ralf Wehrspohn[1], Prerak Dhawan[2], Carsten Rockstuhl[2], and Alexander Sprafke[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale), Germany — [2]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

The frontside of crystalline silicon (c-Si) solar cells oftentimes is micro- or nanotextured to increase light in-coupling, and thus conversion efficiency. Current state-of-the-art textures comprise micron sized pyramidal structures, whereas future ultrathin c-Si solar cells demand new approaches such as submicron nanophotonic structures. However, directly nanotexturing the Si surface degrades its electronic properties strongly, such that a possible gain in absorption does not necessarily translate into an increased conversion efficiency. In this work, we aim to maintain the electronic properties of a planar c-Si interface by leaving it intact but place a nanophotonic structure on top. This structure consists of a nanstructured SiOxNy layer. Moreover, changing the stoichiometry (x,y) during deposition enables us to smoothly vary its refractive index between $n \approx 1.5 - 3.0$. Inspired by transformation optics, we aim to mimic the optical properties of strongly non-planar textures such as black silicon by a planar layer of smoothly varying spatial-dependant refractive index. In this contribution we will present experimental results on the microstructure as well as on the optical properties of our fabricated structures.

HL 7.16 Mon 13:00 P2/EG

**Exciton-polariton emission in copper halides** — •E. Krüger[1], S. Merker[2], S. Blaurock[2], R. Hildebrandt[1], A.L. Pereira[1], L. Käferstein[1], H. Krautscheid[2], M. Grundmann[1], and C. Sturm[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany — [2]Universität Leipzig, Institut für Anorganische Chemie, Germany

Copper halides (CuI, CuBr, and CuCl) have recently attracted research interest since they combine intrinsic p-type conductivity with large bandgaps (3.1 eV - 3.4 eV) and high exciton binding energies (62 meV - 190 meV), making them promising candidates for applications in transparent optoelectronics [1].

Here, we present an overview of the optical properties of solution grown Cu-halide bulk single crystals, focusing especially on spectral- and time-resolved measurements of the near-band-edge luminescence for temperatures between 10 K and room temperature. The line shape of the emission lines at low temperatures is interpreted in terms of exciton-polaritons and their dispersion relation [2]. The different decay characteristics of free and localized states are explained by their coupled interaction. In addition to observation of an anomalous temperature-dependent bandgap shift to higher energies with increasing temperature we present in detail the temperature-dependent decay characteristics of the polariton emission and discuss the corresponding relaxation mechanisms.

[1] M. Grundmann et al., pss (a) **210**, 1671 (2013)
[2] E. Krüger et al., APL Mater. **9**, 121102 (2021)

HL 7.17 Mon 13:00 P2/EG

**Persistent spectral holeburning of the donor-bound exciton transition in ultra-pure $^{28}$Si:P** — •Nico Eggeling[1], Michael Oestreich[1], Eduard Sauter[1], Jens Huebner[1], and N. V. Abrosimov[2] — [1]Leibniz Universität Hannover, Germany — [2]IKZ Berlin, Germany

We utilize persistent spectral hole burning to determine the origin of dynamic and static spectral broadening of the donor-bound exciton transition in ultra-pure $^{28}$Si:P with 99.995% isotopic enrichment [1]. From time-dependent measurements of the spectral hole width and frequency shift we try to determine the impact of donor-acceptor interaction on the spectral transition broadening. The donor-acceptor pair recombination is on the order of seconds in the investigated sample with a donor concentration of $1.2 \times 10^{15}\mathrm{cm}^{-3}$ and an acceptor concentration of estimately $4.6(10) \times 10^{13}\mathrm{cm}^{-3}$. We expect to observe an impact of the recombination dynamics on the measured frequency and width of spectral holes. These results could lead to a better understanding of spin initialization for donors in $^{28}$Si:P, which are a promising candidate for quantum computation [2].

[1] Sauter, E., Abrosimov, N. V., Hübner, J., & Oestreich, M., Phys. Rev. Lett. **126(13)**, 137402 (2021).
[2] Morello, A. et al., Adv. Quant. Tech. **3(11)**, 2000005 (2020).

HL 7.18 Mon 13:00 P2/EG

**Manipulating the luminescence of a rare-earth doped spacer** — •Sören Lerner[1], Francesco Vitale[1], Thomas Siefke[2], Uwe Zeitner[2,3], and Carsten Ronning[1] — [1]Institute of Solid State Physics, Friedrich-Schiller Universität, Helmholtzweg 3, 07743 Jena, Germany — [2]Institute of Applied Physics, Friedrich Schiller Universität, Albert-Einstein-Straße 15, 07745 Jena, Germany — [3]Fraunhofer Institute for Applied Optics and Precision Engineering IOF, Albert-Einstein-Straße 7, 07745 Jena, Germany

The coupling of rare-earth elements with surface plasmon polaritons can lead to a change of their emission properties. We implant rare-earth elements in a nanometric silica spacer on top of an aluminum layer by ion beam implantation. The luminescence properties of such systems were examined by photo- and cathodoluminescence measure-

ments. Placing zinc oxide nanowires on top of this two-layer system allows for additional coupling with surface plasmon polaritons, which generate a high electric field density in the spacer layer. The respective effects and the possibilities of tailoring the emission will be discussed.

HL 7.19 Mon 13:00 P2/EG

**Coupling of Excitons and Plasmons with Phonons in Raman scattering for 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

CuI is an intrinsic p-type with potential for opto-electronic applications. Via resonance effects, various of its fundamental properties may be accessed. For CuI we investigate phonon-exciton- and phonon-plasmon-interactions by Raman spectroscopy.

We present Raman spectra with excitation wavelength of 532 nm, 355 nm and 325 nm for single crystals and thin films. Each excitation wavelength indicates different fundamental Raman scattering processes. With 532 nm fundamental modes as well as second order Raman singals are observed and analyzed [1]. For doped samples with $p = 10^{18}\,\mathrm{cm}^{-3}$, phonon-plasmon coupling is observed which is compared with Hall measurements. By 355 nm excitation, slightly above the bandgap, a phonon damped-plasmon mode coupling modifies the Raman spectra [2]. Finally with a 325 nm a transition close to $\mathrm{E_g}+\Delta_0$, indicates a cascade exciton scattering process. This is dominated by the Fröhlich interaction and n-LO overtones up to $n = 7$ are observed [3]. For each excitation wavelength, an overview of possible applications and possible limits for CuI is shown.

[1] J. Birman, J., Phys. Rev., **131**, 1489, 1963.
[2] A. Mlayah *et al.*, J. Appl. Phys., **69**, 4064, 1991.
[3] Y. Zhang, J. Semicond., **40**, 091102, 2019.

HL 7.20 Mon 13:00 P2/EG

**Raman spectra of CuI alloys with Ag and Br** — •A.L. Pereira[1], R. Hildebrandt[1], J. Bredow[1], C. Dethloff[1], V. Gottschalch[2], S. Vogt[1], H. Krautscheid[2], M. Grundmann[1], and C. Sturm[1] — [1]Universität Leipzig, Felix Bloch Institute for Solid State Physics, 04103 Leipzig, Germany — [2]Universität Leipzig, Institute of Inorganic Chemistry, 04103 Leipzig, Germany

CuI is a p-type semiconductor with a wide band gap of 3.1 eV that has potential for (opto-) electronic applications [1]. By alloying CuI with isoelectronic Ag or Br its properties such as e.g. the charge carrier concentration, lattice constant or band gap can be tuned.

We present our investigations on CuI alloys and their phonon properties with Raman spectroscopy. $\mathrm{Ag}_x\mathrm{Cu}_{1-x}\mathrm{I}$ and $\mathrm{CuBr}_x\mathrm{I}_{1-x}$ (both $0 \leq x \leq 1$) thin films were produced with various deposition techniques such as solid-state reaction, close distance sublimation, sputter deposition and pulsed laser deposition. Raman spectroscopy measurements were conducted at low temperatures and the phonon modes were analyzed regarding their energetic position, broadening and intensity. This was supported by an oscillator strength model [2]. The Cu(Br,I) alloy revealed a nonlinear dependence of the Raman shift on the composition. In the (Ag,Cu)I alloy an apparent three-mode behavior due to a defect mode was observed and characterized.

[1] E. Krüger, *et al.*, Appl. Phys. Lett. 113, 172102, 2018.
[2] G. Livescu, *et al.*, J. Phys. C: Solid State Phys. 19 2663, 1986.

HL 7.21 Mon 13:00 P2/EG

**Excited-state properties of PbWO4 from ab initio calculations** — •Ather Ahmad and Kai-Thomas Brinkmann — II. Phys. Inst. Gießen

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. the CMS at the LHC in CERN. New generation crystals (PWO-II) with improved properties were developed for the PANDA experiment at FAIR in Darmstadt. To reduce absorption of the scintillation light within the crystals, the lead tungstate is doped with Lanthanum and Yttrium. This results in a change of the electronic and optical properties.
In order to assess the functionality of the calorimeter, we first need to analyse these electronic and optical properties of lead tungstate. In our work, we investigate these properties of lead tungstate containing different impurities and defects with ab initio calculations to derive its radiation hardness and scintillation mechanism.

This project is supported by HFHF and HGS-hire

HL 7.22 Mon 13:00 P2/EG

**Multiphoton absorption induced photoluminescence in CuI** — •Andreas Müller[1], Sebastian Henn[1], Evgeny Krüger[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

Two- and three-photon absorption induced photoluminescence (2PAPL, 3PAPL) are nonlinear optical processes useful for energy upconversion or, in contrast to near-to-the-surface single-photon absorption, excitation within the bulk material.

In this work, we report on low temperature (30 K) 2PAPL and 3PAPL in transparent conducting CuI crystals ($E_g = 3.1\,\mathrm{eV}$), analyzed employing excitation energy and density-dependent, steady-state, and time-resolved photoluminescence. Using an excitation energy that corresponds to half of the bandgap energy, the observed intensity dependence on the excitation power shows an almost parabolic behavior. By a further reduction of the photon energy, the cubic contribution of the excitation power on the intensity increases, and for low excitation energies, an almost cubic behavior is obtained. We describe the experimental findings, taking into account the sum of the two- and three-photon transition rates and including the Gaussian spectral intensity distribution of the laser. Through this analysis, the ratio of the cross-sections for the two- and three-photon absorption is estimated to be $10^{-5}\,\mathrm{cm}^2/\mathrm{s}$.

HL 7.23 Mon 13:00 P2/EG

**Optical properties of the organic semiconductor Dimethylanthradithiophene (DMADT)** — •Anncharlott Kusber and Martin Knupfer — IFW Dresden, Helmholtz Straße 20, D-01069 Dresden, Germany

This work presents an analysis of the optical properties of anti- and syn-dimethylanthradithiophene. We have produced 120 nm thick thin films by physical vapour deposition. Using optical spectroscopy, we were able to characterize the films in the visible range. Davydov splitting, due to the existence of two molecules in the unit cell, was observed. Besides that, we measured the exciton dispersion by using electron energy-loss spectroscopy. There we found a positive dispersion of the lowest lying excitation. Comparing the measured values and the calculated coupling strengths, we came to the conclusion that both materials are very weak J-aggregates and that charge transfer exciton coupling is the dominant process and determines the delocalization of the lowest lying excitations.

HL 7.24 Mon 13:00 P2/EG

**Highly dipolar molecule on single crystals: Impact of chemical affinity on the interface formation** — •Baris Öcal and Selina Olthof — Department of Chemistry, University of Cologne, Greinstraße 4-6, 50939 Cologne, Germany

Merocyanines are functional dyes with interesting electronic properties due to their resonant structure between charged and uncharged states. Their bandgap can be widely tuned via the donor and acceptor strength, which makes them interesting as active material in organic-based solar cells, especially since they show very strong absorption. Their physical properties can be further improved by ordering them. The ordering of the molecules is closely related to initial growth on the substrate underneath and interaction between this substrate and molecule. In my work, I investigate the effect of substrate/molecule and molecule/molecule interactions on the electronic structure by photoelectron spectroscopy methods. Highly dipolar HB238 merocyanine has been chosen to observe the chemical interaction and its effect of the charge states of the molecule easier. Surfaces such as SiC/graphene, Au(100), Ag(100) and Cu(100) are used as templating substrates due to their different chemical affinity and ordered structure. Thickness dependent X-ray Photoelectron spectroscopy (XPS) measurements helps us to understand the chemical effect of substrate on the charge states, while Ultraviolet Photoelectron Spectroscopy (UPS) measurement gives information on the molecular phase changes such as dimerization, orientation change. We find that chemical interaction of the substrate significantly affects molecule/molecule interaction.

HL 7.25 Mon 13:00 P2/EG

**Spontaneous orientation polarization in phosphine oxides and how to control it** — •Albin Cakaj, Markus Schmid, Alexander Hofmann, and Wolfgang Brütting — Institut für Physik, Universität Augsburg, Germany

The orientation of small organic molecules in amorphous thin films prepared by vapor-deposition is an important aspect in further improvement of organic semiconductor devices. This feature can influence the optical and electrical properties of organic light emitting diodes (OLEDs) drastically. Due to their asymmetric molecular structure, microscopic properties like the permanent dipole moment (PDM) can show preferential alignment and lead to a macroscopic film polarization in the organic layer. This so-called spontaneous orientation polarization (SOP) affects the charge injection and accumulation behaviour in a device. In our studies, we investigated the electrical and optical orientation of a group of organic molecules, characterized by P=O double bonds, and how to control it by their design and the film-growth conditions. Many of these phosphine oxides have a large PDM, due to a strong electronegative oxygen. However, the magnitude of their SOP is often affected by the presence of multiple molecular conformers. Thus, using less polar species with only one P=O bond yields superior performance with record-high SOP of up to 160mV/nm, even though optical measurements hint to almost no preferred orientation on average.

HL 7.26 Mon 13:00 P2/EG

**Impact of solution processing on the photophysical properties of TADF emitters** — •Konstantin Rausch, Rishabh Saxena, and Anna Köhler — Soft matter Optoelectronics, University of Bayreuth, Germany

Continuous innovation of thermally activated delayed fluorescence (TADF) compounds has led to the rapid development of these materials as emitters in efficient vacuum-deposited organic light emitting diodes (OLEDs). However, the cost of device fabrication, inefficient use of materials and limitation on pixel size are some detracting features of vacuum-deposition. An alternative cost- and materials-efficient fabrication technique is solution processing. In this regard, it is important to understand the impact of different processing conditions, such as varying solvents and host materials, on the photophysical properties of TADF emitters. In general, a donor-acceptor (D-A) strategy is adopted for the chemical design of TADF emitters. Recent studies suggest that conformational flexibility associated with the D-A dihedral angle leads to a distribution of reverse intersystem crossing rates (k_RISC); a parameter that determines the efficiency of the TADF process. In this study, we perform inverse Laplace transform fitting of emission decay, obtained using time-resolved photoluminescence measurements, to extract this distribution. Furthermore, we investigate the impact of different film-preparation methods (spin-coating and evaporation), matrix polarity and conformational rigidity of TADF emitter on the RISC rate distribution with an aim to optimize the performance of solution-processed TADF OLEDs.

HL 7.27 Mon 13:00 P2/EG

**single molecule spectroscopy of emitters in hexagonal boron nitride(hBN)** — •osama farooqui and klas lindfors — department of chemistry, university of cologne

Efficient interaction of light with atoms or molecules has been found crucial in the study of materials that can be used in the development of high-speed communication devices [1]. The central goal of this project is to observe and investigate the light emission and absorption processes in heterostructures of two- and one-dimensional materials and single emitter molecules.

Previously, single terrylene diimide (TDI) molecules on glass substrate have been investigated using single molecule spectroscopy. In order to address the problem of stability of the molecules, hBN is used to encapsulate emitter molecules to avoid chemical reactions with the ambient environment. The preliminary data of time traces of triisopropylsilyl pentacene (TIPS-pentacene) molecules encapsulated in hBN flakes shows that the molecules do not get photobleached over 1 hour at room temperature. However, fast photoblinking was observed in the time traces of the molecules. The cause of fast photoblinking could be the interaction of the molecules with close-by two-level systems, which appears to be related to hBN flakes.

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

HL 7.28 Mon 13:00 P2/EG

**Electronic and optical properties of p-type delafossite transparent conducting oxides: Density Functional Theory calculations** — •Moufdi Hadjab[1,2] and Olga Guskova[2] — [1]Mohamed Boudiaf University of Msila, Msila, Algeria — [2]IPF Dresden, Germany

Transparent conducting oxides (TCO) possessing high optical transparency and electrical conductivity have been studied widely due to their applications in optoelectronics. Delafossite materials with chemical formula AIBIIIO2 are among the promising p-type TCOs. In this study, we have investigated physical properties of three novel semiconductors to address some problems related to the photovoltaic industry. The structural, electronic and optical properties of delafossite transparent conducting oxides CuMO2 have been studied using the Full-Potential Linearized Augmented Plan Wave method based on DFT as implemented in Wien2k computational code. The LDA and PBE generalized gradient approximation have been utilized as the exchange-correlation term for calculating the structural and electronic parameters. Moreover, Tran-Blaha modified Beck-Johnson potential has been used to achieve better degree of accuracy in calculations of the electronic and optical properties. The observations have been compared with published theoretical and experimental data. The ternary delafossite transparent conducting oxide compounds can be considered as an alternative material in photovoltaic applications.

HL 7.29 Mon 13:00 P2/EG

**Simulating multi-component target ablation: A new pulsed laser deposition technique** — •Arne Jörns, Holger von Wenckstern, and Marius Grundmann — University of Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group

Laterally and radially segmented targets allow the fabrication of functional thin films with lateral and vertical composition spreads, respectively [1]. The latter also enables the creation of material libraries consisting of homogeneous thin films with discrete material composition. However, fabrication of such targets is technically demanding with respect to powder blending, insufficient hardening or thermic decomposition due to deviating sintering temperatures of the source powders for the respective segments.

In this work we present a new target design and deposition technique for pulsed laser deposition in order to create vertical composition spreads as well as discrete composition material libraries but bypassing the above mentioned drawbacks. Simulations for the expected material contents will be presented. Then, experimentally determined elemental distributions and growth rates are compared to calculated values. Electrical and optical properties of samples obtained by such techniques will be reported.

[1] H. von Wenckstern et al.,Phys. Status Solidi 2020, 257, 1900626

HL 7.30 Mon 13:00 P2/EG

**Wide bandgap aeromaterials and prospects for their applications** — •Vladimir Ciobanu, Tudor Braniste, Eduard Monaico, and Ion Tiginyanu — National Center for Materials Study and Testing, Technical University of Moldova, Chisinau, Moldova

We report on the fabrication of aeromaterials based on GaN, Ga2O3, TiO2 and Zn2TiO4 using hydride vapor phase epitaxy (HVPE) or Atomic Layer Deposition (ALD) approaches. The fabrication process is based on growth of the preferred material on sacrificial templates consisting of interconnected ZnO microtetrapods. During the epitaxial growth of GaN at high temperatures and corrosive environment, the ZnO is etched away and, consequently, hollow microtetrapods with the wall thickness of the tubes in the range of 20 - 100 nm are obtained. Further, GaN can be transformed into Ga2O3 through an annealing process at temperature as high as 800 °C. Alternatively, ALD approach is used to fabricate aero-TiO2 or aero-Zn2TiO4 materials using sacrificial ZnO templates.

The fabricated materials demonstrated new interesting properties: aero-GaN exhibits good electromagnetic shielding in X-band and THz region, on the other hand aero-Ga2O3 is completely transparent at GHz and THz frequencies, up to 3 THz. We also established that aero-GaN is characterized by dual hydrophilic-hydrophobic behavior. This phenomenon enabled one to demonstrate novel liquid marbles. Due to high active surface area of developed aero-Ga2O3 decorated with noble metal nanodots, aero-TiO2 and aero-Zn2TiO4, these materials are shown to be promising for photocatalytic applications.

HL 7.31 Mon 13:00 P2/EG

**Graded $Zn_xMg_{1-x}O$ layers as building blocks for ultra-compact wavemeters** — Philipp Firme, •Christoph Brunhuber, Lukas Trefflich, Peter Schlupp, Daniel Splith, Holger von Wenckstern, Chris Sturm, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, 04103 Leipzig, Germany

Recently, a new design for a monolithic, ultra-compact wavemeter was proposed, which can be used in a wide spectral range [1]. The building blocks of this wavemeter are two vertically stacked, photosensitive layers, separated by a transparent, insulating layer. In order to achieve a spectral sensitivity, the top layer must consist of a material with a vertical absorption gradient. Here, we discuss the suitability of vertically graded $Zn_xMg_{1-x}O$ layers as top layer of such an ultra-compact wavemeter with wurtzite photosensitive ZnO layer as backside. The layers were deposited by pulsed laser deposition, using a vertical continuous composition spread (VCCS-PLD) technique. In doing so, we were able to achieve out-of-plane composition gradients from $x = 1.0$ up to $x \approx 0.5$. XRD $2\theta - \omega$-scans do not indicate a phase separation, and confirm the wurtzite phase. The Mg incorporation was also confirmed by photoluminescence spectroscopy. The suitability of the films as building blocks for the wavemeter was tested by photocurrent measurements. By radiation with monochromatic light of different wavelengths, a response similar to the theoretically calculated one [1] is obtained.

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

HL 7.32 Mon 13:00 P2/EG

**Synthesis of bismuth ferrite hollow spheres and their application in the photocatalytic degradation of dyes** — •Valeria Sanchez[1], Thomas Cadenbach[2], Alexis Debut[3], Karla Vizuete[3], and Maria J. Benitez[1] — [1]Departamento de Física, Facultad de Ciencias, Escuela Politécnica Nacional, Ladrón de Guevara E11-253, Quito, Ecuador — [2]Colegio de Ciencias e Ingenierías, Universidad San Francisco de Quito, Diego de Robles y Vía Interoceánica, Quito, Ecuador — [3]Centro de Nanociencia y Nanotecnología, Universidad de las Fuerzas Armadas ESPE, Av. Gral. Rumiñahui s/n, Sangolquí, Ecuador

In this work, we show the synthesis and application of next generation semiconductor photocatalysts, i.e. GdxBi1-xFeO3 (x = 0, 0.05. 0.10, 0.15) hollow spheres which function as both, an advanced adsorption material and photocatalytic active semiconductor. The presented spheres were prepared by two distinct novel synthetic protocols, i.e. via a citric acid/urea/ethylene glycol assisted hydrothermal method and via an evaporation induced self-assembly strategy. In both cases, we study the mechanism of formation of phase pure GdxBi1-xFeO3 hollow spheres with a narrow size distribution by varying synthetic conditions such concentration, temperature and treatment time. The samples were characterized by X-ray powder diffraction, scanning electron microscopy and UV-vis diffuse reflectance spectroscopy. All synthesized materials were applied in the photocatalytic degradation of dyes under visible light irradiation. The photocatalysts show superior efficiencies which outperformed previously reported BiFeO3 materials.

HL 7.33 Mon 13:00 P2/EG

**Monitoring Phase Transitions in (Hot-)Pressed $FAPbI_3$ Films by In-Situ Reflection Measurements** — •Lorenz Kiel[1], Christina Witt[1], Konstantin Schötz[1], Nico Leupold[2], Ralf Moos[2], Anna Köhler[1], and Fabian Panzer[1] — [1]Soft Matter Optoelectronics, University of Bayreuth, Bayreuth 95440, Germany — [2]Department of Functional Materials, University of Bayreuth, Bayreuth 95440, Germany

In recent years, a remarkable increase in efficiencies of halide perovskite-based solar cells has been achieved. Record cells on laboratory scale, realized with the perovskite formamidinium lead iodide ($FAPbI_3$), are now competing with established silicon devices.[1] However, phase stability of $FAPbI_3$ is still challenging as the photoactive black $\alpha$-phase is prone to degrade in the inactive yellow $\delta$-phase or intermediate orange and red phases.[2, 3] To address this issue, we evaluate the temperature and pressure dependence of occurring phase transitions using in-situ reflection measurements during (hot-)pressing $\delta$-$FAPbI_3$ powder, and analyze associated strain in the resulting thick films. We show that for our powder based thick films the phase transitions occur at significantly lower pressure and temperature compared to literature reports. The correlation of these parameters with resulting film properties like film morphology suggests strain to be decisive for the phase transition and phase stability.

[1] Jeong et al. Nature 2021, 592.
[2] Cordero et al. Nanomaterials 2021, 11.
[3] Cordero et al. J. Phys. Chem. C 2020, 124.

HL 7.34 Mon 13:00 P2/EG

**Phase diagram of two-dimensional ferroelectric large polarons** — •Florian Kluibenschedl, Georgios Koutentakis, and Mikhail Lemeshko — Institute of Science and Technology Austria (ISTA), Am Campus 1, 3400 Klosterneuburg, Austria

We present a minimal, coarse-grained, two-dimensional model of charge transport in lead halide perovskites, which provides an intuitive explanation for the recently proposed formation of ferroelectric large polarons [1]. The phase-diagram analysis reveals the presence of three phases characterized by the distinct order of the molecular dipole moments which is strongly dependent on the tunneling anisotropy of the carriers. The most striking outcome is the formation of ferroelectric domains that amplify the anisotropy in the carrier tunneling dynamics which has been argued to lead to improved optoelectronic properties. These results provide the groundwork for realizing a top-down approach for understanding the complex carrier dynamics in hybrid organic-inorganic perovskites.

[1] F. Wang, Y. Fu, M. E. Ziffer, Y. Dai, S. F. Maehrlein, and X.-Y. Zhu. Journal of the American Chemical Society 2021 143 (1), 5-16. DOI: 10.1021/jacs.0c10943

HL 7.35 Mon 13:00 P2/EG

**Optical spectroscopy on hBN-encapsulated perovskites** — •Lisa Böhme, Eugen Klein, Rico Schwartz, Christian Klinke, and Tobias Korn — University of Rostock, Institute of Physics, 18059 Rostock, Germany

Perovskites shows promising optoelectronic properties that can be used in a wide range of technologies. For example, they play a central role in the development of more efficient and low-cost solar cells and are also used in LED or low-threshold lasers. However, they pose experimental challenges that need to be solved: perovskites degrade in contact with air and lose their attractive properties. A possibility to avoid this is encapsulation in hexagonal Boron Nitride (hBN). We have examined how lead-halogen perovskites with organic ligands can be encapsulated and whether they retain their stability. We use the Scotch-Tape method to exfoliate hBN crystals and deposit perovskite crystals on top using drop casting. To check the successful encapsulation of the perovskites, photoluminescence measurements were taken over different time periods and at different temperatures. Our measurements showed that the fully encapsulated perovskites remained stable for more than ten days.

HL 7.36 Mon 13:00 P2/EG

**Reflection Electron Energy Loss Spectroscopy of Organic and Perovskite Semiconductors** — •Seren Dilara Öz and Selina Olthof — Department of Chemistry, University of Cologne, Greinstraße 4-6, 50939 Cologne, Germany

The analysis of fundamental semiconductor properties, such as energy level positions and bandgaps, are important to enhance our understanding of these materials and to further improve their performance in applications. In this context, many spectroscopic tools such as ultraviolet photoelectron spectroscopy or UV-vis measurements are exploited. In this project, we explore the use of reflection electron energy loss spectroscopy (REELS) which is a rarely used technique in order to investigate the surface density of states (DOS) and bandgap of organic and perovskite based semiconductor materials.

This measurement technique records the energy loss due to inelastic electron scattering processes which excites electronic transitions. It presents an intriguing technique to gain insights on the joint valence and conduction band density of states over a wide energy range. Due to the extreme surface sensitivity, the band gap of ultra-thin layers can be accessed.

In this work, we try to understand the observed energy loss spectra in order to establish guidelines to investigate surface properties of semiconductor materials. For that reason, information gathered using REELS are compared to UPS, IPES, and UV-vis measurements. Our results show that the REELS technique can be used as an effective tool to explore surface properties of perovskite and organic semiconductors.

HL 7.37 Mon 13:00 P2/EG

**Combinatorial synthesis of $BaZrS_3$ thin films: Influence of off-stoichiometry on optoelectronic and electronic properties** — •Adriana Röttger, Marin Rusu, Hannes Hempel, Daniel Abou-Ras, Orestis Karalis, Ibrahim Simsek, and Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Deutschland

The chalcogenide perovskite $BaZrS_3$ is composed of earth-abundant elements and has potential applications for photovoltaic energy conversion. In this work, compositionally graded $BaZrS_3$ thin films are synthesized from oxide precursors deposited by pulsed laser deposition.

The compositional gradient in a range of 0.8<[Ba]/[Zr]<1.3 enables a high throughput characterization approach of structural, optical and optoelectronic properties. Sulfurization was performed in a tube furnace using $H_2S$ in Ar gas at 1000°C. For all the examined compositions, $BaZrS_3$ forms as the main phase. Under Ba excess, Ruddlesden-Popper phases $Ba_3Zr_2S_7$ and $Ba_4Zr_3S_{10}$ emerge, while excess Zr forms $ZrO_2$ on the Zr-rich side. Optical absorption spectroscopy mapping shows that the band-gap energy exhibits a minimum at $1.0 < [Ba]/[Zr] < 1.1$ and ranges from 1.65 to 2.1 eV. Analysis of the optical constants $n$ and $k$ by ellipsometry mapping verified this trend. Low-temperature photoluminescence spectroscopy revealed deep defect states present for all compositions. Using time-resolved photoluminescence spectroscopy and optical -pump-terahertz probe spectroscopy, we found longer carrier lifetimes on the Ba-rich side, while the Zr-rich side features a higher mobility of charge carriers.

HL 7.38 Mon 13:00 P2/EG

**Defect tolerance of halide perovskites solar absorbers via machine learning** — •Anoop K. Chandran[1], Christoph Friedrich[1], Uwe Rau[2], Stefan Blügel[1], Thomas Kirchartz[2], and Irene Aguilera[3] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [2]IEK5-Photovoltaik, Forschungszentrum Jülich, Germany — [3]Institute of Physics, University of Amsterdam, The Netherlands

The deformation potential measures the changes in the bandgap of materials upon compression of the bonds, which helps to identify the bonding or anti-bonding nature of the valence and conduction bands. Previous works indicate that the bonding or anti-bonding nature impacts a material's tendency to exhibit shallow or deep intrinsic defect levels. Our high-throughput search is based on all-electron density functional theory calculations. Among 1173 studied halide perovskites, only 18% present a favourable anti-bonding valence band. We also establish the calculation of the deformation potential as an effective way to determine the bonding or anti-bonding nature near the band edges. However, subsequent supercell calculations reveal no explicit connection between the nature of the band edges and the defect tolerance. Deep learning neural networks require large datasets. To overcome this limitation, we devised a novel approach for the one-shot binary classification of the deformation potentials. Instead of learning to classify a single material, the network learns the similarity or the difference between two materials.

HL 7.39 Mon 13:00 P2/EG

**Dressed-state analysis of two-color excitation schemes** — •Thomas Bracht[1,2], Tim Seidelmann[3], Yusuf Karli[4], Florian Kappe[4], Vikas Remesh[4], Gregor Weihs[4], Vollrath Martin Axt[3], and Doris E. Reiter[2] — [1]Institut für Festkörpertheorie, WWU Münster, DE — [2]Condensed Matter Theory, TU Dortmund, DE — [3]Theoretische Physik III, Universität Bayreuth, DE — [4]Institut für Experimentalphysik, Universität Innsbruck, AT

For coherent control of a few-level quantum emitter, typically pulses with an energy resonant to the transition energy are used, which requires sophisticated filtering of the signal. However, two-color excitation protocols were recently employed to circumvent the necessity for filtering.

Here I present an analysis of two-color excitation schemes, using the laser dressed states of the system. It can be shown, that the two-color excitation approach can be understood as a driving of transitions between the dressed states. We investigate how these transitions depend on the pulse parameters and explain how the different combinations of laser energies can excite the system. In addition to the results for a simple two-level system (2LS), we consider a three-level exciton-biexciton system (3LS) that is typically found in semiconductor quantum dots and often used to generate entangled photon pairs. While in the 2LS, we can give clear conditions for the applicability, in the 3LS, due to strong state mixing, the conditions are less obvious. Nonetheless, we can find regimes of parameters to drive the system into either the exciton or the biexciton in the 3LS.

HL 7.40 Mon 13:00 P2/EG

**Controlling the dimensions of top-down GaN nanowire ensembles via self-assembled metal islands** — •Rose Mary Jose, Jingxuan Kang, Miriam Oliva, Thomas Auzelle, Abbes Tahraoui, Oliver Brandt, and Lutz Geelhaar — Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany

The large surface-to-volume ratio of semiconductor nanowires and their potential for enhanced light absorption are attractive for photoelectrochemical applications. In this context, large-scale nanowire arrays are needed. For top-down fabrication, a scalable and rapid way to form a nano-island mask is the dewetting of a metal film.

In this work, we study how Pt films evolve upon thermal treatment into nano-islands which serve as a shadow mask for the top-down etching of GaN nanowire ensembles. To gain control over the nano-island ensembles' dimensions, we explore variations of the annealing conditions, Pt film thickness, and the surface energy by investigating Pt dewetting on GaN, SiNx, and SiOx surfaces. The islands' size and density are determined by the initial Pt film thickness. However, nano-island diameter and spacing are coupled by a fixed ratio. Therefore, individually controlling the spacing between nano-islands and their diameter is challenging in this approach.

Nanowire arrays are fabricated using Pt dewetting masks by plasma etching followed by KOH wet etching. The resulting nanowires' dimensions are consistent with those of the original nano-islands. In our experiments, diameters in the range 30 nm-200 nm and lengths of 500-1000 nm are demonstrated.

HL 7.41 Mon 13:00 P2/EG

**Investigation of SiNWs [100] and [111] applying DFT with doping** — •Nedhal Al-Nuaimi, Hilser Florian, and Gemming Sibylle — Chemnitz University of Technology, Chemnitz (Germany)

We present an ab initio study of Silicon nanowires (SiNW) with p-type impurities (doping) of Boron (B) and n-type impurities of Phosphorus (P) using Abinit and VESTA Software. We compare total energy and band dispersion in the [100] and [111] directions with that of pure bulk (semiconductor) silicon. The resulting band structure shows metallic behaviour due to additional states within the band gap. Furthermore dangling bonds lead to localized surface states without dispersion. Saturating these states can cause shifts in the electrostatic potential and may be used to tune the sensing properties of SiNWs.

HL 7.42 Mon 13:00 P2/EG

**Growth and characterisation of local droplet etched InAs quantum dots in an InGaAs matrix** — •Nikolai Spitzer, Hans-Georg Babin, Andreas Wieck, and Arne Ludwig — Ruhr-Universität Bochum, Lehrstuhl für Angewandte Festkörperphysik, Universitätsstraße 150, 44801 Bochum

We present a new local droplet etching (LDE) method for selforganized InGaAs quantum dots (QDs). We use gallium droplets to etch on an InGaAs matrix layer and fill the nanoholes with InAs. The impact of the indium concentration in the InGaAs-layer and of the deposited InAs amount after etching is investigated by atomic force microscopy and photoluminescence spectroscopy.

HL 7.43 Mon 13:00 P2/EG

**Enhancement of Quantum Dot Emission in the Telecom C-Band via Photonic Micro Cavities** — •Raphael Joos, Christian Rupp, Sascha Kolatschek, Stephanie Bauer, Cornelius Nawrath, Robert Sittig, Ponraj Vijayan, Michael Jetter, Simone Luca Portalupi, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Potential quantum technology applications such as quantum communication rely on the availability of carrier of quantum information. For that matter single-photons can be utilized as „flying-qubits“ imprinting information in their polarization state. For these applications it is beneficial to operate at the telecom C-band which offers reduced dispersion and minimum loss in optical fibers. In the recent years InAs quantum dots (QDs) have shown to be capable of emission of single and entangled photons in the telecom C-band. However, as-grown QD structures have limited collection efficiency of the emitted light due to total internal reflection. To tackle this issue photonic cavity structures can be employed which can enhance the photon extraction efficiency and decrease the decay time due the underlying Purcell effect. While there are different approaches to photonic structures ranging from planar cavities to Gaussian micro lenses, this work mainly deals with circular Bragg grating structures. These offer high collection efficiency in a broadband manner as well as a cavity spectrum which potentially allows simultaneous Purcell enhancement of exciton and biexciton.

HL 7.44 Mon 13:00 P2/EG

**Voronoi-Cell Analysis of Density Modulated InAs Quantum Dots** — •Peter Zajac[1], Nikolai Bart[1,2], Christian Dangel[2], Kai Müller[3], Andreas D. Wieck[1], Jonathan Finley[2], and

Arne Ludwig[1] — [1]Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany — [2]Walter Schottky Institut and Physik Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [3]Walter Schottky Institut and Department of Electrical and Computer Engineering, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

InAs quantum dots (QDs) grown by molecular beam epitaxy exhibit a density modulation upon growth on top of a GaAs gradient layer [1]. The local variation of the nucleation probability is ascribed to the roughness of the underlying GaAs layer. It is of interest to study the QD formation on such a surface under the scope of the capture-zone model [2]. Here, the results of AFM data analysis with focus on correlations between Voronoi cell areas and QD size parameters such as height and volume are presented.

[1] Bart, N., Dangel, C. et al. Wafer-scale epitaxial modulation of quantum dot density. *Nat. Commun.* **13**, 1663 (2022).
[2] Löbl, Matthias C., et al. Correlations between optical properties and Voronoi-cell area of quantum dots. *Phys. Rev. B* **100**, 155402 (2019).

HL 7.45 Mon 13:00 P2/EG

**Enhancing the extraction efficiency of photons from low intensity decay processes with solid immersion lenses** — •Patricia Kallert[1], Björn Jonas[2], Eva Schöll[1], Tim Langer[1], Dirk Reuter[1], Artur Zrenner[1], and Klaus D. Jöns[1] — [1]hqpd lab, PhoQS Institute and Department of Physics, Paderborn University, Germany — [2]Photonic Quantum Engineering Group, Walter Schottky Institute, and Department for Electrical and Computer Engineering, Technical University of Munich, Germany

Single photons are basic building blocks for photon-based quantum technologies, such as quantum computation and communication concepts. A promising source offering high single-photon purity and indistinguishability are semiconductor quantum dots in photodiodes. A major drawback of this platform is the low extraction efficiency. Due to the refractive index mismatch of the semiconductor and the surrounding environment, total internal reflection occurs already for very small angles of incidence on the interface. In this study, the enhancement capability and the practical limits of using solid immersion lenses of hemispherical and Weierstrass geometry are investigated and compared. The hemispherical lens is insusceptible to misalignment but offers a mediocre enhancement in collection efficiency. In contrast, the Weierstrass geometry is sensitive to nonperfect alignment but improves the extraction by a factor of up to 2.9. Avoiding the need of the fabrication of complex structures as micropillars and other cavities, consequently, we can triple the detection of photons from low-intensity decay processes.

HL 7.46 Mon 13:00 P2/EG

**Magnetic Field-Dependence of the Auger Recombination Rate in a Self-Assembled Quantum Dot** — •Fabio Rimek[1], Hendrik Mannel[1], Marcel Zöllner[1], Arne Ludwig[2], Andreas D. Wieck[2], Axel Lorke[1], and Martin Geller[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

A quantum dot (QD) is an ideal system to study electron-electron interaction in a confined nanostructure [1]. The Auger recombination is a special case, where the recombination energy is transferred to a third charge carrier that leaves the dot [2] or is excited to a higher energy level. Therefore, the Auger effect destroys the radiative recombination of the charged exciton (trion) - an effect, which should be minimized for future applications that use spin states as stationary qubits, which can be transferred to photons via the QD trion transition. In this work, we investigate how the Auger rate is affected by an external magnetic field, applied perpendicular to the plane of the dots. In the magnetic field, the trion transition of a QD is no longer spin degenerate and splits up. We use two-color, time-resolved resonance fluorescence to investigate the quenching of the trion recombination due to the Auger effect. Two color excitation allows us to excite two quantum dot transitions (both trions or one trion and one exciton) and neglect spin relaxation as well as spin-flip Raman scattering. This ensures that we can directly measure the Auger and the tunneling rate of an electron into the dot. [1] A. Kurzmann et al., Nano Lett. **16**, 3367-3372 (2016).
[2] P. Lochner et al., Nano Lett. **20**, 1631-1636 (2020).

HL 7.47 Mon 13:00 P2/EG

**Towards solid-state quantum emitters strongly coupled to crossed nanobeam cavities** — •Jan-Gabriel Hartel, Oscar Camacho Ibarra, and Klaus D. Jöns — hqpd lab, PhoQS Institute and Department of Physics, Paderborn University, Germany

The strong coupling regime of quantum electrodynamics, theoretically described via the Jaynes-Cummings model, offers insight into purely quantum mechanical effects in the interaction of a two-level system and a single mode light field. An extension of this model to the interaction of a two-level system with two resonant modes yields the possibility of free exchange of the excitation between the light modes as well as subsequent applications in quantum gates. While the fundamental case has been experimentally studied, the realization of this extension has proven to be elusive due to the technological challenges of fabricating a stable coupled cavity system.

In this work, we seek to approach this realization by exploring nanofabrication of on-chip crossed nanobeam cavity systems, realized via Bragg mirrors. We numerically explore heuristic extensions of existing design recipes for 1D nanobeam cavities, based on the creation of a localized defect mode. We emphasize the challenges of conserving high Q-factors at the specified resonance frequency while minimizing coupling between the crossed cavities, developing novel design ideas.

HL 7.48 Mon 13:00 P2/EG

**Towards frequency-converted polarization-entangled photon pairs from semiconductor quantum dots** — •Tim Strobel[1], Andre Bisquerra[1], Tobias Bauer[2], Nand Lal Sharma[3], Marlon Schäfer[2], Stefan Kazmaier[1], Cornelius Nawrath[1], Lukas Wagner[1], Ankita Choudhary[3], Michael Jetter[1], Caspar Hopfmann[3], Christoph Becher[2], Simone L. Portalupi[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Science and Technology ($IQ^{ST}$) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Fachrichtung Physik, Universität des Saarlandes, Campus E2.6, 66123 Saarbrücken, Germany — [3]Institute for Integrative Nanosciences, Leibniz IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

Fiber-based distribution of entangled, single photon pairs is a key requirement for future developments of terrestrial quantum networks. Quantum repeater schemes at telecom wavelengths can overcome the restriction set by fiber transmission losses over long distances. In this context semiconductor quantum dots (QDs) are promising candidates as deterministic sources of on-demand polarization-entangled photon pairs. Here, we investigate photons emitted via the biexciton-exciton cascade of GaAs QDs grown via Al droplet etching and integrated into a GaP solid immersion lens. To be compatible with existing fiber network infrastructures, quantum frequency conversion is employed to convert the QD emission from 780nm to telecom wavelengths.

HL 7.49 Mon 13:00 P2/EG

**Strongly driven germanium qubit** — •Bashab Dey and John Schliemann — Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany

Hole qubits in germanium heterostructures are promising candidates for coherent control and manipulation of the spin degree of freedom by electric dipole spin resonance. The suppression of contact hyperfine interaction due to p-type character of the holes, possibility of nuclear-spin free isotopes and absence of valley degeneracies in germanium are favourable for sustaining longer spin coherence and relaxation times in these qubits. We study the time dynamics of a germanium qubit confined laterally by a parabolic potential and strongly driven by coherent circularly polarized radiation in presence of p-cubic Rashba spin-orbit coupling and perpendicular magnetic field. We calculate the transition rates between the lowest (Zeeman-split) levels of the qubit using Floquet theory. We observe peculiar beating patterns in the Rabi oscillations which depend on the strength of the driving field. When the driving frequency is resonant with Zeeman gap, the maxima of the oscillations is a decreasing function of driving amplitude which is in contrast to that of a harmonically driven two-level system. Furthermore, the time period of oscillations, time interval between the beating nodes and the number of oscillations between the nodes also decrease with the radiation amplitude.

HL 7.50 Mon 13:00 P2/EG

**Swing-Up Dynamics in Quantum Dot Cavity Systems** — •Nils Heinisch, Nikolas Köcher, David Bauch, and Stefan Schumacher — Physics Department and CeOPP, Paderborn University, Germany

In this work, we further investigate the recently proposed [1] and experimentally demonstrated [2] SUPER-scheme (Swing-UP of the quantum EmitteR population). In the SUPER-scheme optical excitation of a quantum emitter is achieved using two off-resonant red-detuned Gaussian pulses. Here, we expand the studies to quantum dot cavity systems and aim for high quality photons, generated during the decay process following the excitation. After successful proof-of-principle studies with a two-level system, we present the successful single-photon and photon-pair generation using the SUPER-scheme for excitation of diamond-shaped exciton-biexciton quantum dot model systems. For a more realistic simulation we also take phonons into account. For all systems studied it can be concluded that a cavity neither hinders the swing-up process nor degrades the quality of the generated photons which is in contrast to excitation schemes using resonant Gaussian pulses. [1] T. K. Bracht et al., PRX Quantum 2, 040354 (2021). [2] Y. Karli et al., Nano Letters 22, 6567 (2022).

HL 7.51 Mon 13:00 P2/EG

**Time-Resolved Wave-Function Mapping in Self-Assembled Quantum Qots** — •Jens Kerski[1], Daniel Hecker[1], Nelson Creutzburg[1], Arne Ludwig[2], Andreas D. Wieck[2], Martin Geller[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

The static and dynamic properties of self-assembled quantum dots (QDs) are often modeled using the QD's single particle wavefunctions. Although this approximation is very successful, the influence of the electron-electron interaction on the few-particle wave-functions and their nonequilibrium dynamics has not yet been studied in detail.

We investigate an ensemble of InAs/GaAs QDs, embedded in a high electron mobility transistor. The QDs are tunnel-coupled to a two-dimensional electron gas (2DEG). By applying a voltage pulse to the gate, we induce charge carriers from the 2DEG to tunnel into targeted quantum dot states. We monitor the temporal evolution of the conductivity $\sigma_{2D}$ of the 2DEG, which is sensitive to the transfer of charge into the QDs. A rate-equation-based evaluation of $\sigma_{2D}$ allows us to separate tunneling processes into different equilibrium or non-equilibrium QD states. We use an in-plane magnetic field perpendicular to the tunneling direction for wave-function mapping [1, 2] of the quantum dot states. This allows us to study the shape and dynamics of the (excited) electron states.

[1] W. Lei et al., Phys. Rev. Lett. 105, 176804 (2010).
[2] D. Zhou et al. J. Appl. Phys. 134, 064401 (2022).

HL 7.52 Mon 13:00 P2/EG

**Development and deterministic nanofabrication of quantum dot based single-photon sources with emission in the 780 nm-930 nm range** — •Dinara Basharova[1], Stephan Reitzenstein[1], Sven Rodt[1], Caspar Hopfmann[2], Nand Lal Sharma[2], Normen Auler[3], and Dirk Reuter[3] — [1]Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden, 01069 Dresden, Germany — [3]Center of Optoelectronics and Photonics, Universität Paderborn, 33098 Paderborn, Germany

Important goals of quantum technology are to demonstrate the elementary building blocks of a quantum repeater and to integrate them into the infrastructure of a quantum network. A network of quantum repeaters allows the distribution of quantum entanglement, thereby enabling secure exchange of information between multiple parties. To implement such building blocks, we use semiconductor heterostructures (HS) with GaAs quantum dots (QDs) integrated into circular Bragg gratings (CBG). GaAs QDs are excellent single-photon emitters with almost negligible multi-photon emission probability and photon extraction efficiencies exceeding 60%. For this purpose, we deterministically integrate QDs on structures with back-side distributed Bragg reflector and in hybrid approach with backside Au mirror for comparison. In-situ electron beam lithography (iEBL) is an ideal technique for deterministic fabrication of such QD-based quantum light sources. The fabricated QDs are characterized by microphotoluminescence and quantum optical spectroscopy.

HL 7.53 Mon 13:00 P2/EG

**Fabrication of electrically controllable quantum dots in PIN diodes integrated within circular Bragg gratings** — •Setthanat Wijitpatima[1], Normen Auler[2], Sven Rodt[1], Dirk Reuter[2], and Stephan Reitzenstein[1] — [1]Institute of Solid-State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Center of Optoelectronics and Photonics, Universität Paderborn, 33098 Paderborn, Germany

A quantum repeater is one emerging device of the decade that has been promised to play a crucial role in quantum communication. To produce an ideal quantum light source with high single-photon purity, nanophotonic structures must be fabricated on self-organized semiconductor quantum dots, which pose challenges due to their random occurrences and requirements of exact spatial and spectral integration. In addition to nanophotonic enhancement, such devices can be designed to allow an electrical manipulation of the excitonic state of quantum dots. Here, we propose a design that allows electrical controls via a PIN diode integrated within circular Bragg gratings (CBGs). Numerical simulations are done to optimize the design to yield the photon extraction efficiency (PEE) of 0.69 at N.A.=0.8. The deterministic fabrication is done with the use of cathodoluminescence (CL) scans and electron beam epitaxy (EBL), and the fabricated devices are characterized by electric-field dependent micro-photoluminescence ($\mu$PL) measurements.

HL 7.54 Mon 13:00 P2/EG

**Patterned growth of vertical zinc oxide nanowires on sputtered zinc oxide thin films** — •Jan Böhmer, Lukas Jäger, Alexander Koch, and Carsten Ronning — Institute of Soild State Physics, Friedrich Schiller University Jena, Max-Wien-Platz 1, 07743 Jena

Because of the wide band of zinc oxide, ZnO nanowires have promising applications in short wavelength optoelectronics, like building photodetectors or laser emitters using nanowire arrays. ZnO nanowires can be easily grown by vapor transport techniques in a high temperature furnace on silicon substrates utilizing the vapor-solid-liquid (VLS) mechanism. However, the nanowires produced in this way typically show random orientations and often overlap each other. A pre-deposited thin film of aluminum doped zinc oxide (Al:ZnO or AZO) by RF sputtering on the substrate creates a polycrystalline ZnO surface with a preferred orientation, on which the nanowires can grow epitaxially. The ZnO nanowires grown this way are almost all orientated perpendicular to the substrate surface resulting in vertical/upstanding nanowires. By now pattering the pre-deposited AZO thin films, selective area growth (SAG) of nanowires is possible. In this contribution, we will discuss our growth results and our goal to control the exact position of nanowire growth to create ordered nanowire arrays.

HL 7.55 Mon 13:00 P2/EG

**Energy transfer between Si quantum dots and protoporphyrin molecules as a function of distance, orientation and size** — •Athanasios Koliogiorgos[1] and Tomas Polcar[2] — [1]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [2]Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, Czech Republic

Organic molecules such as protoporphyrin IX (PPIX) can be attached to bulk or nanostructured silicon to enhance its optical and electronic properties. In this study, the interaction between PPIX molecules (donor) and Si nanocrystals (acceptor) up to 2.5 nm for varying distances and orientations is studied by DFT, semi-empirical and TDDFT methods. Simulations show an effect on electronic structure, indicative of electron charge transfer in parallel orientation and very small distances and non-electron energy transfer for different orientations and larger distances. An absorption-emission spectral overlap is observed. We use the Transition Density Cube method to calculate the electronic couplings and energy transfer rates between donor and acceptor. The Si quantum dots with the smallest size yield larger couplings than the larger nanocrystals. The coupling is enhanced by adding a plasmon nanoparticle as a bridge between donor and acceptor. Results using Au nanoparticles show increased energy transfer rates up to four orders of magnitude and lower distance dependence.

HL 7.56 Mon 13:00 P2/EG

**The internal photoeffect from a single solid-state quantum emitter: Excitation energy and band-structure dependence** — •B. Maib[1], M. Zöllner[1], F. Rimek[1], P. Lochner[1], H. Mannel[1], A.D. Wieck[2], A. Ludwig[2], A. Lorke[1], and M. Geller[1] — [1]University of Duisburg-Essen and CENIDE, Germany — [2]Ruhr-University Bochum, Germany

The coherence time is one of the limiting factors for using single quantum emitters, like self-assembled quantum dots, in future applications

of quantum information processing. Besides spin and charge noise [1] the physical limits are given by the Auger recombination [2] and an internal photoeffect [3] that is present even for resonant excitation.
We have studied in detail the photoeffect in a single self-assembled quantum dot for different energies of a non-resonant laser that excites a single electron from the bound quantum dot state into the continuum of the conduction band. These measurements are realized by time-resolved two-color resonance fluorescence (RF) excitation. The first resonant laser drives the exciton transition, while the second pulsed laser simultaneously excites the photoelectron to the final state in the conduction band, caused by the internal photoeffect.
The results can be used to reduce the internal photoeffect and therefore suppress the photoemission, which would increase the coherence time in such a single photon emitter even under resonant excitation.
[1] A. V. Kuhlmann, Nature Physics, **9**, 570-575 (2013).
[2] A. Kurzmann, Nano Letters **16**, 3367-3372 (2016).
[3] P. Lochner, Phys. Rev. B, **103**, 075426 (2021).

HL 7.57 Mon 13:00 P2/EG

**Calibrating Photoluminescence Yield for Quantum emitters in Planar Photonic Heterostructures** — •Timo Kruck, Hans-Georg Babin, Andreas D. Wieck, and Arne Ludwig — Ruhr-Universität-Bochum; Lehrstuhl für angewandte Festkörperphysik, Bochum, Deutschland

When performing photoluminescence (PL) measurements the spectral intensity of the emitted radiation strongly depends on the dielectric structure surrounding the quantum emitter. Here we show a method for calibrating PL measurements to obtain the unaltered spectrum of the optically active medium [1]. For this purpose, the spectral reflectivity and the wavelength dependent standing wave field are used. The reflectivity, which is determined by reflectometer measurements , and a simulation based on the transfer matrix method are used to compensate for the true layer thickness. This is then used to calculate the standing wave field, the outcoupling efficiency and the quantum yield. To validate the method, the calibrated spectra are compared with cleaved-edge PL measurements where the QDs are excited from the side and the light is also collected from the side.
[1] Babin et al.; Nanomaterials 2021, 11(10), 2703;

HL 7.58 Mon 13:00 P2/EG

**Nanowire-based light absorber patterning for artificial photosynthesis** — •Juliane Koch[1], Jiajia Qiu[2], Peter Kleinschmidt[1], Huaping Zhao[2], Yong Lei[2], and Thomas Hannappel[1] — [1]TU Ilmenau, Institute for Physics, Fundamentals of energy materials, Ilmenau, Germany — [2]TU Ilmenau, Institute for Physics, Applied nanophysics, Ilmenau, Germany

Due to the increased degrees of freedom in device structures and properties, III-V nanowires (NWs) have been predicted to outperform planar devices. In the context of energy conversion in solar cells and photoelectrochemical devices, the kinetics and transport behavior of different charge carriers in light absorbers are closely related to the selected materials and their shape. A key factor for commercially relevant development is the enhanced light absorption, in particular in an uniform NW array, combined with lower costs and material usage (e.g. of III-Vs) for nanowire-based light absorbers. This may ultimately require fabrication techniques with homogenous patterning over a large range. In this work we demonstrate the fabrication techniques for creation of a NW array and key requirements during MOVPE NW growth. By applying a surface patterning technique with anodic aluminum oxide (AAO) templates, arrays of gold droplets can be deposited on a surface, which acts as a catalyst for NW growth during metalorganic vapor phase epitaxy (MOVPE). Under defined process parameters vertical III-V semiconductor NW can be achieved via vapor-liquid-solid (VLS) growth in a horizontal MOVPE system.

HL 7.59 Mon 13:00 P2/EG

**Enhancing spatial resolution for terahertz waveform near-field microscopy** — •Fabian Brütting, Moritz Heindl, and Georg Herink — Experimental Physics VIII, University of Bayreuth, Germany

The quantum confined Stark-effect induces field-driven modulations in the optical transitions of quantum emitters. Harnessing this ultrafast interaction in colloidal quantum dots enables us to image THz near-field waveforms with fluorescence microscopy in the visible spectrum [1]. The spatial resolution of fluorescence microscopy is principally not diffraction-limited and can be extended to the few-nanometer scale using super-resolution techniques such as stimulated emission depletion (STED) microscopy. The efficient depletion of quantum dot emission presents a key requirement [2]. In this contribution, we present our investigations on the STED process in the quantum dots employed as field-probes in the luminescence-based Quantum-probe field microscopy (QFIM) scheme.
[1] Heindl, M. B. et al., Ultrafast imaging of terahertz electric waveforms using quantum dots. Light Sci. Appl. 11, 5 (2022).
[2] Hanne, J. et al., STED nanoscopy with fluorescent quantum dots. Nat. Comm. 6, 7127 (2015).

HL 7.60 Mon 13:00 P2/EG

**Investigation of the biexciton decay in semiconductor In(Ga)As/GaAs quantum dots** — •Christopher Buchholz, Sebastian Krehs, and Artur Zrenner — Universität Paderborn, Paderborn, Deutschland

The biexciton-exciton cascade is a widely used promising emission mechanism in quantum dots for generating entangled photon pairs with high fidelity. An often overlooked critical parameter for the quality of the emitted photons is the different lifetimes of electron and hole. Since the lifetimes of excitonic states can be influenced via external electrical fields (quantum confined stark effect), we studied this parameter in Schottky-contacted GaAs heterostructures. We approached this challenge by placing the quantum dots at different distances to the n-contact, 40 nm and 80 nm, respectively. The quantum dots were first characterized by voltage-dependant photoluminescence (PLV) measurements under above-band excitation and further investigated by photocurrent spectroscopy (PC) under resonant excitation and PLV under two-photon excitation (TPE). From the resonances in the PC measurements, the electron lifetime was extracted, whereas the TPE measurements showed the occurrence of the biexciton and charged exciton states as a function of the voltage. The results suggest that an increased distance to the n-contact leads to a decreased tunneling rate of electrons into the quantum dot. At the same time, the tunneling from the quantum dot is not affected.

HL 7.61 Mon 13:00 P2/EG

**Influence of the quantum dot geometry on higher excited states** — •Jan Kaspari and Doris E. Reiter — Condensed Matter Theory, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund

The energetic structure and absorption spectra of semiconductor quantum dots are strongly dependent on the dot geometry. In particular the higher excited states, typically denoted as p- or d-shell, can become highly mixed and depend strongly on the specific dot. We derive a theoretical model to describe higher excited quantum dot states based on the envelope function approximation. The four-band Luttinger theory as well as the direct and short-range Coulomb interactions are treated within a configuration interaction approach. The quantum dot confinement is approximated by an anisotropic harmonic potential. We show that a variation of the size of a cylindrical symmetric quantum leads to energetic shifts of higher excited quantum dot states. Breaking this cylindrical symmetry significantly alters the absorption spectrum as further energy splittings in the energetic structure appear and state mixtures change which results in differences of oscillator strenghts of some peaks. Our results give insight into the quantum dot energy structure especially for higher excited states, which become relevant in radiative Auger processes or for ultrafast quantum logic operations.

HL 7.62 Mon 13:00 P2/EG

**Towards remote on-chip two-photon interference in gallium arsenide based-photonic integrated circuits** — •Ulrich Pfister[1], Moritz Speidel[1], Florian Hornung[1], Stephanie Bauer[1], Robert Sittig[1], Eric Reutter[2], Michael Jetter[1], Simone L. Portalupi[1], Jürgen Weis[2], and Peter Michler[1] — [1]Institut für Halbleiter und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, Germany — [2]Max-Planck-Institut für Festkörperforschung (MPI), University of Stuttgart, Heisenbergstraße 1, Germany

InGaAs quantum dots (QDs) are a promising source of single and indistinguishable photons for the on-chip realization of two-photon interference (TPI) with remote QDs. One of the challenges is the inhomogeneously distributed emission frequency of the QDs, which makes frequency tuning necessary. We show that strain-induced emission frequency tuning is applicable for ridge waveguides and it can be considered a promising step towards remote on-chip TPI [1]. Additionally, a successful TPI with one single QD and an on-chip multimode interference beamsplitter as a part of a Mach*Zehnder interferometer has

been realized and the feasibility of remote on-chip TPI with MOVPE-grown InGaAs QDs is discussed.
[1] Hepp, S. *et al.*, Appl. Phys. Lett. **117**, 254002 (2020)

HL 7.63 Mon 13:00 P2/EG

**Quantum frequency conversion of entangled photon pair from GaAs Quantum dot to Sn-vacancy center in Diamond** — •Ankita Choudhary, Tim Pokart, Nand lal Sharma, Moritz Langer, and Caspar Hopfmann — Institute for Integrative Nanosciences, Leibniz IFW Dresden, Helmholtzstraβe 20, 01069 Dresden, Germany

The distribution of entangled photons in future long-distance quantum networks requires both on-demand and high-fidelity entangled photon pair generation as well as their temporary storage in low dephasing quantum memory systems. While GaAs quantum dots have proven to be excellent entangled photon pair sources, this is system suffers from strong dephasing of its spin qubits. Diamond color centers on the other hand are excellent quantum memories, but not ideal entangled photon pair sources. In order to combine the complementary properties of both material system in a hybrid quantum network approach, the efficient conversion between the operating photon energies without the loss of quantum information using quantum frequency conversion is required. In this study we present quantum frequency conversion from of 780nm to 619nm, i.e. from GaAs quantum dot emission to the zero-phonon line of the diamond Sn vacancy center, using sum frequency generation in a periodically poled lithium niobate crystal and an infrared laser pump of about 3 *m wavelength. We find that a conversion efficiency of at least 25% can be achieved.

HL 7.64 Mon 13:00 P2/EG

**Design of circular Bragg resonators in the telecom band for efficient emission of entangled and indistinguishable photons from semiconductor quantum dots** — •Dustin Siebert, David Bauch, Klaus D. Jöns, Stefan Schumacher, and Jens Förstner — Electrical Engineering Department, Physics Department, CeOPP and PhoQS, Paderborn University, Germany

The generation of indistinguishable and entangled photons via the biexciton-exciton cascade in semiconductor quantum dots can be tailored by a photonic environment providing an increased emission rate through the Purcell effect and a cavity feedback [1,2].

Circular Bragg resonators exhibit exactly these properties and enable good collection efficiency over a large bandwidth. We developed an optimization strategy based on a two-step process. First, we use a batch of 2D electromagnetic simulations within Bayesian global optimization and finally polish the optimum through Nelder-Mead local optimization based on full 3D simulations.

The optical properties obtained are then used within a quantum mechanical simulation of the carrier dynamics in the semiconductor quantum dots including phonon interaction [3]. After optimization, we achieve a tremendous enhancement of the indistinguishability of the emitted photons even considering that real structures might suffer fabrication imperfections.

[1] E. Schöll, et al., Phys. Rev. Lett. 125, 233605 (2020) [2] F. Sbresny, et al., Phys. Rev. Lett. 128, 093603 (2022) [3] D. Bauch et al., Phys. Rev. B 104, 085308 (2021)

HL 7.65 Mon 13:00 P2/EG

**Origin of Antibunching in Resonance Fluorescence** — •Lukas Hanschke[1], Eva Schöll[1], Eduardo Zubizarreta Casalengua[2,3], Melina Peter[4], Ailton Garcia Jr.[4], Saimon F. Covre da Silva[4], Santanu Manna[4], Armando Rastelli[4], Kai Müller[5], Fabrice P. Laussy[3], Elena del Valle[2], and Klaus D. Jöns[1] — [1]PhoQS, CeOPP, and Department of Physics, Paderborn University — [2]Departamento de Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid — [3]Faculty of Science and Engineering, University of Wolverhampton — [4]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz — [5]Walter Schottky Institute, Technical University of Munich

Resonance fluorescence, the coherent emission of a quantum two-level system under weak resonant driving, exhibits sub-natural linewidth and inherits the coherence properties of the excitation laser. While previous experiments suggest that this emission also maintains antibunched, our results prove recent theoretical insights into the origin of the antibunching and the underlying interplay between the coherent and incoherent emission of the quantum system. This allows us to specifically manipulate the composition of the resonance fluorescence by frequency filtering and interference with the excitation laser field to enable single photons with sub-natural linewidth [PRL 123, 170402 (2020)].

HL 7.66 Mon 13:00 P2/EG

**Near Fourier-Transform Limited Blinking Free Quantum Dots** — •Eva Schöll[1], Lukas Hanschke[1], Melina Peter[2], Ailton Garcia Jr.[2], Patricia Kallert[1], Francesco Salusti[1], Saimon Filipe Covre da Silva[2], Santanu Manna[2], Armando Rastelli[2], and Klaus D. Jöns[1] — [1]PhoQS, CeOPP, and Department of Physics, Paderborn University, Warburger Straße 100, 33098 Paderborn, Germany — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, 4040 Linz, Austria

Tailored quantum light sources are crucial building blocks for applications in quantum technologies. Al droplet etched GaAs Quantum Dots are promising candidates for such sources, as they show very good characteristics for example in terms of single-photon purity, indistinguishability on short time scales and entanglement fidelity. However, these QDs usually exhibit an unstable charge environment, which leads to reduced coherence on long time scales, broadened linewidths and blinking. Embedding the QDs into a p-i-n diode structure enables energy tuning via the Stark effect and stabilizes the charge environment. Here we demonstrate a solid-state single-photon source with no signs of blinking on up to ms time scales and near Fourier-transform limited linewidths. This opens up possibilities for experiments for a fundamentally deeper understanding of quantum level schemes and realization towards a quantum network, where quantum interference between separate sources is required.