HL 39: Poster III

The third poster session covers most recent results on the optical and thermal properties of semiconductors, as well as on nitrides and organic semiconductors, and semiconductor lasers.

Time: Wednesday 15:00–18:00 Location: P3

HL 39.1 Wed 15:00 P3

Termperature dependent electroluminescence spectroscopy of far-UVC-LEDs with varying AlGaN quantum well thickness — •Max Dittmer[1], Jakob Höpfner[1], Markus Blonski[1], Tim Kolbe[2], Sylvia Hagedorn[2], Hyun Kyong Cho[2], Jens Rass[2], Sven Einfeldt[2], Tim Wernicke[1], Markus Weyers[2], and Michael Kneissl[1] — [1]TU Berlin, Insitute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Insitut (FBH), Berlin Germany

AlGaN far-UVC-LEDs with emission wavelengths below 240 nm require AlGaN layers with such high aluminium molefractions that p-doping with magnesium is inefficient due to its high ionization energy. An alternative method of p-doping is distributed polarization doping (DPD), which induces charge carriers by polarization charges. We will present the results of temperature dependent electroluminescence spectrocopy on 233 nm AlGaN LEDs with DPD gradient, grown by metal organic vapor phase epitaxy (MOVPE). We investigated the impact of the quantum well (QW) width from 1.3 nm to 7.6 nm. Most importantly we found the 2.6 nm LED to be the most efficient at room temperature. The LEDs exhibit an S-shape in the emission energy in dependence of the temperature and the highest internal quantum efficiency of 55%, was measured at 200 K.

HL 39.2 Wed 15:00 P3

MATRIX: GaN diode arrays for proton monitoring and imaging — •Nico Brosda[1], Stéphane Higueret[2], Thê-Duc Lê[2], Andreas Wieck[1], Maxime Hugues[3], Matilde Siviero[3], and Jean-Yves Duboz[3] — [1]Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Université de Strasbourg, CNRS, IPHC UMR 7178, F-67000 Strasbourg, France — [3]Université Côte d'Azur, CNRS, CRHEA, 06560, Valbonne, France

The MATRIX project is pioneering advancements in proton therapy for cancer treatment by developing novel, highly durable detectors that enhance real-time control of irradiation doses. Proton detection is achieved by measuring the current induced in the active regions of PIN GaN diodes. Our GaN-based devices are fabricated as linear diode arrays of 128 elements and two-dimensional imaging arrays up to 11×11 elements, covering an area of $1\,\mathrm{cm}^2$ with up to $500\,\mu$m spatial resolution. Thanks to the microelectronics processes, a much higher resolution can be obtained if needed. Results concerning the sample structure and fabrication process are presented. The design of bonding contacts proved to have a significant impact on the measured signal and, thus, the imaging quality. A bonding fanout on the GaN samples introduced notable signal distortions at the edges of the proton irradiation field. The underlying electron external emission mechanism responsible for this distortion was modeled, and a correction method was developed. An adapted sample design improved the device quality and removed the signal distortion. These findings pave the way for optimizing future GaN-based proton detector arrays.

HL 39.3 Wed 15:00 P3

Investigating the Electrical Properties of Distributed Polarization Doped $Al_xGa_{1-x}N$ Heterostructures via Capacitance-Voltage Measurements — •Thibaut Ehlermann[1], Marcel Schilling[1], Massimo Grigoletto[1,2], Jakob Höpfner[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin — [2]Ferdinand-Braun-Institut (FBH)

Distributed Polarization Doping (DPD) enables the generation of charge carriers in wide-bandgap semiconductors like AlGaN by utilizing the material's inherent polarization properties without the introduction of impurities. Linearly graded AlGaN DPD layers were grown by metal-organic vapor phase epitaxy (MOVPE). The starting Al mole fraction was always 100%. The thickness and end mole fraction were varied. The charge carrier concentration N_A was determined from CV-measurements. For a 100 nm thick AlGaN DPD layer (x=100% –> 60%), the charge carrier concentration is $N_A = 1.4 \cdot 10^{18}\,\frac{1}{\mathrm{cm}^3}$, closely matching the theoretical value of $N_A = 1.72 \cdot 10^{18}\,\frac{1}{\mathrm{cm}^3}$, based on the calculated intrinsic polarization. Thicker DPD layers lead to a lower doping concentration and AlGaN DPDs (x=100% –> 80%) result in lower doping concentrations in agreement with the calculated values. The consistency of the results suggest that DPD is a reliable and promising way for p-type doping in AlGaN.

HL 39.4 Wed 15:00 P3

Temperature Dependence of the Quantum Efficiency of UV LEDs emitting from 226 nm to 300 nm — •Max Eysell[1], Jakob Höpfner[1], Marcel Schilling[1], Norman Susilo[1], Anton Muhin[1], Massimo Grigoletto[1,2], Tim Kolbe[2], Arne Knauer[2], Sylvia Hagedorn[2], Markus Weyers[2], Jens Rass[2], Hyun Kyong Cho[2], Tim Wernicke[1], Sven Einfeldt[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

UV-LEDs are of huge interest for e.g. air, surface, and water disinfection. However, the widespread application of UV-LEDs is constrained by their external quantum efficiency (EQE) which is decreasing further as the emission wavelength shortens. To gain insight into the carrier transport and recombination mechanisms, a detailed analysis of the EQE of UV-LEDs and the three contributors: the carrier injection, the radiative recombination and the light extraction was performed.

The emission power of LEDs with emission wavelengths of 226 nm, 233 nm, 265 nm and 305 nm are investigated by temperature dependent electroluminescence measurements in the range of $25-80°C$. A reduction in emission power and EQE has been observed going from UVB to the far-UVC spectral range. A thermal droop in the emission power was observed for all samples which is caused by the decline of all three contributions. The magnitude of this thermal droop becomes higher with decreasing wavelength which we attribute to an increased electron leakage suggested by Schrödinger-Poisson drift-diffusion simulations.

HL 39.5 Wed 15:00 P3

Theoretical Study on the (In, Ga)N/GaN heterojunction — •Maximilian Lauer[1,2], Jan M. Waack[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

Semiconductor materials have a wide range of applications and their electronic properties can be easily tuned by alloying and changing their composition x. Understanding the properties of semiconductor alloys, such as indium gallium nitride $In_xGa_{1-x}N$, is therefore an important area of research. Two such properties are the band gap of the semiconductor and its band alignment with substrate and conduction materials.

While the band gap of the random alloy (In, Ga)N is a well-established quantity, the band alignment is less well understood.

Our research aims to better understand the band alignment and interface states at a GaN/(Ga,In)N heterojunction and its impact on the electronic properties of the system.To achieve this, we performed DFT calculations using the Korringa-Kohn-Rostoker (KKR) formalism with the coherent potential approximation (CPA). From these calculations we computed the layer-resolved density of states (DOS) for varying $In_xGa_{1-x}N$ compositions. This approach can be further used to simulate the effects of doping on the electronic properties or to study the transport properties of such a system.

HL 39.6 Wed 15:00 P3

Moiré exciton polaritons in twisted photonic lattices at room temperature — •Tobias Schneider[1], Chunzi Xing[2], Yu Wang[3], Xiaokun Zhai[2], Xinzheng Zhang[3], Haitao Dai[2], Xiao Wang[4], Anlian Pan[4], Zhenyu Xiong[5], Hao Wu[5], Yuan Ren[5], Stefan Schumacher[1,6], Xuekai Ma[1], and Tingge Gao[2] — [1]Physics dept. and CeOPP, Paderborn University, Germany — [2]Department of Physics, School of Science, Tianjin University, Tianjin 300072, China — [3]The MOE Key Laboratory of Weak-Light Nonlinear Photonics and International Sino-Slovenian Join Research Center on Liquid Crystal Photonics, TEDA Institute of Applied Physics and School of Physics, Nankai University, Tianjin 300457, China — [4]College of Materials Science and Engineering, Hunan University, Changsha 410082, China — [5]Lab of quantum detection and awareness, Space Engineering University Beijing 101416, China — [6]PhoQS, Paderborn University, Germany

Due to their support of many exotic physical phenomena such as Mott insulators or the fractal quantum Hall effect, moiré lattices have attracted great interest. In this work, rhombic optical moiré lattices are realized in microcavity exciton polaritons[1]. These lattices consist of two stacked 1D periodically patterned stripes which are twisted to a specific angle. This structure allows the resulting bands to be tuned via modulating the lattice parameters such as the periodicity, the potential depth of the stripes, and the rotation angle. In addition, moiré polaritons in twisted 2D honeycomb lattices are also observed. [1] C. Xing et al., arXiv:2408.02431 (2024).

HL 39.7 Wed 15:00 P3

Ultradoped GeSn plasmonic antennas for IR photodetection — •Guillermo Godoy[1,2], Ali Azimi[3], Fritz Berkmann[3], Oliver Steuer[1], Slawomir Prucnal[1], Shengqiang Zhou[1], Ing-Song Yu[4], Inga A. Fischer[3], and Yonder Berencén[1] — [1]Helmholtz Zentrum Dresden Rossendorf, Dresden Germany — [2]Dresden University of Technology, Dresden Germany — [3]BTU Cottbus-Senftenberg, Cottbus Germany — [4]National Dong Hwa University, Hualien Taiwan

Ligth mater interaction due to localized surface plasmon resonances (LSPRs) can generate hight electical field enhacement, enabling biosensing and hot-electron photodetection devices. While metallic nanoparticles like Au and Al are commonly used, their optical losses increase at longer wavelengths, limiting applications in the mid-infrared (MIR) range, such as air pollution detection. Highly doped group-IV semiconductors, particularly GeSn alloys, offer a cost-effective alternative with lower losses and CMOS compatibility. The cut-off wavelength for plasmonic resonances depends on the carrier effective mass, and GeSn alloys with its lower electron effective mass enables plasmonic resonances from shorter wavelengths.This work explores strategies to achieve highly doped GeSn alloys for plasmon-enhanced photodetection, utilizing MBE or CVD-grown GeSn layers on Si substrates. These layers will be doped in-situ or ex-situ via ion implantation, followed by non-equilibrium annealing to enhance crystal quality and dopant activation, showcasing their potential for advancing MIR photodetection.

HL 39.8 Wed 15:00 P3

Optical and phonon properties of In-rich InGaN alloys and InN/InGaN multiple quantum well structures — •Svitlana Polesya[1], Masako Ogura[1], Sergiy Mankovsky[1], Gregor Koblmüller[2], and Hubert Ebert[1] — [1]University of Munich, 81377 Munich, Germany — [2]Technical University of Munich, 85748 Garching, Germany

In two-dimensional systems like multiple quantum well structures, thermalization of hot carriers can be strongly suppressed. InN/InGaN multilayered (ML) materials are seen as promising candidates to show this property. In order to optimize these materials, ab initio calculations have been performed on the electronic and phonon band structure, as well as on the optical properties of In-rich $In_xGa_{(1-x)}N$ alloys and the short period ML systems $[InN]_m/[In_xGa_{(1-x)}N]_n$. All calculations have been done with the VASP package. The HSE exchange-correlation potential has been used with further GW0 corrections. Electron-hole interactions were taken into account by solving the Bethe-Salpeter equation. The calculations on alloys were done via the superlattice technique considering for each In concentration x all non-equivalent atomic arrangements. This is crucial as the atomic distribution has a significant impact on the phonon band structure of the alloys. For the layered $[InN]_m/[In_xGa_{(1-x)}N]_n$ system the optical properties were calculated for various concentrations x. The important role of the interface between the quantum well ($[InN]_m$) and the quantum barrier ($[In_xGa_{(1-x)}N]_n$) on the optical properties as well as phonon band gap is shown.

HL 39.9 Wed 15:00 P3

Ultra-sensitive absorption measurements of perovskites nanocrystals, protein crystals and photo-switchable lipids — •Ayesha Khan[1], Simone Strohmair[1], Ines Amersdorffer[1,2], David Hunger[3], and Thomas Hümmer[1,2] — [1]Qlibri GmbH, Munich, Germany — [2]Ludwig Maximilian University of Munich, Munich, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

Optical studies of nano-scale systems through spectroscopy and imaging can reveal intrinsic optical properties of materials including resolving the exitonic fine structure of systems. However, due to diminutive absorption of nano-scale systems, it is challenging to perform absorption spectroscopy. For a nano-scale system placed inside an optical resonator, the light passes through the sample thousands of times, enhancing the absorption and thus, allowing measurements.

Here we present the use of a fiber-based, open-access micro-cavity to image and obtain hyperspectral maps of absorption for different nanoscale, solid state materials including perovskites nanocrystals, protein crystals and photo-switchable lipids.

The successful measurements of different nano-scale systems promise that fiber-based microcavities can become standard tools for absorption measurements of these systems.

HL 39.10 Wed 15:00 P3

Intensity-dependence of the excitonic third-harmonic generation in bilayer MoS2 — •Ruixin Zuo[1], Matthias Reichelt[1], Cong Ngo[1], Xiaohong Song[2], and Torsten Meier[1] — [1]Department of Physics, Paderborn University, D-33098 Paderborn, Germany — [2]School of Physics and Optoelectronic Engineering, Hainan University, Haikou 570288, China

The large exciton binding energies make layered transition metal dichalcogenides an ideal platform for exploring exciton physics in two-dimensional systems. We numerically and theoretically investigate three-photon transitions to the excitonic states in a bilayer MoS2 and demonstrate that beyond the linear order intraband transitions dominate over interband transitions. Beyond the perturbative limit, transitions to and from the continuum that represent fifth- and higher-order nonlinearities contribute to the excitonic response at the third harmonic where they destructively interfere with the third-order excitations. Applying an in-plane static electric field characteristically modifies the k-resolved fourth-order and higher-order nonlinearities and accordingly the interference at the excitonic resonance. We demonstrate that the yield of the third harmonic generation may rise with increasing static field strength. This finding can be interpreted to arise from a shift from destructive to constructive interference between the lowest- and higher-order excitations. Exciton ionization prevails at even higher static field strengths and results in a decrease of the third harmonic generation.

HL 39.11 Wed 15:00 P3

Implementation and Validation of a Herzberg-Teller Approach for Phonon-Assisted Photoluminescence — •Tobias Dittmann, Torben Steenbock, and Gabriel Bester — Insitut für physikalische Chemie, Universität Hamburg

Phonon-assisted PL from electronically excited states leads to the occurrence of phonon side-bands, which can shape the PL spectrum. A Franck-Condon framework based on Huang-Rhys factors efficiently describes phonon side-bands in nanostructures containing up to a few hundred atoms.[1] However, the FC approximation is usually not suited for the emission from a dark state. Therefore, we extend the method towards a Herzberg-Teller (HT) level which allows a more accurate description of the emission from a dark state. Additionally, our method includes the description of spin-orbit effects, offering an advantage over other implementations of the HT framework, particularly for structures containing heavy elements.

In a first stage of the project, we investigate various graphene quantum dots and observe that the inclusion of HT terms introduces both quantitative and qualitative differences compared to the FC spectrum. These findings underscore the critical importance of incorporating HT terms for accurate modelling. In future work, we intend to apply this method to bigger structures containing heavy elements, in order to benefit from the advantages of our implementation.

[1] Wu, Han, Dittmann, Wang, Zhang and Bester, Nanoscale, 2024, DOI: 10.1039/D4NR02458C

HL 39.12 Wed 15:00 P3

Electronic structure and energy landscape of $B_{Si}Si_i$-related defects — Aaron Flötotto[1], Wichard Beenken[1], Kevin Lauer[1,2], Stefan Krischok[1], and •Erich Runge[1] — [1]Technische Universität Ilmenau, Institute for Physics, Ilmenau, Germany — [2]CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany

Boron is an important dopant for silicon. Together with an adjacent interstitial Si atom, it forms the so-called $B_{Si}Si_i$ defect, which has been proposed as a source of light-induced degradation (LID) in solar cells made from boron-doped Czochralski-grown silicon. Furthermore, the $B_{Si}Si_i$ defect is an intermediate configuration in many models for boron diffusion in silicon.

In a recent comprehensive density-functional-theory-based study [1], we have calculated the energy landscape around the $B_{Si}Si_i$ defect and related defects involving one B atom and one interstitial Si atom for different chemical potentials of electrons corresponding to neutral, positively, and negatively charged supercells. Among the found meta-

stable defect configurations, we identify possible recombination centers based on the defect-dependent electronic density of states and the minimal energy paths between them. The resulting potential energy landscape is checked against empirical models for boron diffusion and LID.

[1] A. Flötotto et al., Phys. Rev. Mater. (accepted)

HL 39.13 Wed 15:00 P3

Origin of strong interband transitions in antimony — •Julia Vehndel, Nils Holle, Sebastian Walfort, and Martin Salinga — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Straße 10, 48149 Münster

In recent years, phase change materials (PCMs) have attracted considerable interest as photonic memory elements due to a high contrast in optical properties between crystalline and amorphous states. In order to identify ideal PCMs for specific applications, the intricate connection between electronic structure, bonding and permittivity needs to be understood.

Here, we employ ab-initio simulations based on density functional theory to calculate the optical properties of the single-elemental PCM antimony in the visible and near-infrared. We analyze the permittivity in k-space for both crystalline and amorphous states. Most strikingly, the strong interband transitions at lower energies can be related to the electron and hole pockets in the first Brillouin zone of the crystalline state.

HL 39.14 Wed 15:00 P3

Optical properties of α-$(Cr_xGa_{1-x})_2O_3$ — •Dmitry Sayenko, Clemens Petersen, Jakob Seifert, Christiane Dethloff, Holger von Wenckstern, Chris Sturm, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany

Due to its high bandgap energy in the order of $4.6-5.0\,\mathrm{eV}$ and its high predicted electrical breakdown field of about $8\,\mathrm{MV\,cm^{-1}}$, Ga_2O_3 is a promising material for transparent electronic devices and high power applications [1]. Of special interest is the corundum-structured α-phase as it has the largest band gap energy of the Ga2O3 polymorphs. Further, its band gap energy can be tuned by alloying with Cr without changing its crystal structure. Here we present the dielectric function of α-$(Cr_xGa_{1-x})_2O_3$ as a function of the cation composition. The sample was grown by combinatorial pulsed laser deposition. As expected, the onset of absorption increases with increasing Ga concentration from around $3.2\,\mathrm{eV}$ for $x \approx 0.74$ to $4.2\,\mathrm{eV}$ for $x \approx 0.13$. Whereas we observe for all concentrations a negative birefringence in the visible range, i.e. $n_{\mathrm{eo}} < n_{\mathrm{o}}$, the polarization of the energetically lowest transition changes with Cr concentration. For large Cr concentration the absorption sets in at first for light polarized perpendicular to the c-axis whereas for large Ga concentration the first absorption is observed for light parallel to the c-axis. This change of the polarizability leads to a decrease of the birefringence with decreasing Cr concentration, but $n_{\mathrm{eo}} < n_{\mathrm{o}}$ holds for all x.

[1] M. Higashiwaki *et al.*, Appl. Phys. Lett. **100**, 013504 (2012).

HL 39.15 Wed 15:00 P3

Calibration methods in Raman spectroscopy — •Susanne Moritz, Ron Hildebrandt, Chris Sturm, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany

For low symmetry materials, polarization resolved measurements are required for a precise investigation, especially of the Raman tensor [1, 2]. Here we present strategies for calibrating and determining the polarization state of the incident and scattered light. In addition to the polarizing optics, e.g. polarizers, we also consider the impact of all involved optical elements such as mirrors and beam splitters. We show, that these non-idealities can have an impact on the determined Raman tensor elements. Taken into account the non-idealities of the polarizing optics the uncertainty of the deduced tensor elements can be reduced by 20%.

[1] C. Kranert *et al.*, Phys. Rev. Lett. **116**, 127401 (2016).
[2] C. Kranert *et al.*, Sci. Rep. **6**, 35964 (2016).

HL 39.16 Wed 15:00 P3

Spectral Signatures and Kinetics of Y6 Aggregates and Disordered Phase via Absorption Spectroscopy — •Daniel Kroh[1,2], Xinyue Xu[2], Trevor Smith[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, EPII, Universität Bayreuth, Bayreuth, Germany — [2]School of Chemistry, University of Melbourne, Melbourne, Australia

Recent advancements in single-junction organic solar cells (OSCs) utilizing non-fullerene acceptors (NFAs) have significantly increased power conversion efficiencies (PCEs) to over 19%. This remarkable progress is largely attributed to the introduction of the "Y-series" NFAs, with Y6 being the most notable example. Motivated by these achievements, numerous research groups are investigating the relationship between film morphologies and their exceptional optoelectronic properties, especially when blended with the donor material PM6.

In our study, we employed temperature-dependent steady-state UV-Vis absorption and photoluminescence spectroscopy combined with Franck-Condon analysis to identify the spectral signatures of two types of aggregates and the disordered phase of Y6 in solution. We observed that all three phases are also present in neat Y6 films and blend films with PM6. Through transient absorption measurements, we further explored the excitation kinetics and transient absorption spectral signatures of these phases, providing deeper insights into their behavior.

HL 39.17 Wed 15:00 P3

Empowering Thermoelectric Performance of ZnSb via Bonding Interaction Regulation — •Meng Jiang[1,2], Fangyi Hu[1], Qihao Zhang[2], Lianjun Wang[2], Wan Jiang[2], Matthias Wuttig[1], and Yuan Yu[1] — [1]Physical Institute 1, RWTH Aachen University, Aachen, 52074, Germany. — [2]Donghua University, Shanghai, 201620, China.

ZnSb compounds have garnered significant attention due to its green nature, low cost and high Seebeck coefficient. However, its thermoelectric performance has been limited by a relatively low power factor and high lattice thermal conductivity. Recent studies have demonstrated that regulating bonding interactions offers an effective strategy to optimize the thermoelectric properties. Specifically, metavalent bonding shows unprecedented success in predicting and optimizing a series of high-performance thermoelectric materials. This reignites research interest in ZnSb. We explored a one-step synthesis strategy for ZnSb and specifically investigated optimizing mechanisms of Cd and Mg. By regulating bonding interactions to optimize electrical conductivity, the room-temperature power factor was enhanced from 2.5 to 4 μW cm-1 K-2. This improvement, coupled with a reduction in lattice thermal conductivity, resulted in a zT of 0.6 at 600 K. Our work highlights the potential of bonding interaction regulation as an effective approach for enhancing the thermoelectric performance of ZnSb. More, future research would focus on unraveling the intricate mechanisms linking bonding and microstructure to achieve even higher performance.

HL 39.18 Wed 15:00 P3

Challenges and Opportunities for Thermoelectric Coolers — •Fangyi Hu, Meng Jiang, Matthias Wuttig, and Yuan Yu — I. Physikalisches Institut (IA), RWTH Aachen University, 52074 Aachen, Germany

Thermoelectric (TE) materials allow a direct interconversion between heat and electricity, providing an eco-friendly and sustainable energy solution. Particularly, thermoelectric coolers based on the Peltier effect achieve high-precision temperature control without any refrigerant. Bi2Te3-based materials have beenused in commercial TE cooling due to their high near-room-temperature figure-or-merit (ZT). Yet, the low earth abundance of Te restricts the large-scale application of this compound. Discovering Te-free materials with comparable cooling performance is an urgent task. This requires a small bandgap and low thermal conductivity for the material at low temperatures. The recently developed concept of metavalent bonding provides a new avenue for discovering potential candidates. Besides materials, the device design and effective heat dissipation on the hot side are of critical importance. This Poster will summarize the challenges and opportunities for TE cooling materials and devices. We hope that it can shed light on the development of new TE coolers.

HL 39.19 Wed 15:00 P3

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

We modeled PBDB-T:ITIC heterojunctions by applying DFT on dimers built of various conformers of a PBDB-T segment and the ITIC molecule. These variations represented the non-uniformity of the interface between the donor and the acceptor in the organic solar cell.

Based on this model, we calculated electronic and optical properties most relevant for charge separation at the interface using DFT and TD-DFT, respectively. For almost half of our modeled dimers, we found that the band offsets between them and the pristine donor and acceptor materials resulted in charge carrier trapping leading to inefficient charge separation as well as non-geminate recombination. When we calculated the exciton binding energy by TD-DFT using either the B3LYP or the HSE06 functional, we obtained very different qualitative and quantitative results. We, therefore, compared our results with experimental data from ultraviolet photoelectron spectroscopy, CV, ERIS, PL, absorption spectroscopy, EQE and EL. Finally we discuss the impact of our findings on characteristic photovoltaic parameters, particularly the open circuit voltage and the short-circuit current.

HL 39.20 Wed 15:00 P3

Investigation of the optical coupling of lasing ZnO nanowires — •Ann-Kathrin Kollak, Lukas Raam Jäger, Francesco Vitale, and Carsten Ronning — Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Semiconductor nanowires offer potential for miniaturizing optical circuits. Good candidates for this application are ZnO nanowires, because their bottom-up growth via the Vapor-Liquid-Solid (VLS) mechanism allows for high quality crystal structures. When optically pumped, ZnO nanowires simultaneously act as an active medium and a laser cavity, emitting UV light mainly waveguided to their end facets. To study the interaction of these nanometer-scale lasers via evanescent field coupling, two nanowires were positioned in contact next to each other on a SiO_2 substrate using a nanomanipulator. In a micro-PL (photoluminescence) setup, the nanowire pair was optically excited using the third harmonic of an Nd:YAG laser (355 nm). The pair's emission was collected with the same setup, allowing the investigation of the spatially resolved PL and lasing spectra, as well as their linear polarization parallel to the substrate. The data obtained indicate that ZnO nanowire cavities can couple with one another. Depending on the geometry of the nanowire pair and the pumping conditions, optical modes that extend into both cavities can appear in addition to modes confined to only one nanowire. In other cases, the coupled modes dominate the lasing behavior.

HL 39.21 Wed 15:00 P3

Impact of stress current on reverse-bias electroluminescence images of 850 nm oxide-confined VCSELs — •Arndt Jaeger[1], Nikolay Ledentsov Jr.[2], Sebastian Haberkern[1], Helmut Meinert[1], Alexander Moll[1], Ilya E. Titkov[2], Oleg Yu. Makarov[2], and Nikolay N. Ledentsov[2] — [1]Esslingen University of Applied Sciences, Flandernstrasse 101, 73732 Esslingen, Germany — [2]VI Systems GmbH, Hardenbergstrasse 7, 10623 Berlin, Germany

Vertical-cavity surface-emitting lasers (VCSEL) employing different doping of the cavity region are studied utilizing reverse current-voltage (IV) characteristics as well as reverse bias electroluminescence (ReBEL). Reverse IV characteristics exhibits avalanche breakdown enabling an estimation of the electric field in the cavity region. ReBEL emission is observed at locations where avalanche breakthrough current has its maximum. The oxide-confined VCSELs are characterised before and after high current operation. Virgin devices have a homogeneous device center in ReBEL images. Upon a short high current burn-in VCSELs evolved a homogeneous ring at the oxide-aperture perimeter. This ring structure decays into 2 point-like areas after long-term current stress. These observations in ReBEL images can be understood in terms of recently published VCSEL simulation results which gave evidence of local current crowding at the oxide-aperture during high current laser operation.

HL 39.22 Wed 15:00 P3

Tuning nanowire lasers via hybridization with organic molecules — •Philipp Swatosch, Edwin Eobaldt, Marco Grünewald, Olga Ustimenko, Kalina Peneva, and Carsten Ronning — Friedrich Schiller Universität Jena, Deutschland

Among the numerous nanomaterials, semiconductor nanowires have drawn significant scientific interest as promising candidates for nanoscale coherent light sources and all-optical circuits. This attention is due to their exceptional waveguiding properties and inherent ability to lase under high excitation. However, precise control over their lasing characteristics, such as emission wavelength and lasing threshold, is essential for various applications. In this regard, hybridizing nanowires with customized molecules presents a potential approach, providing new control mechanisms through efficient charge and energy transfer processes at the heterointerface. To demonstrate this concept, we hybridized ZnO nanowires with perylene-based organic dyes. These chromophores are particularly advantageous as their optical gap can be easily tuned over a wide spectral range through chemical functionalization. This study employs comparative micro-photoluminescence measurements to investigate the impact of these molecules on the lasing properties of the nanowires.

HL 39.23 Wed 15:00 P3

Development of a VCSEL-chip in the red spectral range with integrated photodiode for chlorophyll fluorescence analysis — •Raphael Buffler, Michael Zimmer, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum-Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart

Chlorophyll fluorescence analysis provides information on photosynthetic activity of plants and thus also on their health. Changes in the environmental conditions can be monitored on large scale and, water and nutrients can be added as needed. In order to induce the fluorescence of chlorophyll in the range from 660 nm to 750nm , optical excitation at 650 nm can be used. In this work, a semiconductor chip will be developed that contains both, the light source for excitation and the photodiode for fluorescence detection. The chip is based on the AlGaAs & AlGaInP material systems, which can realise the band gaps for the required wavelengths. The light source is designed as a vertical-cavity surface-emitting laser (VCSEL), which allows for the vertical emission of the excitation light and the vertical irradiation of the photodiode. A stacked arrangement is used, where the VCSEL is grown by metal-organic vapor-phase epitaxy (MOVPE) on top of the photodiode structure on a GaAs wafer. First electro-optical characteristics of the VCSEL and the photodiode such as P-U-I curves, emission wavelength and photodiode responsivity are presented.

HL 39.24 Wed 15:00 P3

Monolithic 850 nm VCSEL array for Quantum Key Distribution via the Decoy State Protocol — •Katharina Dahler, Michael Zimmer, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The need for secure data communication has increased in recent years. In contrast to classical key distribution, the use of quantum key distribution (QKD) offers fundamental advantages, such as complete secrecy. However, QKD poses numerous challenges regarding the use of single photons. With this in mind, the decoy-state protocol offers the possibility of realizing QKD with classical light sources such as attenuated semiconductor lasers. Here, we present the electro-optical characterization of a monolithic 850 nm vertical-cavity surface-emitting laser (VCSEL) array, for QKD via the BB84 and decoy state protocol. The complete VCSEL array consists of eight individual VCSELs arranged in a coplanar contact design, with four VCSELs serving as signal states and four as decoy states. A highly homogeneous growth is needed due to the requirement of indistinguishable light pulses regarding the emission wavelength. In order to realize the four necessary polarization states and to counteract the electro-optical effect, each VCSEL features a monolithically integrated surface grating in the top layer of its light emission window. Electro-optical device characteristics regarding light polarization via surface gratings and spectral homogeneity of the VCSEL array are presented.

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A machine learning potential for tellurium — •Andrea Corradini, Giovanni Marini, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Elemental tellurium has drawn attention in recent years, due to its possible technological application as switching device in phase change memories [1]. Recent computational studies are addressing the behaviour of elemental Te under operating conditions with a focus on the crystallization dynamics [2]. In addition, experiments have found anomalous thermodynamic maxima in undercooled liquid Te around 615 K, i.e. 130 K below the melting point [3]. Thermodynamic maxima behave in a very similar way as those in undercooled liquid water. Hence the question whether elemental Te shows a liquid-liquid phase transition, analogously to what is claimed for water. In this work, we develop a robust machine learning potential to study elemental Te and try to answer this question.

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[1] Shen et al., Science 374, 1390*1394 (2021)
[2] Zhou et al., arXiv:2409.03860 [cond-mat.mtrl-sci]
[3] Sun et al., PNAS 119 (28), e2202044119 (2022)