HL 46: Optical Properties

Time: Thursday 9:30–13:00 Location: H15

Invited Talk HL 46.1 Thu 9:30 H15

Exploring Auto-Oscillations in Semiconductor Electron-Nuclear Spin System — •Alex Greilich, Nataliia E. Kopteva, Vladimir L. Korenev, and Manfred Bayer — Experimentelle Physik 2a, TU Dortmund University, Dortmund, Germany

We demonstrate self-sustained auto-oscillations in a dissipative electron-nuclear spin system (ENSS) in semiconductors, where spontaneous breaking of translational symmetry in time produces robust limit-cycle dynamics across a broad range of parameters, including laser power, temperature, and magnetic field. These periodic oscillations exhibit coherence times extending to hours, reflecting ideal "time atom" ordering within the auto-oscillatory system.

Additionally, we uncover synchronization within excited subsystems without additional modulation, identifying its microscopic origins. Under periodic driving, modulation of parameters such as excitation power and pump polarization yields parametric resonances, signaling a transition to discrete auto-oscillatory behavior. Key phenomena include frequency entrainment, Arnold tongues, bifurcation jets, and a devil's staircase, showcasing the ENSS's versatility in exploring nonlinear dynamics, with broad implications for both fundamental physics and semiconductor applications.

HL 46.2 Thu 10:00 H15

Material selective Nonlinear Optics on Transition-metal Dichalcogenide - ZnO Nanowire Hybrid Structures — •Maximilian Tomoscheit, Benedikt Mathes, Edwin Eobalt, Alexander Zaunick, Carsten Ronning, and Giancarlo Soavi — Institute of Solid State Physics, Friedrich Schiller University Jena

The nonlinear optical (NLO) properties of any material are described by the complex tensor $\chi^{(n)}$, where, for each element of the tensor, the imaginary part mainly appears close to optical resonances. A direct measurement of the complex NLO suscebility is challenging because any NLO measurement is proportional to $|\chi^{(n)}|^2$. A second harmonic generation (SHG) interference measurement from two different materials with $\chi^{(2)}_\nu$ ($\nu = 1, 2$), is also proportional to $\left|\chi^{(2)}_1\right| \left|\chi^{(2)}_2\right| \cos\theta$, where θ is the phasemismatch. For a hybrid system with non overlapping resonances, if the SH photon energy is off-resonant for one material and resonant for the other, the interference term directly probes the complex NLO suscebility of the resonant material. In this work, we study SH interference in a transition-metal dichalcogenide (TMD) ZnO-nanowire (NW) hybrid structure, and we characterize the complex NLO suscebility of the TMD close to the A-exciton resonance. To be able to measure such interference, the ZnO NW needs to be placed along the armchair direction of the TMD, in our case WSe_2. Preliminary measurements and the results of SH polarization and wavelength dependent measurements will be be presented in this talk.

HL 46.3 Thu 10:15 H15

Nonempirical hybrid functional based on metaGGA — •Stefan Riemelmoser[1], Xun Xu[1,2], and Alfredo Pasquarello[1] — [1]École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland — [2]Beijing Computational Science Research Center, Beijing, China

Semi-local density functionals such as PBE typically underestimate experimental band gaps by 50%. Hybrid functionals address this "band gap problem" by admixing a fraction of exact exchange to semi-local exchange. The optimal mixing parameter depends on the specific material and can be identified as the inverse dielectric constant. Recently, we have show that dielectric constants obtained using the r^2SCAN metaGGA functional are significantly more accurate than dielectric constants obtained using PBE. This can be understood through the improved treatment of electronic self-interaction within the metaGGA framework.

In this talk, we will show that a dielectric-dependent hybrid functional based on r^2SCAN can outperform the standard PBE based hybrid in terms of band gaps. Particularly impressive improvements are obtained for narrow gap semiconductors such as Ge and InAs, where PBE wrongly predicts a metallic phase, but r^2SCAN can open a gap. The hybrid functional based on r^2SCAN also yields accurate effective masses and ionization potentials. Finally, we showcase that our new hybrid functional is an excellent choice for semiconductor applications such as defect calculations.

HL 46.4 Thu 10:30 H15

Room-temperature polariton condensate in a two-dimensional hybrid perovskite — •M. Struve[1], C. Bennenhei[1], H. P. Adl[1], K. W. Song[2], H. Shan[1], N. Mathukhno[1], J. Drawner[1], F. Eilenberg[3], N. P. Jasti[4], D. Cahen[4], O. Kyriienko[2], C. Schneider[1], and M. Esmann[1] — [1]Institut for Physics, Carl von Ossietzky Universität Oldenburg — [2]University Exeter, United Kingdom — [3]Frauenhofer IOF, Jena — [4]Weizmann Instutute of Science, Israel

Chemically synthesized 2D halide perovskites form naturally grown quantum well stacks. Their large binding energy, tunable emission spectra and high oscillator strength makes them promising platforms for room temperature polaritonics but bosonic condensation and polariton lasing at ambient conditions are yet to be shown. In this work we demonstrate cavity exciton-polariton condensation of 2D Ruddelson-Popper iodine perovskites $(BA)_2(MA)_2Pb_3I_{10}$ crystal at room temperature [1]. A polariton condensation threshold of $P_{th}\approx6.8$ fJ with a strong non-linear response is observed. The emergence of spontaneous spatial coherence across the condensate with interferometric measurements is confirmed with a first-order autocorrelation reaching $g^{(1)}\approx0.6$. With our results we lay the foundation for a new class of 2D halide perovskite based room-temperature polariton lasers that offer great potential for hetero-integration with other van-der-Waals materials and combination with photonic crystals. [1] M.Struve et al., arXiv 2024, https://doi.org/10.48550/arXiv.2408.13677

HL 46.5 Thu 10:45 H15

Determination of optical losses at 265 nm in multimode AlGaN waveguides — •Verena Montag[1], Martin Guttmann[2], Bruno Marx[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut, Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany

Many applications for ultraviolet photonic integrated circuits (UV PICs) like, e.g., biochemical sensing, solar-blind communication, and UV Raman spectroscopy require materials with a large bandgap energy to enable low optical losses. Currently, no ideal material has been identified that enables low loss waveguides and simultaneously the implementation of active and passive components in the UV spectral range. AlGaN is a promising material which is already successfully employed for the fabrication of UV light emitting diodes (UV-LEDs) and UV lasers. However, the optical properties of AlGaN, especially the absorption losses in AlGaN waveguides have not yet been studied in detail in the UVC spectral range. In this work, 200 μm wide AlGaN waveguides, UV-LEDs, and detectors were monolithically fabricated on AlN/sapphire wafers and the waveguide losses are determined. We were able to measure photocurrents > 1 nA using an integrated AlGaN-based photodiode. Also, an exponential decrease of the photocurrent with increasing waveguide length could be observed. However, Monte Carlo ray tracing simulations show that apart from absorption losses in the AlGaN waveguides also scattering losses from surface roughness have to be considered in order to fully explain the results.

15 min. break

Prize Talk HL 46.6 Thu 11:15 H15

Development and Application of Computational Simulations to Optimize Organic Photovoltaic Modules — •Annika Janssen — Technische Hochschule Nürnberg — Laureate of the Georg-Simon-Ohm-Prize 2025

Organic photovoltaics (OPV) is one of the emerging solar technologies and has the possibility of more cost-effective and sustainable production compared to conventional silicon cells. The printing technique considered in this thesis is doctor blade printing. In research, this is mainly used to produce OPV, as it is fast and the coating physics is similar to slot-die coating, the technique that is most commonly used for large-scale R2R printing. To produce large modules, a homogeneous coating is important, since the thickness of the layers has an influence on the efficiency of the device. In this work, the influence of the film thickness on the efficiency is investigated experimentally on cell level and the influence of layer thickness variations is studied by means of electrical finite element method (FEM) simulations for large-area modules. Formulas describing the behavior of the injected ink during printing are established. A special focus was put on the analysis of the non-accelerated and the accelerated printing. Using simulations, this work shows that a homogeneous coating achieved by accelerating the doctor blade can improve the efficiency of organic solar modules by 16.22 %.

HL 46.7 Thu 11:45 H15

Ultraflat excitonic dispersion in single layer g-C3N4 — •Francesca Martini, Pietro Nicolò Brangi, Pier Luigi Cudazzo, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Single-layer graphitic carbon nitride (g-C3N4) is widely regarded as one of the most promising two-dimensional photocatalysts for hydrogen generation via water splitting. Despite its extensive study, limited information is available on its excitonic dispersion and velocity, critical parameters for achieving high charge mobility and efficient photogeneration. In this work, we employ many-body perturbation theory and the Bethe-Salpeter equation to provide a comprehensive description of the optical absorption and finite-momentum energy loss function for both s-triazine and tri-s-triazine structures. Our findings reveal the exciton dispersion and velocity, emphasizing the significant role of localized nitrogen lone pairs in producing remarkably flat excitonic bands with velocities that are two orders of magnitudes smaller than the typical one in two-dimensional materials and of the same order or smaller than the optical phonon frequencies in single layer g-C3N4. As the time-scale for inter-site exciton hopping is longer or similar to a phonon period, our results point to a highly non-conventional exciton propagation.

HL 46.8 Thu 12:00 H15

Investigation of PLD-grown β-CuI — •Aaron Giess, Lukas Trefflich, Gabrielle Benndorf, Marius Grundmann, and Chris Sturm — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany

Copper iodide (CuI) is a transparent semiconductor that is currently of great interest due to its inherent p-type behavior and its high exciton binding energy of 62 meV. Typically, CuI crystallizes in the zincblende structure (γ-CuI) at room temperature. However, CuI can also crystallize in other phases, which are thermodynamically not stable at ambient pressure and temperature. One of these phases is the rhombohedral phase, which is often also called β-phase. Under certain growth conditions, this β-phase appears simultaneously with the γ-phase.

We grew closed thin films of CuI on c-sapphire, using pulsed laser deposition. The influence of the growth-parameters on the occurrence of β-CuI seems to be a multidimensional problem. The most important parameter is the film thickness, with thinner films favouring a higher fraction of the β-phase. The appearance of the β-phase causes additional features in the 2θ-ω scan in XRD, the dielectric function and the optical transmittance. Furthermore, photoluminescence spectra reveal a change of the emission spectra with time, which indicates that a photobleaching processes takes place.

HL 46.9 Thu 12:15 H15

Luminescent Microthermometers Based on ALD-encapsulated Ga_2O_3:Cr DBR Microcavities — •Ruben Neelissen[1], Daniel Carrasco[1,2], Anton Schäning[1], Marco Schowalter[1], Andreas Rosenauer[1], Emilio Nogales[2], Bianchi Mendez[2], Martin Eickhoff[1], and Manuel Alonso-Orts[1] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany. — [2]Departamento de Fisica de Materiales, Plaza Ciencias 1, Universidad Complutense de Madrid, 28040 Madrid, Spain.

The ability to measure temperature non-invasively, accurately and reliably is an ever reoccurring challenge in various fields such as micro- and nanosystems. Luminescent thermometry sensors can operate in environments where electronic counterparts are ineffective, thanks to their capability for remote sensing while being minimally intrusive.

Gallium oxide (β-Ga_2O_3) is a semiconductor with an ultra-wide bandgap of 4.8 eV and high resilience. Chromium-Ions (Cr^{3+}) in β-Ga_2O_3 result in two well-defined peaks, superimposed to a red-NIR emission, which can be utilized for temperature sensing.

In this work [1] it is demonstrated how confined light of β-Ga_2O_3:Cr microcavities (MCs) can be enhanced by encapsulating them in ALD-grown distributed Bragg reflectors (DBRs). With increasing temperature, the resonant wavelength redshifts due to changes in both the refractive index and the optical length of the MCs. A temperature accuracy of < 0.5 °C for temperatures above -80 °C is demonstrated.

[1] M. Alonso-Orts et al. In: *Advanced Materials Technologies* (2024), p. 2400881.

HL 46.10 Thu 12:30 H15

Theoretical and Experimental Study of Lead Tungstate (PWO-II) Crystal Properties for Electromagnetic Calorimetry — •Ather Ahmad[1], Pavel Orsich[1], Valera Dormenev[1], Hans-Georg Zaunick[1], Kai-Thomas Brinkmann[1], Simone Sanna[2], Martin Becker[3], and Limei Chen[3] — [1]II. Physikalisches Institut, Gießen, Germany — [2]Institut für Theoretische Physik, Gießen, Germany — [3]I. Physikalisches Institut, Gießen, Germany

Lead tungstate ($PbWO_4$ or PWO) is widely recognized as a high-performance scintillator for electromagnetic calorimeters due to its fast response, high density, and radiation hardness. PWO scintillator material is used in several experiments, such as CMS at the LHC (CERN), and the next-generation PWO-II crystals, which are doped to enhance their properties, have been optimized for the PANDA experiment at FAIR in Darmstadt.

To gain a deeper understanding of the material's performance, we have combined theoretical and experimental approaches to study the electronic and optical properties of PWO-II. Raman spectra and light transmission measurements were conducted on PWO-II samples and compared with results from density functional theory (DFT) calculations. In our models, we consider the crystal phases stable at room temperature, revealing characteristic differences in both Raman spectra and light transmission between these phases.

These combined efforts aim to refine the characterization of PWO-II and support the development of advanced calorimeter materials.

HL 46.11 Thu 12:45 H15

Rabi splitting mediated dual electromagnetically induced transparency in metamaterial — •Amit Haldar[1], Kshitij V Goyal[1], Ruturaj Puranik[2], Vivek Dwij[2], Shriganesh Prabhu[2], and Shovon Pal[1] — [1]NISER, HBNI, Jatni, India. — [2]TIFR, HBNI, Mumbai, India.

Electromagnetically Induced Transparency (EIT) and strong coupling are pivotal phenomena in light-matter interactions with profound implications for quantum and material sciences. EIT, resulting from destructive interference in three-level quantum systems, creates a transparency window within an absorption spectrum [1] and is classically emulated in metamaterials via bright-dark-mode interference. This enables applications such as slow-light devices, sensors, and cloaking technologies. Strong coupling, achieved when the interaction strength between a quantum emitter and an electromagnetic field surpasses system losses, leads to hybridized states (Rabi splitting), facilitating coherent energy exchange and insights into coupling mechanisms [2]. This study combines these phenomena using terahertz metamaterials to achieve tunable transitions between single and dual EIT states through strong coupling. This integration enhances the tunability of metamaterial-based devices and deepens our understanding of EIT and strong coupling, bridging classical and quantum perspectives for future applications.

[1] S. Y. Chiam *et al.*, *Phys. Rev. B* **80**, 153103 (2009).
[2] H. S. Kim *et al.*, *Nano Lett.* **20**, 6690 (2020).