HL 35: Optical Properties II

Time: Wednesday 16:30–19:00 Location: POT/0251

HL 35.1 Wed 16:30 POT/0251

Polarization-Angle-Resolved Raman Spectroscopy for Reliable Raman Tensor Analysis — •Hans Tornatzky[1], Jonas Rose[1], Luca Choi[2], Moritz Meissner[1], Zbigniew Galazka[3], and Markus R. Wagner[1,2] — [1]Paul Drude Institut — [2]Technische Universität Berlin — [3]Institut für Kristallzüchtung

Phonons are fundamental to materials, shaping the physical properties that underlie device functionality. Accurate knowledge of their quantitative description, specifically the Raman tensor, is essential for a detailed understanding of materials and for reliable modeling and optimization of structures and devices.

This talk presents state-of-the-art approaches for determining relative Raman tensor elements using polarization-angle-resolved Raman (PARRS) spectroscopy, alongside discussion of major challenges and sources of error encountered in the process. We also introduce a newly developed fitting procedure that enables robust disentanglement of strongly overlapping signals arising from different modes, permitting precise extraction of their characteristics – energy, FWHM, symmetry, and tensor elements – with enhanced reproducibility.

These techniques are demonstrated across several materials recently studied by our group, including rutile GeO_2, Ga_2O_3, and $LaInO_3$.

HL 35.2 Wed 16:45 POT/0251

Characterization of Exciton-exciton entanglement in different phases: A many-body investigation in low dimensions — •Fangzhou Zhao[1], Carlos Mejuto-Zaera[2], Vojtech Vlcek[3], and Angel Rubio[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Laboratoire de Physique Théorique, LPT, CNRS, Toulouse, France — [3]UCSB, Santa Barbara, USA

There have been emerging experimental investigations on exciton-exciton correlations, especially in moiré superlattices. However, theoretical understanding of exciton-exciton interactions - which requires an accurate treatment of four-point Green's functions and the validity of a bosonic description of excitons- remains relatively underdeveloped. We construct an exactly solvable one-dimensional model to investigate exciton-exciton correlations and entanglement using many-body exact techniques. We identify phase boundaries separating excitonic phases with different degrees of binding, and extrapolate the data to the thermodynamic limit to infer properties in large systems. We also apply a wavefunction projection technique to characterize the strength of entanglement between excitons, as well as the strength of entanglement between the electron and hole inside an exciton. Our results show that, over a broad parameter range, excitonic correlations remain weak, validating the applicability of many-body perturbation theory in most cases. We also explored the quantum confinement effect of multi-exciton state in 1D systems and uncovered the conditions under which the confinement effects emerge.

HL 35.3 Wed 17:00 POT/0251

Excited-state trions in a quantum well — Sourabh Jain[1], Mikhail Glazov[2], and •Ashish Arora[1] — [1]Indian Institute of Science Education and Research, Pune 411008 India — [2]St. Petersburg, Russia

Recently, excited-states of trions were discovered in a layered semiconductor raising strong interest in many-body physics of Coulomb-bound quasiparticles in solids [1]. Here, we report on the observation of an excited 2s state of a trion in a GaAs quantum well (QW) using magneto-optical Kerr effect (MOKE) spectroscopy under out-of-plane magnetic fields up to 6 T [2]. This resonance appears slightly below the 2s exciton in energy. Strikingly, the 2s trion is found to be bound only for magnetic fields larger than 1 T. The signature of the 2s trion is absent in the magneto-reflectance spectra, while it is detectable in the MOKE spectra signifying the importance of the powerful technique. Similar to the 1s states, the 2s trion shows an opposite degree of magnetic-field-induced polarization compared to its exciton counterpart, in agreement with our theoretical calculations. This transfer of oscillator strength between the complexes establishes an optical fingerprint of the 2s excited trion. Our work addresses a four-decade old problem of excited-state trions in a quantum well, and opens scope for further investigations of many-body physics in solids. [1] Phys. Rev. Lett. 123, 167401 (2019) [2] Phys. Rev. Lett. 134, 246902 (2025)

HL 35.4 Wed 17:15 POT/0251

Directional lasing and optical coupling in indium phosphide nanowires — •Lukas Raam Jäger[1], Wei Wen Wong[2], Hark Hoe Tan[2], and Carsten Ronning[1] — [1]Friedrich-Schiller-Universität Jena, Fürstengraben 1, 07743 Jena, Germany — [2]The Australian National University, Canberra ACT 2600, Australia

Indium phosphide (InP) nanowires (NWs) are promising nanoscale light sources due to their strong optical confinement and compatibility with selective-area epitaxy. We investigate optical coupling in vertically standing lasing InP NWs using finite-difference time-domain simulations and angle-resolved photoluminescence. Single NWs lase in the TE01 mode for diameters above about 250 nm and exhibit far-field patterns shaped by interference of emission from the top and bottom facets. Coupled NW structures enable controlled emission engineering. In NW pairs, coupling splits the TE01 mode into two hybrid modes with orthogonal directional lobes, in good agreement with experiment. Mode selection is highly sensitive to subtle geometric differences, while asymmetric pumping has negligible effect. Extending this concept to arrays of NW pairs shows that array-level interference can further narrow the emission lobes. Triplet NW structures exhibit three distinct hybrid modes with characteristic far-field patterns. These results demonstrate designable directional nanoscale emitters based on coupled NW lasers.

HL 35.5 Wed 17:30 POT/0251

Optical emission of monolayer-hybridized nanowire lasers — •Moritz Willems, Edwin Eobaldt, Alexander Zaunick, Aurelia Eberhard, Lukas Jäger, Xiao Chen, and Carsten Ronning — Friedrich Schiller Universität, Jena, Deutschland

Semiconductor Nanowires have attracted substantial scientific interest as foundation for nanoscale coherent light sources and all-optical circuits, based on to their remarkable waveguide properties and their intrinsic ability to lase. 2D-Materials offer a functional environment that enables influencing the lasing characteristics, including emission wavelength and lasing threshold, of ZnO nanowires. These hybrid structures thus allow for electrical and optical charge and energy transfer. Deterministic nanowire integration is achieved through stage-assisted transfer using PDMS and tip-assisted nanomanipulation. Comparative micro-photoluminescence measurements are used to investigate how the 2D-materials influence and modify the lasing behaviour of individual nanowires.

HL 35.6 Wed 17:45 POT/0251

Bandgap and exciton engineering in two-dimensional transition $Mo_{1-x}W_xSe_2$ alloys for next-generation photonics. — •Muhammad Hussain[1], Omid Ghaebi[1], Mohammad Monfared[2], Marco Gruenewald[1], Umer Ahsan[3], Fedor Lipilin[3], Jan Luxa[3], Zdenek Sofer[3], Ulf Peschel[2,4], and Giancarlo Soavi[1,4] — [1]Institute of Solid-State Physics, Friedrich Schiller University Jena, Germany — [2]Institute of Condensed Matter Theory and Optics, Friedrich Schiller University Jena, Germany. — [3]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic — [4]Abbe Center of Photonics, Friedrich Schiller University Jena, Germany

Alloys of 2D transition metal dichalcogenides (TMDs), provide a unique platform for bandgap engineering at the atomic scale. In this work, we investigate the nonlinear optical response of $Mo_{1-x}W_xSe_2$ alloys focusing in particular on second harmonic generation (SHG) and two-photon photoluminescence (TP-PL) [1]. We find that alloyed TMDs exhibit enhanced nonlinearities compared to their pristine counterparts. By combining SHG and TP-PL and the respective optical selection rules, we are able to extract the energy difference between 1s and 2p exciton states in samples of different alloy composition. By doing this, we find that the exciton binding energy in such alloys varies with the W composition (x). This can be used as a knob to tune not only the optical bandgap, but also the exciton binding energy by changing the alloy composition.

[1] M. Hussain, et al. Adv. Opt. Mater. 13, 01000 (2025).

15 min. break

HL 35.7 Wed 18:15 POT/0251

Photoluminescence of single color centers in hBN below the diffraction limit — •Iris Niehues[1], Daniel Wigger[2], Korbinian Kaltenecker[3], Annika Klein-Hitpass[1], Johannes Binder[4], Andrzej Wysmołek[4], and Rainer Hillenbrand[5] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Physics, University of Münster, Germany — [3]Department of Physics, Ludwig-Maximilians-Universität München, Germany — [4]Faculty of Physics, University of Warsaw, Poland — [5]CIC nanoGUNE BRTA, Spain

Color Centers in hexagonal boron nitride (hBN) are promising quantum light sources due to their stable single-photon emission at room temperature. Using a scattering-type near-field optical microscope, we investigate photoluminescence (PL) properties of hBN grown via metalorganic vapor phase epitaxy. Our experiments employ the microscope in tapping mode to detect PL signals influenced by the metallic AFM tip. We demonstrate near-field optical excitation and emission via the tip's nanofocus, creating a sub-diffraction limited tip-enhanced (TE)PL hotspot [1]. Additionally, an "arc" forms around the emitter, explained by constructive interference between direct beams between the optics and the emitter and indirect beams scattered from the tip. This tip-assisted (TA)PL method can be used to map in-plane dipole orientations of hBN color centers at the nanoscale.

[1] I. Niehues et al., Nanophotonics 14(3), 335-342 (2025)

HL 35.8 Wed 18:30 POT/0251

Role of lattice temperature for the optical properties of boron nitride — •Peter Kratzer[1] and Andre Schleife[2] — [1]Faculty of Physics, University Duisburg-Essen, 47057 Duisburg, Germany — [2]Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, USA

We carried out a computational study of boron nitride both in its cubic (c-BN) and hexagonal (h-BN) polytypes as a prototypical system for the renormalization of optical properties in semiconductors by lattice vibrations. While band-gap renormalization due to electron-phonon coupling is a well-explored concept in semiconductor physics, this topic has gained renewed attention in the context of pump-probe spectroscopies where high fluences may lead to local lattice excitation. With this motivation, we performed first-principles calculations of c-BN and h-BN supercells using the DFT+GW method, treating lattice excitation via explicit atomic displacements. Finally, the frequency-dependent dielectric function and the optical absorbance are obtained including many-particle effects on the level of the Bethe-Salpeter equation. The results show that the atomic displacements in the 2x2x2 supercells used in this study have little effect in c-BN but lead to a considerable narrowing of the optical gap in h-BN. In h-BN, the band splitting due to 'frozen' phonons gets even amplified on the GW level of theory. The binding energy of approximately 0.5eV of the exciton derived from the band edges, however, is found to be only weakly affected by the atomic displacements.

Financial support from CRC 1242 is gratefully acknowledged.

HL 35.9 Wed 18:45 POT/0251

Half-saddle excitons in monolayer SnS2: a first-principles study — •Vinicius Alves Bastos[1], Fulvio Paleari[2], Eleonora Luppi[3], Marco Gibertini[1,2], and Alice Ruini[1,2] — [1]Dipartimento di Scienze Fisiche, Informatiche e Matematiche, UNIMORE, Modena (Italy) — [2]CNR-Nano, Modena (Italy) — [3]Laboratoire de Chimie Théorique, Sorbonne Université and CNRS, Paris (France)

Monolayer SnS2 has been demonstrated as a visible-light absorber with promising characteristics for applications in fuel cells and thin film photovoltaics [1]. Motivated by that, we have performed a first-principles study of bound excitons in this system within the GW-BSE formalism [2]. We have gone beyond previous works by analysing the exciton symmetries, electron-hole contributions, and transition dipoles. We find a richer structure of bound excitons than previously reported, e.g., deeply bound dark excitons with binding energies of about 0.9 eV and a very strong bright exciton at 2.9 eV, in good correspondence with the experimental absorption peak. Also, the bound excitons are localized around the direct band gap at the M point, which exhibits a saddle point at the top valence band and a minimum at the bottom conduction band. Consequently, we show that linearly polarized light can be used to completely select two of the three inequivalent M saddles, as previously demonstrated in graphene [3]. PNRR MUR project ECS_00000033_ECOSISTER

[1] Y. Sun et al., Angew. Chem. Int. Ed. 51, 8727 (2012). [2] D. Sangalli et al., J. Phys. Condens. Matter. 31, 325902 (2019). [3] S. Sharma et al., arXiv preprint, arXiv:2503.21376 (2025).