HL 21: Optical Properties 1

Time: Wednesday 15:00–18:30 Location: H32

HL 21.1 Wed 15:00 H32

Dynamics of exciton-polariton emission in CuI — •E. Krüger[1], M. Bar[1], S. Blaurock[2], L. Trefflich[1], R. Hildebrandt[1], A. Müller[1], O. Herrfurth[1,3], G. Benndorf[1], H. von Wenckstern[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 — [3]now at: Active Fiber Systems GmbH, Germany

Copper iodide (CuI) is a promising candidate for transparent optoelectronic applications due to its large band gap of 3.1 eV and high exciton binding energy of 62 meV [1]. Here we present spectral- and time-resolved measurements of the near-band-edge luminescence of CuI bulk crystals for temperatures between 10 K and 250 K. The line shape of the emission lines at low temperatures is interpreted in terms of defect-bound exitons and exciton-polaritons [2]. The different decay characteristics of free and localized exciton states are explained by their coupled interaction. Based on the rise time of bound excitons, the defect density is estimated to be about $1{\times}10^{17}\mathrm{cm}^{-3}$, which is in good agreement with the density of free holes at room temperature. The decay times of the free exciton polaritons increase with increasing temperature up to 360 ps. For the emission of bound excitons, decay times between 180 ps and 380 ps are observed at low temperatures.

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

HL 21.2 Wed 15:15 H32

Coherent phonon oscillations and transient critical-point parameters in femtosecond pump-probe ellipsometry spectra — •S Zollner[1], C Emminger[1,2,3,4], S Espinoza[5], S Richter[3,5,6], M Rebarz[5], O Herrfurth[3,7], M Zahradnik[5], R Schmidt-Grund[8], and J Andreasson[5] — [1]NMSU, Las Cruces, NM, USA — [2]Masaryk University, Brno — [3]Uni Leipzig — [4]Humboldt Universität, Berlin — [5]ELI Beamlines, Dolni Brezany, Czech Republic — [6]Lund University — [7]Active Fiber Systems GmbH, Jena — [8]TU Ilmenau

Spectroscopic ellipsometry measures the dielectric function of materials, which is related to the electronic band structure of semiconductors, and allows the study of critical points and their parameters (energy, broadening, amplitude, phase angle). At ELI Beamlines, femtosecond pump probe ellipsometry measurements can be performed with a white-light continuum probe beam, resulting in a time resolution of 120 fs. We report the transient dielectric function of Ge as a function of delay time between the pump and probe beams near the E_1 and $E_1 + \Delta_1$ critical points. The changes of the critical-point amplitudes are attributed to band filling at the L-point, intervalley scattering, carrier diffusion, lattice heating, and recombination. We also calculate the derivatives of these spectra using a novel Fourier analysis technique and determine the critical point parameters. We find oscillations of the critical-point energies with a period of 11 ps, related to the propagation of coherent acoustic phonons (strain waves) generated by the pump pulse. The amplitude of these oscillations shows that the strain is hydrostatic (isotropic) and has a magnitude of 0.1%.

HL 21.3 Wed 15:30 H32

Temperature dependence of the mid-infrared dielectric function of InSb from 80 to 800 K — Melissa Rivero Arias[1], Cesy Zamarripa[1], Jaden Love[1], Carola Emminger[1,2,3,4], and •Stefan Zollner[1] — [1]New Mexico State University, Las Cruces, NM, USA — [2]Masaryk University, Brno, Czech Republic — [3]Uni Leipzig — [4]Humboldt Universität, Berlin

We describe measurements of the mid-infrared dielectric function of bulk InSb near the direct band gap using Fourier-transform infrared spectroscopic ellipsometry from 80 to 800 K in an ultra-high vacuum cryostat. Indium antimonide is the zinc blende compound semiconductor with the smallest direct band gap (E_0=0.18 eV at 300K) due to its heavy elements, the large resulting spin-orbit splitting and Darwin shifts. It has a low melting point of 800 K. Previously, the band gap of InSb has only been measured up to room temperature and estimated from Hall effect measurements of the effective mass up to 470 K. Calculations indicate that InSb should undergo a topological phase transition from semiconductor to semi-metal at 600 K. It is interesting to see in the data if this transition occurs below the melting point of InSb.

HL 21.4 Wed 15:45 H32

Ultra-fast change of the absorption onset in undoped cubic GaN — •Elias Baron[1], Martin Feneberg[1], Rüdiger Goldhahn[1], Michael Deppe[2], Donat J. As[2], Shirly Espinoza[3], and Martin Zahradník[3] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Department Physik, Universität Paderborn, Germany — [3]ELI Beamlines, Institute of Physics, Czech Academy of Science, Dolní Břežany, Czech Republic

Nitride semiconductors are essential for modern applications, which means that an example for nitride research is necessary. For this, the cubic zincblende phase is predestined on account of isotropic properties. We present our investigation of thin film zincblende GaN, deposited by plasma-assisted molecular beam epitaxy on 3C-SiC/Si substrates in (001) orientation, by time-resolved spectroscopic ellipsometry, based on a pump-probe approach in the visible and ultra violet spectral range. The 266nm pump beam excites the cubic GaN far above the band gap and therefore creates up to $\approx 5 \times 10^{20}\mathrm{cm}^{-3}$ electron-hole pairs, which influence the dielectric function due to many-body effects like band gap renormalization and Burstein-Moss shift. By varying the delay time between pump and probe beam from femto- to nanoseconds, a time-resolved change of the absorption onset due to the relaxation and recombination of electron-hole pairs in the context of many-body effects is observed and concur with comparable steady-state measurements of highly n-type doped GaN.

15 min. break

HL 21.5 Wed 16:15 H32

Strain-induced bandgap transition in III-V semiconductors — •Badal Mondal and Ralf Tonner-Zech — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, 04103 Leipzig, Germany

In the interest of a deep and thorough understanding of the effect of strain on the electronic properties, we have developed a systematic strategy for the analysis of composition-strain-bandgap relationship in III-V semiconductors. Using the tool of computational method, modern *ab-initio* density functional theory (DFT), we have shown that depending on the nature and strength of applied strain in the system the material behavior can change substantially. Namely, a direct bandgap semiconductor can transform to an indirect bandgap semiconductor and vice versa. This ultimately enables us to construct the 'bandgap phase diagram' [1] by mapping the different direct-indirect transition points with composition and strain. By combining the advanced tools of machine learning with DFT, we have further developed an efficient approach to extend the scope in multinary systems. In combination with the thermodynamic phase diagram, we have shown that this new way of mapping the effect of strain will significantly improve the future developments in terms of strategic choice of certain application-oriented best-suited material systems or vice versa.

[1] https://bmondal94.github.io/Bandgap-Phase-Diagram/, 2022

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HL 21.6 Wed 16:30 H32

Probing free carrier and exciton dynamics in bulk gallium selenide with two-dimensional electronic spectroscopy — •Jonas Allerbeck[1,2], Thomas Deckert[2], Laurens Spitzner[3], and Daniele Brida[2] — [1]nanotech@surfaces Laboratory, Empa, Überlandstrasse 129, 8600 Dübendorf, Switzerland — [2]Department of Physics and Materials Science, Université du Luxembourg, 162a Avenue de la Faïencerie, L-1511 Luxembourg, Luxembourg — [3]Department of Physics, University of Konstanz, Universitätsstrasse 10, 78457 Konstanz, Germany

Multidimensional optical spectroscopy employing a sequence of three or more pulses is a powerful technique to disentangle energetic correlations. While the technique has been used to study molecular systems, its application to femtosecond dynamics in solid state materials remains new. In this work, we investigate the ultrafast response of excitons and free carriers in the technologically important semiconductor gallium selenide (GaSe) with 10 fs temporal and 1 THz (4 meV) spectral resolution. 2D spectra resolve the excitation energy of broadband

pulses and reveal strong bleaching at the exciton resonance, which is hidden by the free carrier response in standard pump-probe measurements, allowing to extract an exciton relaxation time of 112 fs at room temperature. Our quantitative mapping of carrier thermalization shows the interplay of spectral diffusion, induced absorption and dephasing, motivating ongoing theoretical investigation and paving the way for future investigation of quasiparticle correlations in functional material systems.

HL 21.7 Wed 16:45 H32

Multistable, co- and counterflowing currents of polariton condensates in concentric ring-shaped and elliptical potentials — •Franziska Barkhausen, Matthias Pukrop, Xuekai Ma, and Stefan Schumacher — Department of Physics and CeOPP, Paderborn University, Germany

Vortices occur in a broad range of nonlinear systems. They have been widely investigated in many physical systems and different materials for their fundamental interest and for applications in data storage and information processing. In polariton condensates in semiconductor microcavities vortices can be supported and trapped by including a ring-shaped potential, for example optically induced using spatially structured non-resonant excitation [1]. Here we theoretically study vortices excited non-resonantly in different fabricated ring-shaped and elliptical external potentials. These kinds of potentials trap the polariton condensate such that different steady-state solutions, oscillating or co- and counterrotating solutions can be formed, depending on the size and number of the potential wells. A single ring potential can stabilize multistable solutions carrying different orbital angular momenta (OAM) which can lead to the beating of different modes and spatially rotating solutions. A concentric arrangement of many rings enables the excitation of Bessel-like solutions [2]. Embedding a standard ring potential in an elliptical one gives rise to phase differences of the condensates in the two rings and to counterflowing condensate currents.

[1] X. Ma, et al., Nat Commun 11, 897 (2020).
[2] F. Barkhausen, et al., Phys. Rev. B 103, 075305 (2021).

HL 21.8 Wed 17:00 H32

Optical properties of transition metal oxide perovskites by the Bethe-Salpeter equation — •Lorenzo Varrassi[1], Peitao Liu[2], Zeynep Ergönenc Yavas[3], Menno Bokdam[4], Georg Kresse[2], and Cesare Franchini[1,2] — [1]Department of Physics, University of Bologna — [2]Faculty of Physics, University of Vienna — [3]Turkish Aerospace Industries- Department of Materials Engineering — [4]University of Twente, Faculty of Science and Technology

The accurate account of optical spectra of semiconductors and insulators requires the explicit treatment of the electron-hole (e-h) interaction. This talk will present a systematic investigation of the role of excitonic effects on the optical properties of transitions metal oxide perovskites. A representative set of fourteen compounds has been selected, including 3d, 4d, and 5d perovskites. Optical conductivities and exciton binding energies are calculated through the Bethe-Salpeter equation (BSE) based on G0W0 approximation. Results are compared with the experimental data.

The origin of spectra's main peaks are investigated through the analysis of the e-h coupling coefficients. A particular emphasis in our analysis was placed on how differences between the electronic band-structures of the studied compounds impact the optical properties and e-h coupling coefficients.

A computationally cheaper model-BSE approach, based on a model dielectric screening, was employed for the calculations of the excitonic binding energies. The quality and validity of the the approach was assessed through a comparison with reference G0W0+BSE values.

15 min. break

HL 21.9 Wed 17:30 H32

Dynamics of phase defects trapped in optically imprinted orbits in dissipative binary polariton condensates — •Jan Wingenbach, Matthias Pukrop, Stefan Schumacher, and Xuekai Ma — Physics Department and CeOPP, Paderborn University, Germany

Polaritons are quasiparticles, formed due to the strong coupling of photons and excitons in planar semiconductor microcavities. In polariton condensates, quantized vortices can form, which makes them promising candidates for novel quantum technological devices [1]. By nonresonant excitation of the condensate, periodic potentials can be generated, which can be used to trap vortices and stabilize phase defects, so-called dark solitons [2]. We study the dynamics of phase defects trapped in a finite, optically imprinted ring lattice in binary polariton condensates. Depending on their topological charge a Magnus force leads to the circulation of vortices in these orbits. This is investigated considering the cross interaction (CI) between the condensates in different spin components and the spin-orbit interaction (SOI). We observe elongated vortices and frozen phase defects, which resemble dark solitons showing finite size in both spin components. When the entire orbit is occupied, a snake instability is triggered, leading to the decay of the dark ring solution. In our system, the motion of vortex constellations is affected by the SOI. [1] X. Ma, et al., Nature Communications 11, 1 (2020). [2] X. Ma, et al., Phys. Rev. Lett. 118, 157401 (2017).

HL 21.10 Wed 17:45 H32

Optimization of Silicon Nanoantenna for Optical Phased Arrays — •Andreas Strauch, Henna Farheen, Viktor Myroshnychenko, and Jens Förstner — University Paderborn - Department of Electrical Engineering and Information Technology, Paderborn, Germany

The classical microwave phased array is a proven antenna technology since the beginning of the last century. Among other things, it leads to significant improvements in radar technology as well as mobile, radio and satellite communications. Beyond that, this principal is not limited to the microwave band and can transfer into the optical spectrum, such as for light detection and ranging (LIDAR). The specific, technical features of the optical phased array (OPA) are the fast, non mechanical variation of directional characteristic (beam steering) during the operation and the great beam focusing through an ensemble of sophisticatedly, interacting single antennas. Besides them, the usage of serveral single antennas increases the redundancy and gives a high operational reliability and signal-to-noise ratio.

We designed, numerically analyzed, and optimized an efficient Silicon on Insulator (SOI) based photonic light transmitter, working in the infrared band, with high antenna gain and sidelobe attenuation (super resolution in principle), high redundancy and noise robustness and most important an electronically, configurable farfield characteristic. In comparison to a reference design, we increased the radiation efficiency from 2.66 to 9% by numerical optimization using evolutionary and natural analogue approaches.

HL 21.11 Wed 18:00 H32

Spatially Resolved Dynamics of Intra 3d Luminescence of Co in ZnO Nanowires Revealed by Nanoscale X-ray Analysis — •Christian Plass[1], Valentina Bonino[2], Maurizio Ritzer[1], Lukas Jäger[1], Jaime Segura-Ruiz[2], Gema Martinez-Criado[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743, Jena — [2]ESRF - The European Synchrotron, 71 Avenue des Martyrs, 38043 Grenoble, France

Color centers in semiconductors have drawn a lot of interest in recent years. They are able to provide high quality single photon sources. Such color centers can for example be obtained by doping ZnO with Co. The underlying emission processes have to be determined in order to achieve quantum emission by such a system. Hence, there is a strong need to evaluate how the dynamics of the luminescence is influenced by elemental composition and local environment of the color centers. High resolution synchrotron based methods like X-ray fluorescence (XRF) and X-ray excited optical luminescence (XEOL) enable insight into such compositional and functional variations. Simultaneous XRF and XEOL measurements of Co doped ZnO nanowires were conducted: The highly focused X-ray nanobeam at the ID16B-NA station of the European Synchrotron Radiation Facility scanned the nanowire and by analyzing the emitted X-ray fluorescence radiation together with the corresponding optical luminescence correlating maps were obtained. As the spatial resolution is about 50nm, we can show how the local composition influences the spectral dynamics of the obtained emission.

HL 21.12 Wed 18:15 H32

Fröhlich polarons in cubic materials — •B. Guster[1], P.M.M.C. Melo[2], B.A.A. Martin[3], V. Brousseau-Couture[4], J.C. de Abreu[2], A. Miglio[1], M. Giantomassi[1], M. Côté[4], J.M. Frost[3], M.J. Verstraete[2], and X. Gonze[1,5] — [1]UCLouvain(UCL), IMCN, Louvain-la-Neuve, Belgium — [2]NanoMat/Q-Mat/CESAM, Université de Liège, Liège, Belgium — [3]Department of Physics, Imperial College London, London, UK — [4]Département de Physique, Université

de Montréal, Montréal, Canada — [5]Moscow, Russia

Most works on polaron models, to understand their characteristics such as radius, effective mass, mobility and energy dispersion, have focused on the original Fröhlich model. Real cubic materials have electronic band extrema that are often degenerate, or anisotropic. In this work, we keep the continuum hypothesis inherent to large polaron models, but go beyond the existing isotropic and nondegeneracy hypotheses, and also include multiple phonon modes. For polaron effective masses, we provide (i) the analytical result for the case of anisotropic electronic energy dispersion, with two distinctive effective masses (uniaxial), (ii) an approximate expression for the case of three distinctive axes (ellipsoidal), (iii) numerical simulations for the 3-band degenerate case, typical of III-V and II-VI semiconductor valence bands. We also deal with the strong-coupling limit, using a variational treatment: we propose trial wavefunctions for the three above-mentioned cases as well, providing polaron radii and energies. We gauge such approaches for the case of a dozen of II-VI and III-V semiconductors, and oxides.