HL 5: Optical Properties I

Time: Monday 9:30–11:45 Location: EW 561

HL 5.1 Mon 9:30 EW 561

Can we predict exciton binding energies from ground-state properties? — •Malte Grunert, Max Grossmann, and Erich Runge — Theoretische Physik I, TU Ilmenau, Germany

Accurate ab-initio exciton binding energies are commonly obtained by solving the Bethe-Salpeter equation on the results of an expensive quasiparticle calculation. Accurate ground-state properties, however, are often much cheaper to evaluate. Establishing reliable connections between cheap ground-state properties and expensive exciton binding energies is therefore desirable - ideally, we would be able to predict the latter based on the former!

A well-known method of predicting exciton binding energies is the Wannier-Mott model, which is however not directly applicable to more localized excitons. Several alternative approaches have been put forward proposing that e.g., the colocalization of electron and hole states [1] or a high JDOS around the bandgap [2] correlates with increasing exciton binding strength.

We investigate and possibly verify these proposed links between exciton binding energies and ground-state properties in several dozen materials across different classes of materials, including simple narrow- and wide-bandgap semiconductors, insulators, and more complex compounds such as transition metal chalcogenides and perovskites. We critically evaluate emerging trends and attempt predictions going beyond the Wannier-Mott model.

[1] M. Dvorak et al., Phys. Rev. Lett., 2013, 110, 016402
[2] E. Baldini et al., Nat. Commun. 2017, 8, 13

HL 5.2 Mon 9:45 EW 561

Conduction band nonparabolicity, chemical potential, and carrier concentration of intrinsic InSb as a function of temperature — •Stefan Zollner, Carlos Armenta, and Sonam Yadav — New Mexico State University, Las Cruces, NM, USA

The goal of our work is to predict the complex dielectric function of intrinsic indium antimonide from 80 to 800 K, which was recently measured using spectroscopic ellipsometry [M. Rivero Arias *et al.*, J. Vac. Sci. Technol. B **41**, 022203 (2023)]. The first step is to find a good analytical description for the nonparabolic band structure of InSb based on $\vec{k} \cdot \vec{p}$ theory. We implement a simple 8×8 $\vec{k} \cdot \vec{p}$ Hamiltonian based on the work of Kane (1956) within the limit of large spin-orbit splittings, where a single nonparabolicity parameter provides a good description of the density of states. We select a value of the momentum matrix element P which yields the experimental effective electron mass for the unrenormalized low-temperature band gap. The temperature-dependence of the effective electron mass is then calculated taking into account only the thermal expansion contribution to the redshift of the direct band gap, not the renormalization due to deformation-potential electron phonon interactions. With this approach, we calculate the temperature dependence of the chemical potential, the thermal Burstein-Moss shift, and the carrier concentration of intrinsic InSb, which is in good agreement with electrical Hall effect measurements. The calculation of the temperature-dependent dielectric function will be the next step.

HL 5.3 Mon 10:00 EW 561

Interplay between excitons and lattice vibrations in the optical properties of monolayer boron nitride — •Giovanni Marini, Matteo Calandra, and Pierluigi Cudazzo — University of Trento, Department of Physics, Via Sommarive 14 Povo(TN)

Monolayer hexagonal boron nitride exhibits a complex optical response, the full understanding of which remains elusive. The photoluminescence spectrum is enriched with satellite features that hint at the existence of substantial couplings between excitons and phonons whose nature is completely unknown. Being photoluminescence experiments always performed in presence of a substrate, the knowledge of the basic properties of the isolated ideal layer constitutes fundamental reference for the interpretation of the experiments and allows disentangling the effect of the substrate. Here, through a cumulant expansion of the charge response function developed in the framework of many body perturbation theory, we performed a first principles study of the exciton-phonon coupling in monolayer boron nitride. Our results allows to identify the different exciton-phonon scattering channels and their effect on the optical properties of this system providing important insights about recent photoluminescence experiments.

HL 5.4 Mon 10:15 EW 561

Optical and Structural Properties of Zinc Oxide Nanoparticles using the Leaf Extract of Silybum marianum (Milk Thistle) — •Ahed AL-Faouri[1], Mahmoud Abu-Kharma[2], and Mahmoud Hatem[3] — [1]Al-Ahliyya Amman University — [2]Al-Balqa Applied University — [3]Al-Balqa Applied University

This study utilized the leaf extract of Silybum marianum (Milk thistle), as an effective bio-reductant, stabilizer, and capping agent for the synthesis of zinc oxide nanoparticles (ZnO-NPs) at ambient temperature. The chosen approach was not only simple and efficient but also demonstrated low-cost, non-toxic, and environmentally friendly characteristics, aligning with green synthesis principles. ZnO -NPs were detected and characterized using a Fourier transform infrared spectroscopy (FTIR), UV-Visible (UV-Vis) spectroscopy, X-ray powder diffraction (XRD), and scanning electron microscope (SEM). UV-Vis spectroscopy showed a sharp peak at 373 nm, and the energy band gap was measured to be approximately 2.77 eV. Furthermore, the UV-Vis analysis was utilized to quantify and interpret a range of optical properties. These properties include the absorption coefficient (α), skin depth (δ), optical density (Dopt), extinction coefficient (k), optical conductivity (σopt), and the optical dielectric constant (ϵ). This thorough exploration of the optical and structural characteristics of the CuO-NPs aids in comprehending their response to light interaction, thereby opening avenues for their practical applications across various fields.

15 min. break

HL 5.5 Mon 10:45 EW 561

Cr-doped Ga_2O_3 microcavities for thermometric applications — •Ruben Johannes Theodorus Neelissen[1], Manuel Alonso-Orts[1], Daniel Carrasco[2], Marco Schowalter[1], Andreas Rosenauer[1], Emilio Nogales[2], Bianchi Mendez[2], and Martin Eickhoff[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.

Monoclinic gallium oxide (β-Ga_2O_3) is a transparent conductive oxide with an ultra-wide bandgap of 4.8 eV and high chemical and thermal resilience. This makes β-Ga_2O_3 very interesting for areas such as high power (opto)electronics.

Previous work [1] focused on chromium doped β-Ga_2O_3 microwires as optical microcavities and their use of thermometric application. Focused ion beam (FIB) fabricated distributed Bragg reflectors (DBRs) enhance the confined light in the microcavities, resulting in strong resonances. With increasing temperature, the resonant wavelength of these peaks redshifts due to changes in both the refractive index and the optical length of the cavities. The operation of these wide dynamic range thermometers with a resolution of 1 K was demonstrated [1].

However, the FIB-fabricated microcavities involve a complex fabrication process, are mechanically unstable and are not resilient to high laser powers. In this work, a new fabrication method involving atomic layer deposition (ALD) was developed.

[1] M. Alonso-Orts et al. In: *Small 18.1* (2022), p. 2105355.

HL 5.6 Mon 11:00 EW 561

Carrier generation and diffusion in Ga(As,Sb) nanowires probed by cathodoluminescence spectroscopy — •Mikel Gómez Ruiz[1], Vladimir Kaganer[1], Akhil Ajay[2], Hyowon Jeong[2], Gregor Koblmüller[2], Oliver Brandt[1], and Jonas Lähnemann[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Germany — [2]Walter Schottky Institut, School of Natural Sciences, Technical University of Munich (TUM)

Semiconductor nanowire (NW) structures emitting at wavelengths used for optical telecommunications are attractive for the integration on silicon-on-insulator waveguides. Here, we study Ga(As,Sb) NWs with a lower bandgap (In,Ga)As insertion on a microscopic scale by cathodoluminescence (CL) spectroscopy to understand the charge carrier transfer to and the recombination in the insertion. In our CL experiments the electron beam, and thus the volume in which electron-

hole pairs are generated, is scanned along the axis of the NW. After their generation and diffusion, the carriers recombine either in the Ga(As,Sb) segment or in the (In,Ga)As insertion, giving rise to spectrally distinct CL bands. The intensity profiles of both emission bands are recorded as a function of the beam position. Although the (In,Ga)As insertion is only about 20 nm long, the corresponding CL band can be observed over a length of more than 400 nm under high excitation conditions. The evolution of these profiles with temperature is studied to determine the diffusion length in the Ga(As,Sb) NW using a model that includes the temperature-dependent generation volume and the diffusion of the cathodogenerated carriers.

HL 5.7 Mon 11:15 EW 561

Excitons in Helium Under Pressure — •Fatema Mohamed[1], Frédéric Pailloux[2], Marie-Laure David[2], Laurent Pizzagalli[2], Lucia Reining[1], and Matteo Gatti[1] — [1]LSI, Ecole Polytechnique, CNRS, Palaiseau, France — [2]Institut Pprime, Université de Poitiers, Poitiers, France

The absorption and the electron energy loss spectra of solid helium at different pressures are calculated using a first principles approach based on the Bethe-Salpeter equation of many-body perturbation theory. The results are used to explain the effect of pressure on HCP helium that has been measured by spectroscopy experiments [1,2]. We found a well defined exciton peak, showing linear pressure dependence, both in the peak position and intensity. We calculated the excitonic dispersion of the loss function along the Γ-M direction for momentum transfers beyond the first Brillouin zone. We found strong parabolic-like dispersion of the spectra, dominated by the screened Coulomb interaction. Near Bragg reflection points we found an anomalous angular dependence of the exciton peak, due to the crystal local field effects, analogously to the plasmon in graphite [3].

References:
1- M.-L. David, et al. Appl. Phys. Lett. 98, 171903, 2011.
2- H. K. Mao, et al. Phys. Rev. Lett. 105, 186404, 2010.
3- R. Hambach, et al. Phys. Rev. Lett. 101, 266406, 2008.

HL 5.8 Mon 11:30 EW 561

UV defect emitters in hexagonal boron nitride — •Nils Bernhardt[1], Luca Choi[1], Benjamin M. Janzen[1], Felix Nippert[1], Angus Gale[2], Igor Aharonovich[2], Milos Toth[2], and Markus R. Wagner[3,1] — [1]Technische Universität Berlin, Insitute of Solid State Physics, Berlin, Germany — [2]University of Technology Sydney, Sydeny, Australia — [3]Paul Drude Institute for Solid State Electronics, Berlin, Germany

Room temperature defect quantum emitters in hexagonal boron nitride have emerged as a source of considerable scientific interest. Recent studies have demonstrated the ability to engineer reliable single photon sources in thin film hBN with reproducible emission properties in all spectral ranges, suitable for applications such as quantum communications. While extensive studies of such emitters in hBN have been conducted in the visible and near-IR spectral range, this work aims to investigate the recently observed UV luminescence of hBN point defects at 4.1eV, likely caused by carbon substitutions at nitrogen sites.

A frequency-quadrupled titanium-sapphire laser at 200 nm is used for pulsed above-bandgap excitation and compared to sub-bandgap pulsed and continuous wave excitation. A direct dependence between the luminescence of the defect and its surroundings is explored to establish a link between the properties of the 2D material samples and the electron-phonon coupling. These results are corroborated by the correlation of AFM, micro-Raman, and micro-PL mapping measurements.