CPP 23: Optical Properties (joint session HL/CPP)

Time: Tuesday 9:30–13:00 Location: POT 112

CPP 23.1 Tue 9:30 POT 112

Can Ge and Si be optoelectronic materials: Hexagonal polytypes — •Martin Keller[1], Abderrezak Belabbes[1,2], Jürgen Furthmüller[1], Friedhelm Bechstedt[1], and Silvana Botti[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörpertheorie und -optik, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Department of Physics, Sultan Qaboos University, P.O. Box 36, PC 123, Muscat, Oman

The group IV elements silicon and germanium crystallize in cubic diamond structure under ambient conditions and feature indirect bandgaps. Therefore they cannot emit light efficiently and are not applicable in active optoelectronic devices. Under high pressure, however, as well as using different growth techniques, several Si and Ge polymorphs, including hexagonal polytypes, have been observed. Lonsdaleite Ge as well as Ge-rich hexagonal alloys have even been found to have a direct bandgap and strongly emit light with varying frequency. Thus hexagonal systems have become of great interest for potential optical emitters that may be integratable with CMOS technology. We have performed extensive ab initio studies of the energetic, structural, elastic and electronic properties as well as the strengths of some dipole transitions of the hexagonal Si and Ge polytypes 2H, 4H and 6H using Density Functional Theory and approximate quasiparticle treatments, and trends between the different geometries are analysed. The results for cubic and hexagonal Si and Ge agree excellently with existing experimental findings. The electronic structures point to promising optical properties.

CPP 23.2 Tue 9:45 POT 112

Many-body effects in the mid-infrared dielectric function of InSb from 80 to 800 K — Melissa Rivero Arias, Cesy Zamarripa, Jaden Love, Carlos Armenta, Carola Emminger, Sonam Yadav, and •Stefan Zollner — New Mexico State University, Las Cruces, NM, USA

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 300 K) due to its heavy elements and the large resulting spin-orbit splitting and Darwin shifts. The band gap is extracted from the dielectric function by fitting with a parametric oscillator model. It decreases from 80 to 450 K following a Bose-Einstein model, then remains constant up to 550 K, and increases again at the highest temperatures. This is explained with a thermal Burstein-Moss shift: The onset of optical absorption increases as electron-hole pairs are thermally excited at the highest temperatures. The intrinsic carrier concentration determined from the Drude tail in the ellipsometry spectra agrees qualitatively with temperature-dependent Hall experiments and calculations based on degenerate Fermi-Dirac statistics.

CPP 23.3 Tue 10:00 POT 112

Polarized Raman scattering study of epitaxially grown GeSn layers with various Sn content — •Agnieszka Anna Corley-Wiciak[1], Omar Concepción[2], Marvin Hartwig Zoellner[1], Detlev Grützmacher[2], Dan Buca[2], Giovanni Capellini[1,3], and Davide Spirito[1] — [1]IHP Leibniz-Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]Peter Grünberg Institute 9 (PGI-9) and JARA-Fundamentals of Future Information Technologies — [3]Dipartimento di Scienze, Università Roma Tre, V.le G. Marconi 446, 00146 Roma, Italy

$Ge_{1-x}Sn_x$ alloys are an excellent candidate for developing mid-infrared light sources integrated with CMOS technology. The challenges in the controlled growth with high crystal quality have highlighted the peculiarity of these alloys, which can be monitored by their vibrational properties. To this purpose, Raman spectroscopy is an effective experimental method to determine these properties, as this technique is non-destructive, contactless, fast, and locally resolved. We use Raman scattering with different polarization configurations to investigate $Ge_{1-x}Sn_x$ ($0.05 \leq x \leq 0.14$) alloys grown by Chemical Vapour Deposition on Ge/Si virtual substrates. Measurements were performed in backscattering geometry with parallel and cross polarizations. In this way, we identify multiple components in the vibrational modes and how they deviate from simplified models. Our results will help to understand the fundamental properties of $Ge_{1-x}Sn_x$ alloys to enable fast assessment for their applications in optoelectronic and thermoelectric.

CPP 23.4 Tue 10:15 POT 112

Eigenmodes and Polarization Structure of Coupled Elliptical Microcavities — •Johannes Düreth[1], Simon Betzold[1], Monika Emmerling[1], Antonina Bieganowska[2], Jürgen Ohmer[3], Utz Fischer[3], Sven Höfling[1], and Sebastian Klembt[1] — [1]Technische Physik, RCCM and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg, Germany — [2]Faculty of Problems of Fundamental Technology, Department of Experimental Physics, Laboratory for Optical Spectroscopy of Nanostructures, Wroclaw, Poland — [3]Department of Biochemistry, University of Würzburg, Germany

Elliptical potentials give rise to a set of eigenmodes called Ince-Gaussian modes. Contrary to hemispherical potentials, the geometric shape leads to a mode splitting of the otherwise degenerate fundamental mode. Theoretically, this behaviour can be exploited to realize interesting topological phenomena like non-reciprocal transport, the non-hermitian skin-effect or engineer artificial gauge fields. On the way to an experimental implementation of such systems, the singular building blocks of these photonic potentials - single and coupled elliptical potentials - have to be experimentally studied.

Here we present an investigation of the mode splitting and polarisation in single elliptical microcavities, as well as an examination of the coupling between differently angled ellipses.

15 min. break

CPP 23.5 Tue 10:45 POT 112

Optical properties of $Ag_xCu_{1-x}I$ alloy thin films — •E. Krüger[1], M. Seifert[2], V. Gottschalch[3], H. Krautscheid[3], C.S. Schnohr[1], S. Botti[2], M. Grundmann[1], and C. Sturm[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany — [2]Friedrich-Schiller-Universität Jena, Institut für Festkörpertheorie und Optik , Germany — [3]Universität Leipzig, Institut für Anorganische Chemie, Germany

Copper iodide (CuI) is a promising wide bandgap semiconductor for applications in transparent optoelectronic devices. In this context, the specific tuning of electrical and optical properties, which can potentially be achieved with ternary alloys such as $CuBr_xI_{1-x}$ [1] and $Ag_xCu_{1-x}I$ [2], is crucial for the development of novel CuI-based devices. In particular, $Ag_xCu_{1-x}I$ is of great interest because the intrinsic conductivity changes from p-type to n-type with increasing Ag content.

Here we present the bandgap energy and spin-orbit splitting in $Ag_xCu_{1-x}I$ alloys as a function of alloy composition and temperature, studied by a combination of experimental and computational methods. The non-linear bandgap dependence on Ag content can be described by a quadratic bowing parameter of 0.54 eV and is dominated by charge carrier redistribution effects in the presence of unequal element-specific bond lengths. The slight increase of the spin-orbit splitting from 640 meV for CuI to about 790 meV for AgI is discussed in terms of decreasing p-d hybridization of the valence bands at the Γ-point.

[1] N. Yamada et al., Adv. Funct. Mater. **30**, 2003096 (2020)
[2] A. Annadi and H. Gong, Appl. Mater. Today **20**, 100703 (2020)

CPP 23.6 Tue 11:00 POT 112

Multipole theory of optical spatial dispersion in crystals — •Óscar Pozo — Centro de Física de Materiales, Universidad del País Vasco, 20018 San Sebastián, Spain

Natural optical activity is the paradigmatic example of an effect originating in the weak spatial inhomogeneity of the electromagnetic field on the atomic scale. In molecules, such effects are well described by the multipole theory of electromagnetism, where the coupling to light is treated semiclassically beyond the electric-dipole approximation. That theory has two shortcomings: it is limited to bounded systems, and its building blocks - the multipole transition moments - are origin dependent. In this work, we recast the multipole theory in a translationally-invariant form that remains valid for periodic crystals. Working in the independent-particle approximation, we introduce 'intrinsic' multipole transition moments that are origin independent and transform covariantly under gauge transformations of the Bloch eigenstates. Electric-

dipole transitions are given by the interbank Berry connection, while magnetic-dipole and electric-quadrupole transitions are described by matrix generalizations of the intrinsic magnetic moment and quantum metric. In addition to multipole-like terms, the response of crystals at first order in the wave vector of light contains band-dispersion terms that have no counterpart in molecular theories. The rotatory-strength sum rule for crystals is found to be equivalent to the topological constraint for a vanishing chiral magnetic effect in equilibrium, and the formalism is validated by numerical tight-binding calculations.

CPP 23.7 Tue 11:15 POT 112

Predicting bandgap in strain-engineered multinary III-V semiconductors — •Badal Mondal and Ralf Tonner-Zech — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, 04103 Leipzig, Germany

The tuning of the type and size of bandgaps of III-V semiconductors is a major goal for optoelectronic applications. Varying the relative composition of several III- or V-components in compound semiconductors is one of the major approaches here. Alternatively, straining the system can be used to modify the bandgaps. By combining these two approaches, bandgaps can be tuned over a wide range of values, and direct or indirect semiconductors can be designed. However, an optimal choice of composition and strain to a target bandgap requires complete material-specific composition, strain, and bandgap knowledge. Exploring the vast chemical space of all possible combinations of III- and V-elements with variation in composition and strain is experimentally not feasible. We thus developed a density-functional-theory-based predictive computational approach for such an exhaustive exploration. This enabled us to construct the 'bandgap phase diagram' [1] by mapping the bandgap in terms of its magnitude and nature over the whole composition-strain space. Further, we have developed efficient machine-learning models to accelerate such mapping. We will show the application to binary [2], ternary and quaternary material combinations and the possible impact on device design.

[1] https://bmondal94.github.io/Bandgap-Phase-Diagram , 2022
[2] https://arxiv.org/abs/2208.10596

CPP 23.8 Tue 11:30 POT 112

GeSn vertical p/n photodetectors formed by 2-step ion implantation — •Shuyu Wen[1,2], Saif Shaikh[1], Oliver Steuer[1], Yonder Berencen[1], Slawomir Prucnal[1], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]Institute of Semiconductors, Chinese Academy of Sciences, Bejing, China

Germanium (Ge) is a promising material in integrated circuit (IC) due to the high mobility of hole carrier and highly compatibility in the Si-base IC technology. However, the indirect band structure of Ge leads to the low radiative recombination efficiency, limiting the application in opto-electronics. Alloying Ge with Tin (Sn) is a promising method to obtain energy band modification even to a direct band. Here, high quality Ge0.97Sn0.03 and Ge0.955Sn0.045 alloy is obtained by CMOS-compatible ion implantation method. Tensile strain leads by Sn alloying and damage recovery after Flash annealing (FLA) are characterized by Raman and XRD measurements. A subsequently phosphors implantation is applied to obtain vertical pn photodetectors (PD). The device shows an extended spectral response comparing with commercial Ge PD. This work provides a new CMOS-compatible method to fabricate photodetectors in short-wave infrared.

15 min. break

CPP 23.9 Tue 12:00 POT 112

Interplay between strain, Sn content and temperature in GeSn-based optoelectronic devices — •Ignatii Zaitsev[1], Agnieszka A. Corley-Wiciak[1], Dan Buca[2], Omar Concepción[2], Michele Virgilio[3], Giovanni Capellini[1,4], Costanza L. Manganelli[1], and Davide Spirito[1] — [1]IHP - Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany — [2]PGI 9, Jülich, Germany — [3]Università di Pisa, Pisa, Italy — [4]Università Roma Tre, Roma, Italy

Several works have shown the subtle interplay between thermomechanical strain, Sn content and band occupation in optoelectronic devices based on CMOS-integratable group-IV materials (Ge, SiGe, SiGeSn). This is especially the case when temperature plays a key role, e.g. devices operating at cryogenic temperature or in presence of high power. Here we provide a theoretical-experimental approach combining 3D FEM calculations, Raman and photoluminescence spectroscopy to fully capture the influence of mechanical and thermomechanical features on the optical properties. We apply this method to strained GeSn microdisks, a device geometry aimed at laser in the MIR range. With the presented methods, we can develop a thorough guidelines for the assessment and design of integrated light emitters.

CPP 23.10 Tue 12:15 POT 112

Excitons in MoS_2 bilayers under pressure — •Jan-Hauke Graalmann[1], Paul Steeger[2], Robert Schmidt[2], Steffen Michaelis de Vasconcellos[2], Rudolf Bratschitsch[2], and Michael Rohlfing[1] — [1]Institute of Solid State Theory, University of Münster, 48149 Münster, Germany — [2]Institute of Physics, University of Münster, 48149 Münster, Germany

Theoretical and experimental studies have shown that the optical spectrum of the MoS_2 bilayer changes under pressure.

Our theoretical investigations are based on DFT, *GdW* and the Bethe-Salpeter equation. For the specific stress conditions of the experiment, our calculations show an effective shift of the excitation energies of the A exciton towards higher energies with increasing pressure. This behaviour can be explained with an approximately constant direct band gap at the K point while the binding energy decreases. Due to a growing valence band splitting for increasing pressures, the interlayer exciton shows a smaller shift. These results are substantiated by measurements using a piston type diamond anvil cell (DAC) to create pressures in the GPa range.

The reason for only small changes of the fundamental band gap is a significant influence of interlayer interaction. The effect of a decreasing gap by biaxial lateral shrinking of each single layer under an external pressure gets counterbalanced by the reduction of the interlayer distance. Furthermore, the real space distribution shows an increased interlayer character for the A and interlayer exciton under pressure.

CPP 23.11 Tue 12:30 POT 112

Optical properties of a vacancy-related complex in 4H-SiC — •Maximilian Schober[1], Nicolas Jungwirth[1], Takuma Kobayashi[2], Johannes A. F. Lehmeyer[2], Michael Krieger[2], Heiko B. Weber[2], and Michel Bockstedte[1] — [1]Institute for Theoretical Physics, Johannes Kepler University Linz, Austria — [2]Lst. f. Angewandte Physik, Friedrich-Alexander-University Erlangen-Nürnberg, Germany

SiC is host to multiple color centers, such as the silicon vacancy, the divancy, and the carbon antisite-vacancy complex, with relevant applications as qubits, single photon sources and in quantum metrology. Recently, the carbon di-vacancy-antisite complex was identified as an annealing product of vacancy related defects [1], and is expected to feature favorable properties for quantum technology. The presence of strongly localized silicon and carbon dangling bonds points to rich photo- and spin physics that has so far not been explored in detail. In this work we probe the basal and axial configurations of $V_C C_{Si} V_C$ for their electronic-, optical- and radiative properties using a theoretical framework of hybrid density functional and many body approaches. We obtain the principal transitions, as well as the associated static- and transition dipole moments of the relevant charge states. Our results suggest a tentative identification of the carbon di-vacancy-antisite with the temperature-stable (TS) center [2].

[1] E. M. Y. Lee *et al.*, Nat. Commun. 12, 63 (2021).
[2] M. Rühl, C. Ott, S. Götzinger, M. Krieger, H. B. Weber, Appl. Phys. Lett. 113, 122102 (2018).

CPP 23.12 Tue 12:45 POT 112

Defects or Dots – what semiconductor physics can bring into optical super-resolution imaging — •Philipp Kellner[1], Jana Sütterlin[1], Paul Konrad[2], Andreas Sperlich[2], and Christian Eggeling[1,3] — [1]Institut für angewandte Optik und Biophysik, FSU Jena, Philosophenweg 7, 07743 Jena — [2]Physikalisches Institut, Julius-Maximilians Universität Würzburg, Am Hubland, 97074 Würzburg — [3]Institut für physikalische Hochtechnologie, Albert-Einstein-Straße 9, 07745 Jena

Super-resolved optical microscopy is a widely used tool throughout the medicine and biology community. Mostly and routinely done with organic dyes super-resolution imaging has led to various insights into cell structures and diffusional dynamics. The fundamental problem occuring with organic dyes is their rather dim brightness and their lack of photostability paired with photo-toxicity. This presentation will shed light on novel semi-conductor-based chromophores, like NV-centers in diamond, defects in hBN and CdTe quantum dots, and their use in optical nanoscale sensing schemes like StED-imaging or fluorescence correlation microscopy.