# HL 16: Semiconductors: Optical, Transport and Ultrafast Properties

Time: Thursday 11:15–12:45 Location: H1

HL 16.1 Thu 11:15 H1

**A Koopman's compliant exchange correlation potential for semiconductors** — •Michael Lorke, Peter Deak, and Thomas Frauenheim — Universität Bremen

Density functional theory is the workhorse of theoretical materials investigations. Due to the shortcoming of (semi-)local exchange correlation potentials, hybrid functionals have been established for practical calculations to describe surfaces, molecular adsorption, and defects. These functionals operate by mixing between semi-local and Hartree-Fock exchange semi-emprically. However, their parameters have to be optimized for every material separately. To treat materials with a more physics driven approach and without the need of parameter optimization is possible with many-body approaches like GW, but at an immense increase in computational costs and without the access to total energies and hence geometry optimization. We propose a novel exchange correlation potential[1] for semiconductor materials, that is based on physical properties of the underlying microscopic screening. We demonstrate that it reprocuduces the low temperature band gap of several materials. Moreover, on the example of defects in semiconductors, it respects the required linearity condition of the total energy with the fractional occupation number, as expressed by the generalized Koopman's theorem. It is shown, that alloys can be treated with a common choice of the functional. We also show that this novel functional can be used as a kernel in linear response TDDFT to reproduce excitonic effects in optical spectra

[1] Physical Review B 102 (23), 235168 (2020)

HL 16.2 Thu 11:30 H1

**Kerr and Faraday rotations of two-dimensional topological flat bands** — Alireza Habibi, Johan Ekström, Thomas Schmidt, and •Eddwi Hasdeo — Department of Physics and Materials Science, University of Luxembourg, Luxembourg, Luxembourg

Flat-band systems are one of main subjects of research in condensed-matter physics especially after the discovery of a strongly correlated phase in twisted bilayer graphene. Flat bands can be observed directly via angle-resolved photo-emission spectroscopy. However, due to the band flatness and the close proximity to the Fermi energy, a flat band is usually difficult to characterize. Here, we propose an alternative characterization method for topological flat bands using photon absorption. In topological bands, the anomalous Hall conductivity can rotate the incident light polarization, resulting in a rotated polarization of the transmitted light (Faraday effect) and the reflected light (Kerr effect). In this work, we employ a model featuring nearly flat bands, for which the bandwidth is much smaller than the band gap. We investigate the dynamical (ac) conductivities of the model in the presence of an external electric field. We contrast how flat bands and dispersive bands can be detected sensitively via Kerr and Faraday rotations. These results can serve as a simple characterization tool to determine the bandwidth or band flatness of topological materials.

HL 16.3 Thu 11:45 H1

**Benchmarking the accuracy of screened range-separated hybrids for bulk properties of semiconductors** — •Stefan A. Seidl, Bernhard Kretz, Christian Gehrmann, and David A. Egger — Technical University of Munich

A recently developed class of functionals, the so called screened range-separated hybrid (SRSH) functionals, only use one empirical parameter to fit the band gap to the accurately calculated band gap from the GW approach. After the tuning procedure of the range-separation parameter, SRSH functionals have been shown to provide accurate electronic-structure and optical properties of semiconductors [1]. This is an advantage over conventional semilocal and hybrid functionals in density functional theory (DFT), where it is known that they predict the structural properties well, but fail in the accurate description of electronic and optical properties. Here, we assess the accuracy of the SRSH functional to compute static and dynamic bulk properties (lattice constants, bulk moduli, atomization energies as well as phonon dispersion relations) of inorganic semiconductors [2]. We find that for these quantities, SRSH is similarly accurate as the two well-established functionals PBE and HSE. This demonstrates that the superior performance of SRSH for electronic-structure and optical calculations does not come at a cost of reduced accuracy for calculations of bulk properties.

[1] D. Wing et al, Phys. Rev. Materials 3, 064603 (2019)
[2] S. A. Seidl et al, Phys. Rev. Materials 5, 034602 (2021)

HL 16.4 Thu 12:00 H1

**Hydrogen-Bonding Ability of the GaAs (001) Surface** — •MARSEL KARMO and ERICH RUNGE — Weimarer Str.32

Thin films of direct-band gap III-V-semiconductors are widely used in optoelectronic devices such as lasers or solar cells. Their production via MOVPE/MOCVD involves hydrogen, which may or may not bind to the semiconductor surface. We study the hydrogen-bonding ability of the paradigmatic GaAs (001) surface via DFT using the VASP code. From the calculated thermodynamic potentials, we derive the phase diagram for the surface reconstructions as function of the availability of hydrogen and arsenic. Furthermore, we calculate the potential surface energy (PES) for a single adsorbed hydrogen which gives information about potential hydrogen bonding sites. For a wide range of the surface chemical potentials the (2x2)-surface with one hydrogen adsorbed to each As-dimer is energetically favored.

HL 16.5 Thu 12:15 H1

**Size-dependent electrical characteristics of highly doped Germanium nanowires** — •ahmad echresh, slawomir prucnal, yordan georgiev, and lars rebohle — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Germanium (Ge) is the most compatible material with silicon (Si)-based complementary metal-oxide-semiconductor processes. Ge has a higher electron and hole mobility compared to Si, leading to improved device performance. Moreover, Ge nanowires (GeNWs) are promising nanostructures for future nano- and optoelectronics due to their unique properties. In this work, ion beam implantation and flash lamp annealing (FLA) were used to dope phosphorous into the top Ge layer of Ge-on-insulator (GeOI) substrates, achieving a highly n-type doped semiconductor. Raman spectroscopy and Rutherford backscattering spectrometry were performed to characterize the crystallinity of the Ge layers after ion beam implantation and FLA. Subsequently, doped GeNWs were fabricated using electron beam lithography and inductively coupled plasma reactive ion etching. Electrical characterization of the GeNWs was conducted using an innovative Hall bar configuration. The effect of nanowire width on transport parameters such as resistivity and carrier mobility was investigated. Moreover, a nickel germanide layer was made using Ni deposition, followed by FLA to create ohmic contacts on n-type GeNWs.

HL 16.6 Thu 12:30 H1

**Extreme ultraviolet laser source for time resolved experiments including a terahertz driver laser** — Torsten Golz, Gregor Indorf, Mihail Petev, Jan-Heye Buss, Michael Schulz, and •Robert Riedel — Class 5 Photonics GmbH, Luruper Hauptstraße 1, 22547 Hamburg

The investigation of ultrafast dynamics in condensed matter and interfaces requires high repetition rates and multiple wavelength laser sources, together with femtosecond resolution. To meet these needs, we have therefore designed an extreme-ultraviolet laser source with output within the range of 21.7 to 50 eV (total flux of $3 \times 10^{12}$ photons/sec), together with a tunable output from 750 - 950 nm with 10 $\mu J$ pulse energy and a pulse duration of $<$40 fs, as well as, a third output for terahertz generation (2 mJ, $<$600 fs at 1030 nm). All three outputs are optically synchronized and can be used, for example, in time- and angle-resolved photoemission spectroscopy (trARPES) experiments.