# HL 13: Theory of electronic structure

Time: Monday 16:15–17:30 Location: EW 202

HL 13.1 Mon 16:15 EW 202

***GW* Method for *f*-electron Systems: Applications to $\mathbf{CeO_2}$ and $\mathbf{ThO_2}$** — •Hong Jiang[1], Ricardo I. Gomez-Abal[1], Xinzheng Li[1], Patrick Rinke[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of California at Sant Barbara, CA 93106

Understanding the physics of $f$-electron systems is regarded as a great challenge in condensed-matter physics today. In many of these materials the strong localization of the $f$-electrons gives rise to large many-body exchange and correlation effects and in addition leads to severe self-interaction errors in the local-density approximation (LDA). Many-body perturbation theory in the $GW$ approximation offers both a quasiparticle perspective and an exact treatment of exchange. It is therefore a promising approach for investigating these systems. In this work we apply the $G_0W_0$ method to $CeO_2$ and $ThO_2$, the "simplest" $f$-electron systems for which the LDA provides a qualitatively correct description, but underestimates band gaps significantly. For both materials, $G_0W_0$ based on LDA provides an accurate description for the fundamental ($p$-$d$) band gap. In $CeO_2$, the highly localized $f$-states fall within the $p$-$d$ gap; the $G_0W_0$ correction increases the $p$-$f$ gap and reduces the $f$-band width considerably. The resultant density of states is in good agreement with experiments. In $ThO_2$, the $5f$-states are more delocalized and overlap with the Th-$6d$ bands; the $G_0W_0$ correction shifts the $5f$-bands more than $6d$-bands, changing the density of unoccupied states considerably. Implications for general $f$-electron systems with partially filled $f$-shell are discussed.

HL 13.2 Mon 16:30 EW 202

**Hybrid density functionals for calculating the lattice dynamics of semiconductors** — •Kerstin Hummer and Georg Kresse — Vienna University, Sensengasse 8/12, 1090 Vienna, Austria

We present the *ab initio* study of the lattice dynamics of group-IV tetrahedral semiconductors, *i.e.*, cubic diamond, silicon, germanium, and grey tin as well as $\alpha$-quartz by a frozen phonon approach. The main objective of this work is to examine the performance of the screened hybrid density functional proposed by Heyd, Scuseria and Ernzerhof (HSE03) [1] for calculating phonon dispersion curves. The HSE03 has been very successful in describing the structural, electronic, and thermochemical properties of many solids comprising insulators, semiconductors as well as metals [2]. Within density functional theory (DFT), the widely utilized exchange-correlation functionals LDA and GGA show deficiencies in accurately describing the shallow $d$ electrons, which is particularly important in the case of germanium and grey tin. While for both, DFT-LDA yields a wrong (metallic) ground state and considerably underestimated phonon frequencies, the HSE03 functional significantly improves the results regarding the ground state solution, the theoretical lattice constant and thus the lattice dynamics. The presented *ab initio* phonon dispersions are compared to experimental data and reviewed in the context of previously reported theoretical findings, where particular emphasis is also placed on analyzing its sensitivity to the lattice constant utilized in the calculations.

[1] J. Heyd *et al.*, J. Chem. Phys. **118**, 8207 (2003)

[2] J. Paier *et al.*, J. Chem. Phys. **124**, 154709 (2006)

HL 13.3 Mon 16:45 EW 202

**An efficient approach to bound excitons: Applications to model and *ab initio* band structures.** — •Frank Fuchs, Claudia Rödl, André Schleife, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik and European Theoretical Spectroscopy Facility (ETSF), Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

The accurate calculation and parameter-free prediction of optical spectra including excitonic effects is highly desirable for both fundamental and applied research. Excitonic effects can be treated in the framework of many-body perturbation theory and the Bethe-Salpeter equation (BSE), by solving an eigenvalue problem for the electron-hole Hamiltonian $\hat{H}$. Although an efficient method for the calculation of excitonic spectra in an extended frequency range is available [1], a comparably efficient approach to bound excitonic states or even dark excitons is lacking. Instead, the diagonalization of $\hat{H}$, with computational costs scaling with the number of pair states $N$ like $O(N^3)$, is required. Thus computational studies are usually limited to well behaved problems and/or are insufficiently converged with respect to N. We present a numerically efficient approach for the calculation of a limited number of excitonic states avoiding the full diagonalization of $\hat{H}$. The approach is tested for its accuracy and performance by numerically solving the BSE for the Wannier-Mott two-band model in **k**-space and real semiconductors like InN and ZnO.

[1] W.G. Schmidt et al. , Phys. Rev. B **67**, 085307 (2003).

HL 13.4 Mon 17:00 EW 202

**Charged defects in a supercell formalism: from an empirical to a fully ab-initio treatment of finite-size effects** — •Christoph Freysoldt and Jörg Neugebauer — MPI für Eisenforschung, Düsseldorf, Germany

Charged point defects govern the charge carrier densities in semiconductors and are crucial for the performance of electronic devices. However, quantifying the thermodynamical, chemical, electrical, and other properties of such defects is a challenge to both theory and experiment. On the theoretical side, *ab-initio* calculations have proven to be a valuable tool. In these calculations, the defect is usually modelled in a periodic supercell with a few dozen to a few hundred atoms. Unfortunately, the supercell approximation introduces artificial electrostatic interactions between the charged defects. A number of correction schemes such as Makov-Payne corrections, potential alignment, scaling laws, or Coulomb truncation are available in the literature, but the magnitude of these corrections for a specific supercell usually scatters widely. The assumptions behind these schemes are often unclear and all schemes lack a stringent theoretical foundation. From a formal analysis within linear-response theory, we propose a new and simple scheme that combines the strengthes of Makov-Payne corrections and potential alignment. Our scheme requires no empirical parameters or fitting procedures. Its reliability (scatter in formation energies <0.1 eV, charge transition levels <0.05 eV) is demonstrated for the Ga vacancy in GaAs.

HL 13.5 Mon 17:15 EW 202

**First-Principles Calculations of Electronic and Optical Properties of MnO and NiO** — •Claudia Rödl, Frank Fuchs, Jürgen Furthmüller, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik and European Theoretical Spectroscopy Facility (ETSF), Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The treatment of the antiferromagnetic transition-metal oxides within many-body perturbation theory (MBPT) remains a challenge. It is well-known for years that density-functional theory (DFT) in the local-density (LDA) and generalized-gradient approximation (GGA) yields very small or even negative gaps for this class of materials. Consequently, quasiparticle calculations using Hedin's GW approximation in the commonly applied one-shot approach underestimate the fundamental gap significantly. That is why we use the non-local HSE03 exchange-correlation functional to obtain a reasonable starting point for a quasiparticle calculation within first-order perturbation theory. We explicitly focus on the compounds MnO and NiO which are usually considered as paradigmatic examples. Furthermore, we examine the optical properties of these materials. We solve the spin-polarized Bethe-Salpeter equation (BSE) and calculate optical absorption spectra including excitonic and local-field effects. In order to keep the computational demand treatable, we utilize the comparably less expensive GGA+U scheme for the subjacent electronic structure calculation.