HL 43.3 Thu 14:30 H14

**GW Calculations Starting from Generalized Kohn-Sham Schemes**

---

**Frank Fuchs**, Jürgen Furrerth Müller, and Friedhelm Beschitted

**Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany**

We start with a calculation of the electronic ground state in the framework of density-functional theory (DFT) within the generalized-gradient approximation (GGA) and use the projector-augmented wave (PAW) method to describe the wave functions. In the case of MnO the main problem consists in obtaining reasonable quasiparticle energies. We compute quasiparticle shifts using Hedin’s GW approximation in a model scheme. To treat magnetic materials one has to extend the usual BSE scheme in order to describe the spin degree of freedom. As a consequence the rank of the BSE Hamiltonian doubles resulting in increased computational cost. The optical spectra are determined by solving an initial-value problem instead of a direct diagonalization of the Hamiltonian.

**Location:** H14
our method, we occupy all included subbands with electrons according to Fermi statistics and subsequently subtract a positive background charge that guarantees charge neutrality. We present results, such as gaps, subband dispersions, masses, and local charge densities, for strained intrinsic InAs/GaSb (001)-superlattices as a function of layer thickness and bias. We find good agreement for the effective bandgap with experimental data [1,2]. [1] L. L. Chang et al., J. Vac. Sci. Technol. 19, 589 (1981). [2] H. Mosheni et al., Appl. Phys. Lett. 71, 1403 (1997).

HL 43.7 Thu 15:30 H14
The impact of self-consistency and vertex corrections in GW calculations. — Maxim Shishkin and Georg Kresse — Institut fuer Materialphysik and Centre for Computational Materials Science, Universitaet Wien, A 1090 Wien, Austria

The GW method is a common choice for accurate calculations of electronic band structures in solids. The commonly used single shot GW approximation (G0W0) is plagued by reliance on DFT wavefunctions and energies, which do not always provide a reasonable input. As a remedy to this problem, we present here the results of self-consistent quasiparticle calculations (scGW) [1] with a full update of both eigenvalues and wavefunctions, performed using the VASP code. The obtained gaps are generally overestimated for most of the materials, which is however not surprising as the higher terms in the many body expansion of the Hamiltonian (vertex corrections) are missing. Indeed, it is shown that addition of vertex corrections decreases the gaps, bringing them into much closer agreement with experiment. We propose that the overestimation of scGW gaps can be caused by an inaccurate description of dielectric properties (underestimated static dielectric constants), resulting from neglect of electron-hole interaction in the calculation of polarizabilities and dielectric matrices. The vertex correction contributions, which includes such electron-hole interactions, lead to an increase of dielectric constants to values close to experiment, and a concomitant decrease of the gaps.