HL 43: Theory of electronic structure

Time: Thursday 14:00–15:45 Location: H14

HL 43.1 Thu 14:00 H14

Analysis of core-valence linearization in G_0W_0 calculation — •Xinzheng Li[1], Ricardo Gomez-Abal[1], Claudia Ambrosch-Draxl[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Insitut der Max-Planck-Gesellschaft, D-14195, Berlin — [2]Department of Material Physics, A-8700, Leoben

In recent years, the *GW* approach, typically applied as the first order correction to the Kohn-Sham (KS) eigenenergies (G_0W_0 approximation), has achieved great success in describing the single-particle excitations in weakly correlated semiconductors and insulators. For implementation simplicity and computational efficiency, most of the existing codes are based on the pseudopotential (PP) method, in which the self-energy is only calculated from the (pseudo-)valence states. It is already well-known in DFT that such a linear treatment of the core-valence exchange-correlation interaction is not always valid. Non-linear core corrections have to be added in such cases. While within G_0W_0-PP, core-valence interaction can only be included at the KS level, its results always show better agreement with experiment than the all-electron calculations available so far. In this talk, we analyze the reasons for this disturbing discrepancy and the validity of the "core-valence linearization" in the G_0W_0-PP scheme. Calculations are performed using our newly developed all electron G_0W_0 code, based on the Wien2k implementation of the FP-(L)APW+lo method. We compare our all-electron results with those obtained by computing the self-energy from the valence states only as well as with G_0W_0-PP calculations for selected materials (e.g. Si, GaAs, NaCl, ...).

HL 43.2 Thu 14:15 H14

Excitonic Effects in MnO: An Application of Spin-Polarized BSE — •Claudia Rödl, Frank Fuchs, Jürgen Furthmüller, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

As it is desirable to calculate optical spectra also for magnetic materials we approach the problem of evaluating excitation properties for collinear spin-polarized systems within the Bethe-Salpeter equation (BSE). As an interesting test material we choose the antiferromagnetic insulator MnO.

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.

HL 43.3 Thu 14:30 H14

GW Calculations Starting from Generalized Kohn-Sham Schemes — •Frank Fuchs[1], Jürgen Furthmüller[1], Friedhelm Bechstedt[1], Maxim Shishkin[2], and Georg Kresse[2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut für Materialphysik and Center for Computational Materials Science, Universität Wien, Austria

The GW approximation of Hedin is arguably the most successful approach for the calculation of quasi-particle (QP) energies in extended systems. Its accuracy has been proven for a variety of systems. Usually, the QP eigenvalues are calculated in a perturbative approach, starting from solutions of the Kohn-Sham equations with an exchange-correlation (XC) potential in local density or generalized gradient approximation (LDA/GGA). However, this standard approach fails for a number of systems such as InN or ZnO with shallow 'semi-core' electrons and a much too small or even 'negative gap' in LDA/GGA. Here we present G_0W_0 calculations for various materials which start from solutions of the generalized Kohn-Sham (gKS) equations for the screened exchange (sX), HSE03, PBE0 and HF model of exchange and correlation. The calculations are performed within the framework of the full potential PAW method. The *GW* calculations, with various gKS solution as input, are found to yield a positive gap and *d*-band positions close to the experimental values for all the functionals investigated here. Furthermore, with exception of HF the resulting gaps are almost the same for all the gKS functionals chosen as starting point.

HL 43.4 Thu 14:45 H14

Electron Localization Function, persistent current and Wigner crystal phase in a one-dimensional quantum ring — •Marc Siegmund and Oleg Pankratov — Lst. für Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr.7, 91058 Erlangen

Due to the absence of long-range order in one-dimensional (1D) systems, the existence of a 1D Wigner crystal has been a long debated subject. It was shown [1] that despite the strong fluctuations, already a small pinning potential can stabilize the crystal phase at moderate electron densities. We confirm the existence of a 1D Wigner phase via studying a persistent current in a one-dimensional quantum ring with a single Gaussian impurity. The current is induced by a magnetic flux penetrating the ring. To calculate the current we use Density Functional Theory with OEP approximation for exchange effects. The Wigner crystallization manifests itself as a drastic decrease of the current at a critical value r_S^c. In the limit of a vanishing impurity potential we find a sharp drop of the current, whereas for a finite potential strength the transition is smooth. We interpret the observed behaviour as a pinning of a Wigner crystal phase at $r_S^c \approx 2.2$ (for 0.3 of the flux quantum). This interpretation is supported by the calculation of the Electron Localization Function [2]. The latter shows the delocalized electron distribution for $r_S < r_S^c$, which drastically changes reflecting a strong localization of periodically arranged electrons at $r_S > r_S^c$.

[1] L.I. Glazman et al., Phys. Rev. B **45**, 8454 (1992)
[2] A.D. Becke and K.E. Edgecombe , J. Chem. Phys. **92**, 5397 (1990)

HL 43.5 Thu 15:00 H14

Self-consistent solutions for non-adiabatic electron dynamics within time-dependent density functional theory — •Günther Schwarz, Ilya V. Tokatly, and Oleg Pankratov — Lst. für Theoretische Festkörperphysik, Universität Erlangen-Nürnberg

Based on recent work in our group [1,2] we implemented a scheme to simulate a finite, one-dimensional electron system self-consistently within time-dependent density functional theory (TDDFT) taking non-adiabatic effects in the exchange-correlation potential v_{xc} into account. This is done by calculating the time evolution of the density within the co-moving Lagrangian reference frame. v_{xc} depends on the Cauchy deformation tensor as the basic variable rather than on the electron density or current.

We simulate the collective behavior of an electron liquid in single and double well structures subjected to time-dependent external electric fields. The evolution of the electron density is compared to the common adiabatic local density approximation. In good agreement with the results of non-self-consistent calculations for an analytic test system [3] we find most prominent non-adiabatic effects in regions with strongly varying deformation. Consequences for laser excitations of quantum well systems are discussed.

[1] I. V. Tokatly and O. Pankratov, Phys. Rev. B **67**, 201103(R) (2003).
[2] I. V. Tokatly, Phys. Rev. B **71**, 165105 (2005).
[3] C. A. Ullrich und I. V. Tokatly, Phys. Rev. B **73**, 235102 (2006).

HL 43.6 Thu 15:15 H14

Self-consistent k.p envelope function method for InAs/GaSb broken gap superlattices — •Till Andlauer, Tobias Zibold, and Peter Vogl — Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, D-85748 Garching

A novel charge self-consistent k.p envelope function method is presented for the calculation of the electronic structure of type-II semiconductor heterostructures with broken gap. Such heterostructures are relevant for the development of infrared lasers as well as infrared detectors. Standard multi-band k.p approaches fail to yield the correct occupation of electronic states in broken gap heterostructures, because strong hybridization of conduction band and valence band states makes it impossible to occupy electron and hole states separately. In

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.

[1] M. van Schilfgaarde, T. Kotani, and S. Faleev, Phys. Rev. Lett., vol. 96, 226402 (2006).