

## O 67: Ab-initio approaches to excitations in condensed matter III

Time: Friday 11:15–12:45

Location: SCH 251

O 67.1 Fri 11:15 SCH 251

**Tackling localized  $d$ -states: a systematic investigation by  $GW@LDA+U$**  — ●HONG JIANG<sup>1</sup>, RICARDO I. GOMEZ-ABAL<sup>1</sup>, PATRICK RINKE<sup>2,1</sup>, and MATTHIAS SCHEFFLER<sup>1,2</sup> — <sup>1</sup>Fritz-Haber-Institut der MPG, Berlin — <sup>2</sup>University of California at Sant Barbara, CA 93106

First-principles modeling of systems with localized  $d$ -states is currently a great challenge in condensed matter physics. Density-functional theory (DFT) in the standard local-density approximation (LDA) proves to be problematic. This can be partly overcome by including local Hubbard  $U$  corrections (LDA+ $U$ ), but itinerant states are still treated on the LDA level. Many-body perturbation theory in the  $GW$  approach offers both a quasiparticle perspective (appropriate for itinerant states) and an exact treatment of exchange (appropriate for localized states), and is therefore promising for these systems. Here we present a systematic investigation of the  $G_0W_0$  method based on LDA+ $U$  ( $G_0W_0@LDA+U$ ) for a series of prototype systems: 1) ZnS with semicore  $d$ -states, 2) ScN and TiO<sub>2</sub> with empty  $d$ -states and 3) late transition metal oxides (MnO, FeO, CoO and NiO) with partially occupied  $d$ -states. We show that for ZnS, ScN and TiO<sub>2</sub>, the  $G_0W_0$  band gap only weakly depends on  $U$ , but for the other transition metal oxides the dependence on  $U$  is as strong as in LDA+ $U$ . These different trends can be understood in terms of changes in the hybridization and screening. Our work demonstrates that  $G_0W_0@LDA+U$  with “physical” values of  $U$  provides a balanced and accurate description of both localized and itinerant states.

O 67.2 Fri 11:30 SCH 251

**Spin-wave excitations in itinerant ferromagnets from many-body perturbation theory** — ●ERSOY SASIOGLU<sup>1</sup>, ARNO SCHINDLMAYR<sup>2</sup>, CHRISTOPH FRIEDRICH<sup>1</sup>, and STEFAN BLÜGEL<sup>1</sup> — <sup>1</sup>Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>Department Physik, Universität Paderborn, 33095 Paderborn, Germany

To study excitation spectra of magnetic materials from first principles we have developed a computational scheme based on many-body perturbation theory. The main quantity of interest is the dynamical transverse spin susceptibility, from which magnetic excitations, including single-particle spin-flip Stoner excitations and collective spin-wave modes as well as their lifetimes, can be obtained. In order to describe spin waves we include appropriate vertex corrections in the form of a multiple-scattering T-matrix, which describes the coupling of electrons and holes with different spin. To reduce the numerical cost for the calculation of the four-point T-matrix we exploit a transformation to maximally localized Wannier functions that takes advantage of the short spatial range of electronic correlation in the partially filled  $d$  or  $f$  orbitals of magnetic materials. Our implementation is based on the full-potential linearized augmented plane-wave (FLAPW) method. As an illustration, we present spin-wave spectra and dispersions for the elementary ferromagnets Fe, Co and Ni calculated with our scheme. The results are in good agreement with available experimental data.

O 67.3 Fri 11:45 SCH 251

**All-electron  $GW$  calculations for SrTiO<sub>3</sub>, BaTiO<sub>3</sub> and PbTiO<sub>3</sub>** — CHRISTOPH FRIEDRICH<sup>1</sup>, ●ANDREAS GIERLICH<sup>1</sup>, ARNO SCHINDLMAYR<sup>2</sup>, and STEFAN BLÜGEL<sup>1</sup> — <sup>1</sup>Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>Department Physik, Universität Paderborn, 33095 Paderborn, Germany

The  $GW$  approximation for the electronic self-energy, which combines bare exchange with the dynamical screening of the many-electron system within the random-phase approximation, yields quasiparticle band structures in very good agreement with experiment. While most implementations today employ the pseudopotential approximation, our recently developed realization (<http://www.flapw.de/spex>) is based on the all-electron full-potential linearized augmented-plane-wave (FLAPW) method, where core and valence electrons are treated on the same footing. Within this method a large variety of materials can be treated, including  $d$ - and  $f$ -electron systems, oxides and magnetic systems. In this work we present results for the perovskite transition-metal oxides SrTiO<sub>3</sub>, BaTiO<sub>3</sub> and PbTiO<sub>3</sub>, which

are widely used in technical applications. Their band gaps are difficult to measure experimentally and have been under debate for a long time. Most *ab initio* studies so far were based on density-functional theory and showed a strong underestimation of the band gap. Here we present all-electron  $GW$  calculations that overcome this problem and yield band gaps very close to the best experimental estimates.

O 67.4 Fri 12:00 SCH 251

**Efficient all-electron  $GW$  calculations of complex semiconductors** — ●CHRISTOPH FRIEDRICH<sup>1</sup>, ARNO SCHINDLMAYR<sup>2</sup>, and STEFAN BLÜGEL<sup>1</sup> — <sup>1</sup>Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>Department Physik, Universität Paderborn, 33095 Paderborn, Germany

The  $GW$  approximation for the electronic self-energy yields quasiparticle band structures in very good agreement with experiment, but almost all implementations so far are based on the pseudopotential approach, which limits their range of applicability. We have developed an implementation (SPEX, <http://www.flapw.de/spex/>) within the full-potential linearized augmented-plane-wave (FLAPW) method, which treats core and valence electrons on an equal footing. Within this method a large variety of materials can be treated, including  $d$ - and  $f$ -electron systems, oxides and magnetic systems. Our implementation employs a mixed product basis for the representation of wave-function products in the interstitial and muffin-tin regions. A basis transformation to the eigenfunctions of the Coulomb potential allows a reduction of the basis-set size without compromising the accuracy, thus leading to a considerable speed-up in computation time. To demonstrate the efficiency of the implementation we present results for complex semiconductors. Financial support from the Deutsche Forschungsgemeinschaft through the Priority Programme 1145 is gratefully acknowledged.

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**X-ray absorption spectra of ice and water: a first principles study with the  $GW$  method** — XIFAN WU<sup>1</sup>, WEI CHEN<sup>2</sup>, and ●ROBERTO CAR<sup>1,2</sup> — <sup>1</sup>Department of Chemistry, Princeton University, Princeton, USA — <sup>2</sup>Department of Physics, Princeton University, Princeton, USA

We calculated the X-ray absorption spectra of ice and liquid water by adopting an approach based on the  $GW$  method to describe the excited electron in presence of a frozen core hole. We used the static Coulomb-hole and screened exchange approximation for the self-energy and used Maximally Localized Wannier functions to make  $GW$  calculations feasible in the large supercell needed to model a disordered system like water. The calculated spectra considerably improve the agreement with experiment, compared with previous DFT calculations. In particular, the three main features observed in experiments are well reproduced in terms of position and intensity for both ice and water. We also find that the difference between the ice and water spectra can be understood in terms of the electronic structures of these systems, manifested by a distorted, tetrahedral hydrogen bond network in the liquid.

O 67.6 Fri 12:30 SCH 251

**Electron-phonon coupling in graphite within the  $GW$ -approximation** — ●LUDGER WIRTZ<sup>1</sup>, MICHELE LAZZERI<sup>2</sup>, CLAUDIO ATTACALITE<sup>3</sup>, and FRANCESCO MAURI<sup>2</sup> — <sup>1</sup>IEMN, Lille France — <sup>2</sup>IMPMC, University “Pierre et Marie Curie”, Paris, France — <sup>3</sup>European Theoretical Spectroscopy Facility, University of the Basque Country, San Sebastian, Spain

A seemingly trivial thing such as the phonon dispersion of graphite continues to present surprises. For most materials (both metals and insulators), density-functional perturbation theory using LDA or GGA gives phonon dispersions in close agreement with experimental results. For graphene and graphite, however, there is a pronounced failure of LDA and GGA for the highest optical phonon branch (HOB) around the Kohn-anomaly at the high-symmetry point K. We evaluate the electron-phonon coupling (EPC) between the  $\pi$ -bands and the HOB in the  $GW$ -approximation. Non-local exchange-correlation effects renormalize the square EPC by almost 80%. This almost doubles the slope of the HOB around K and explains recent experimental results on graphite-phonons using inelastic x-ray scattering and double-resonance

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Raman spectroscopy. The short-coming of LDA and GGA may be partially fixed by the use of hybrid-functionals such as B3LYP (which partially contains exact Hartree-Fock exchange). The use of pure Hartree-

Fock, however, leads to an extremely strong EPC and consequently to an instability of graphene under distortion along the HOB phonon.