HL 51: Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers III

Time: Wednesday 11:15–13:00 Location: TRE Phy

HL 51.1 Wed 11:15 TRE Phy

Dynamical magnetic excitations of nanostructures from first-principles — •Samir Lounis[1,2], Antonio Costa[3], Roberto Muniz[3], and Douglas Mills[1] — [1]Department of Physics and Astronomy, University of California Irvine, California, 92697 USA — [2]Institut für Festkörperforschung and Institut for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [3]Instituto d Fisica, Universidade Federal Fluminense, 24210-340 Niteroi, Rio de Janeiro, Brazil

Within the framework of time-dependent density functional theory combined with the Korringa-Kohn-Rostoker Green function formalism, we present a real space methodology to investigate dynamical magnetic excitations from first-principles [1]. We set forth a scheme which enables one to deduce the correct effective Coulomb potential needed to preserve the spin-invariance signature in the dynamical susceptibilities, i.e. the Goldstone mode. We use our approach to explore the spin dynamics of 3d adatoms and different dimers deposited on a Cu(001) surface[1] and a Cu(111) surface [2] with emphasis on their decay to particle-hole pairs.

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[1] Lounis *et al.* Phys. Rev. Lett. **105**, 187205 (2010); Lounis *et al.* arXiv:1010.1293. [2] Khajetoorians et al. arXiv:1010.1284v2.

HL 51.2 Wed 11:30 TRE Phy

Magnetic order of $LaVO_3/SrVO_3$ superlattices — •Cosima Schuster[1], Ulrike Lüders[2], Udo Schwingenschlögl[3], and Raymond Fresard[2] — [1]Institut für Physik, Universität Augsburg, D-86135 Augsburg — [2]Laboratoire CRISMAT, UMR CNRS-ENSICAEN(ISMRA) 6508, FR3095 Caen — [3]KAUST, PCSE Division, P.O. Box 55455, Jeddah 21534, Saudi Arabia

While stable ferromagnetic ground states are predicted based on model calculations their experimental realizations are scarce. Experimental data obtained on $LaVO_3[m]/SrVO_3$[1] superlattices show that these systems remain magnetic above room temperature for particular values of m, in contrast to the solid solutions with the same composition. To clarify the magnetic and orbital order in these heterostructures, we perform electronic structure calculations based on density functional theory. First, we discuss the magnetic and orbital order of strained $LaVO_3$, for the c/a ratio of the heterostructure, where two types of ordering are nearly degenerate. While both g-type and c-type antiferromagnetic ordering within the $LaVO_3$ favour a non-magnetic interface in case of odd m and a ferromagnetic interface in case of even m, the orbital ordering perpendicular to the interface is different in both cases. A detailed discussion of the particular combinations of the magnetic and orbital order at the interface is given.

HL 51.3 Wed 11:45 TRE Phy

First-principles quantum-mechanical methods for full prediction of NMR parameters in fluorides — •Aymeric Sadoc[1], Florent Boucher[1], Mamata Biswal[2], Monique Body[2], and Christophe Legein[2] — [1]Institut des matériaux Jean Rouxel (IMN) - Université de Nantes, CNRS, 2 rue de la houssinière, BP 32229, 44322 Nantes, France — [2]Institut de Recherche en Ingénierie Moléculaire et Matériaux Fonctionnels (IRIM2F) - Université du Maine, CNRS, Avenue Olivier Messiaen, 72085 Le Mans, France

^{19}F magic angle spinning (MAS) NMR is a powerful structural tool for complex fluoride crystalline materials having multiple crystallographic sites since ^{19}F (I=1/2) isotropic chemical shift (δ_{iso}) is very sensitive to the environment of the fluorine atom. However, in many cases, several fluorine sites have the same multiplicity preventing an unambiguous experimental assignment. Simulation of the response to an external magnetic field is then necessary to complete the analysis. The relation of the measured δ_{iso} values with the calculated isotropic chemical shieldings (σ_{iso}) is needed to interpret of NMR spectra.

^{19}F σ_{iso} values were calculated for alkali, alkaline earth and rare earth of column IIIB fluoride compounds using the GIPAW method implemented in the CASTEP software. Using DFT-PBE, we have established a linear relation between ^{19}F calculated σ_{iso} and experimental δ_{iso} values which enables full prediction of ^{19}F NMR spectra. In the case of complex NMR spectra, this calibration curve is successfully applied for the attribution from first-principles quantum-mechanical of ^{19}F chemical shifts.

HL 51.4 Wed 12:00 TRE Phy

***Ab-initio* study of MnO and NiO in various crystal structures – The failure of (semi)local density functionals** — •Andreas Schrön, Claudia Rödl, and Friedhelm Bechstedt — IFTO, FSU Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Transition-metal oxides (TMOs) are of great interest for applications in e.g. dilute magnetic semiconductors (DMSs) which are supposed to allow for transparent ferromagnets with high critical temperatures. One of the most promising host materials is ZnO which crystallizes in the wurtzite structure. Although TMOs have been investigated a long time experimentally, their theoretical description is still unsatisfying.

The semilocal generalized-gradient approximation (GGA) to density functional theory (DFT) works well for many materials. Here we demonstrate that this approach predicts the wrong ground-state crystal structure for MnO, since it does not account sufficiently for the electron correlation effects in materials with strongly localized electrons. It is usually assumed, that approaches including an additional on-site Coulomb interaction U (GGA+U) or non-local exchange contributions like the hybrid functional HSE03 cure this failure.

The relative energetic ordering of the rock-salt, zinc-blende, and wurtzite crystal structures are investigated for various magnetic orderings. It is shown that neither GGA nor the HSE03 hybrid functional yields the experimentally observed ground-state structure. However, agreement with experiment is obtained if the GGA+U functional with $U > 4$ eV is applied. For NiO, on the other hand, all three functionals yield rock-salt as the equilibrium crystal structure.

HL 51.5 Wed 12:15 TRE Phy

Laser-induced ultrafast demagnetization: First-principles analysis of Elliott-Yafet processes — •Karel Carva[1,2] and Peter M. Oppeneer[2] — [1]Department of Condensed Matter Physics, Charles University, Ke Karlovu 5, CZ-12116 Prague 2, Czech Republic — [2]Department of Physics and Materials Science, Uppsala University, Box 530, SE-75121 Uppsala, Sweden

The laser-induced ultrafast demagnetization phenomenon has attracted a lot of attention since the first successful experiment on the fs timescale in 1996. However even now it is still far from being understood on the microscopic level. A number of possible microscopic mechanisms have been proposed.

Here we concentrate on Elliott-Yafet spin relaxation due to to electron-phonon scattering in Ni. The spin-flip probability associated with electron-phonon scattering in Ni has been estimated - employing the ab initio band structure - to be larger than expected. We calculate the spin-flip Eliashberg function based on ab initio electron-phonon coupling matrix elements to obtain the spin-flip probability with much higher accuracy. We extend this method to the regime of non-equilibrium electron distributions relevant for ultrafast processes. We find significant differences between the efficiency of this spin relaxation mechanism for highly non-equilibrium electron distributions pumped by the laser and thermalized ones (not in equilibrium with lattice).

HL 51.6 Wed 12:30 TRE Phy

Momentum Distribution and Renormalization Factor in Sodium and the Electron Gas — •Valerio Olevano — Institut Neel, CNRS & UJF, Grenoble, France

The homogeneous electron gas or jellium is one of the most fundamental models, canonical workbench to test different many-body theoretical approaches. Although really simple, still is very close to real solids, especially alkali metals, and sodium is one of its nature's closest realization. Here we present theoretical and also experimental results on the momentum distribution and the quasiparticle renormalization factor in sodium. From an x-ray Compton-profile measurement of the valence-electron momentum density, we derive its discontinuity at the Fermi wavevector. This yields for the first time an accurate measure of the renormalization factor, one of the most important quantities in

many-body theory, that we compare with GW and quantum Monte Carlo calculations performed both on crystalline sodium and on the homogeneous electron gas. Our calculated results are in good agreement with the experiment.

References: S. Huotari, J. A. Soininen, T. Pylkkänen, K. Hämäläinen, A. Issolah, A. Titov, J. McMinis, J. Kim, K. Esler, D. M. Ceperley, M. Holzmann, and V. Olevano, Phys. Rev. Lett. 105, 086403 (2010).

HL 51.7 Wed 12:45 TRE Phy

Construction of low energy Hamiltonians using maximally localized Wannier functions — •Roman Kovacik and Claude Ederer — School of Physics, Trinity College Dublin, Ireland

The theoretical description of correlated electron systems, such as e.g. transition metal oxides, is often based on effective tight-binding (TB) models. A systematic way to obtain realistic TB model parameters from first principles calculations is the construction of maximally localized Wannier functions (MLWFs) [1]. The corresponding TB representation is given by the real space Hamiltonian matrix elements in the MLWF basis. We address two important issues: i) how many orbitals to include in the basis set for the TB model representation, and ii) what is the most appropriate reference point to connect the model and Kohn-Sham band structures (i.e. should the Kohn-Sham band structure be considered as "non-interacting" or as mean-field approximation to the interacting case). We use $LaMnO_3$, a prototype material for correlation-driven phenomena, as an example for the construction of model Hamiltonians. In particular, we compare a TB description based only on effective Mn e_g bands with a description that explicitly includes also the O p bands, and we analyze the effects of the Hubbard U and the Jahn-Teller distortion on the corresponding TB parameterizations. In addition, we discuss the suitability of different types of Wannier functions for the calculation of TB parameters.

[1] I. Souza, N. Marzari, and D. Vanderbilt, PRB 65, 035109 (2001).