O 26: Focussed session: Theory and computation of electronic structure: new frontiers II (jointly with HL, DS)

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

Topical Talk O 26.1 Tue 11:15 TRE Phy

Electronic and Optical Excitations in Magnetic Insulators — •Claudia Rödl, Frank Fuchs, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

With the advent of electronic devices exploiting also the spin degree of freedom, magnetic materials attract more and more interest due to potential technological applications. However, describing the excitation properties of insulators with strongly localized and partially occupied d states by means of *ab-initio* methods remains a considerable challenge. Here, we focus on the antiferromagnetic transition-metal oxides (TMO) MnO, FeO, CoO, and NiO and ferromagnetic $CrBr_3$ as prototypical representatives for the class of magnetic insulators.

A perturbative treatment of Hedin's *GW* approximation based on (semi)local approaches to exchange and correlation in the subjacent density-functional calculation fails to reproduce the experimental photoemission spectra. Instead, we use the non-local HSE03 exchange-correlation functional to obtain a reasonable starting point for the *GW* calculation. The spin-polarized extension of the Bethe-Salpeter equation (BSE) is solved to calculate optical absorption spectra including excitonic and local-field effects. The spectra are analyzed in terms of dipole-allowed and dipole-forbidden transitions. For instance, it turns out that the main absorption peaks in the TMOs are due to d-d excitations which are dipole-forbidden at the Γ point. Further, the occurrence of spin-allowed and spin-forbidden Frenkel-like bound excitonic states within the fundamental band gap is investigated.

O 26.2 Tue 11:45 TRE Phy

LSDA+DMFT calculations of FeNi disordered alloys and Fe/Au(001) thin films — •Jan Minar, Jurgen Braun, Ara Cho, and Hubert Ebert — Dep. Chemie und Biochemie, LMU University of Munich, Germany

The combination of the local spin density approximation (LSDA) and the dynamical mean field theory (DMFT) provide a powerful tool to treat correlations beyond plain LSDA. The KKR or multiple scattering approach implemented on this basis allows among others to deal with alloy and surface systems as well as to study spectroscopic properties on equal footing [1].

Here, we present a LSDA+DMFT study of FeNi disordered alloys using the coherent potential approximation (CPA). In particular the influence of correlation effects on magnetic properties will be discussed. Special emphasis will be put on the additional information supplied by the spin-polarised relativistic mode allowing to deal with the spin-orbit coupling induced properties like orbital magnetic moments and dichroism. A detailed comparison to recent angle resolved photoemission with high resolution [3] allows for a discussion on the influence of correlations with the increasing Ni concentration. In the second part the results of fully self-consistent LSDA+DMFT calculations for the Fe/Au(001) system are presented. In particular the creation of quantum well states has been followed by angular resolved photoemission.

1. J. Minar et al., prb 72, 0415125 (2005), J. Sanchez-Barriga et al., prl 103, 267203 (2009) and Phys. Rev. B 82, 104414 (2010)

O 26.3 Tue 12:00 TRE Phy

Effective on-site Coulomb interaction in transition metals from constrained RPA — •Ersoy Sasioglu, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Effective on-site Coulomb interaction (Hubbard U) between localized d electrons in $3d$, $4d$, and $5d$ transition metals are calculated employing the recently developed constrained random-phase approximation (cRPA) within the full-potential linearized augmented plane-wave (FLAPW) method [1] using Wannier functions [2]. The obtained Hubbard U parameters lie between 1 and 5 eV and show a non-monotonic behavior across the transition-metal series. We find that the U depends on the crystal structure, spin polarization, d-electron number and filling of the d orbitals rather than d-character of the elements. For most of the isovalent transition metals, U assumes similar values. The obtained U parameters for the $3d$ series are in good agreement with previous studies as well as available experimental data. Using calculated U parameters we discuss the strength of the electronic correlations and instability of the paramagnetic state towards the ferromagnetic one for $3d$ transition metals. This work has been supported in part by DFG-FOR-1346.

[1] www.flapw.de
[2] F. Freimuth, Y. Mokrousov, D. Wortmann, S. Heinze, and S. Blügel, Phys. Rev. B. **78**, 035120 (2008).

O 26.4 Tue 12:15 TRE Phy

Ab-initio description of spin-dependent transport in disordered alloys — •Diemo Ködderitzsch, Stephan Lowitzer, and Hubert Ebert — Ludwig-Maximilians-Universität München, Department Chemie und Biochemie, Physikalische Chemie, Butenandtstraße 11, D-81377 München, Germany

Spin-orbit induced couplings are the source of many interesting physical phenomena like the anomalous- and spin-Hall-effects (AHE, SHE), which recently received a lot of attention due to their potential application in the field of spintronics. During the last years several theoretical works have dealt with the intrinsic AHE and SHE, based on the band structure of pure materials and only few of them use a parameter free *ab initio* approach.

We present a coherent *ab initio* description of both, the AHE and SHE, that is applicable to pure **and** disordered alloys by treating all sources, i.e. intrinsic as well as extrinisic contributions, on equal footing. We use an implementation of the Kubo-Středa equation employing the fully relativistic Korringa-Kohn-Rostoker (KKR) Green's function method in conjunction with the Coherent Potential Approximation (CPA) alloy theory. For discussing spin currents we employ our recently devised relativistic spin projection scheme [1] and a corresponding generalization of the Kubo-Středa equation. We illustrate the power and versatility of the approach by giving several examples.

[1] S. Lowitzer, D. Ködderitzsch and H. Ebert, Phys. Rev. B 82, 140402(R) (2010).

O 26.5 Tue 12:30 TRE Phy

Applying hybrid-functional and many-body methods to rare earths: a study of Cerium — •Marco Casadei[1], Xinguo Ren[1], Joachim Paier[2], Patrick Rinke[1], Angel Rubio[1,3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG (TH), Berlin, Germany — [2]Humboldt Universitaet (Institut fuer Chemie), Berlin, Germany — [3]UPV/EHV, San Sebastian (Fisica Materiales), Spain

The presence of localized, partially occupied f-electron states dictates many of the peculiar physical properties of rare-earth materials. In particular, the description of the iso-structural α-γ phase transition in Ce metal poses great challenges to density-functional theory (DFT) based approaches since local/semilocal (LDA/GGA) functionals completely fail to produce the phase transition. Here we address this problem by investigating bulk-like Ce clusters of increasing size using hybrid functionals, that incorporate a portion of exact-exchange, and full exact-exchange plus correlation at the level of the random phase approximation (EX+cRPA). In all clusters we find two stable configurations with different lattice constants and distinct electronic and magnetic properties, resembling the bulk situation. However, all hybrid functionals predict that the high volume phase (linked to the γ-Ce phase) is lower in energy at zero temperature, in contrast to experiment. Decreasing the amount of exact-exchange in the hybrid functional eventually restores the correct phase ordering, at the expense of introducing an adjustable parameter. We show that EX+cRPA – a physically meaningful screening of exact-exchange – achieves the same effect from first principles.

O 26.6 Tue 12:45 TRE Phy

Issues with J-dependence in the LSDA+U method for non-collinear magnets — •Eric Bousquet[1,2] and Nicola Spaldin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]Physique Théorique des Matériaux, Université de Liège, B-4000 Sart Tilman, Belgium

We re-examine the commonly used density functional theory plus Hubbard U DFT+U method for the case of non-collinear magnets. While many studies neglect to explicitly include the exchange correction parameter J, or consider its exact value to be unimportant, here we show

that in the case of non-collinear magnetism calculations the J parameter can strongly affect the magnetic ground state. We illustrate the drastic J-dependence of magnetic canting, magnetoelectric response and magnetocrystalline anisotropy by calculating trends in the magnetic lithium orthophosphate family $LiMPO_4$ (M = Fe and Ni) and difluorite family MF_2 (M = Mn, Fe, Co and Ni). These results can be readily understood by expanding the usual DFT+U equations within the spinor scheme. On the flip side, it is clear that non-collinear magnetic systems provide a challenging case for testing the correctness of new exchange correlation functionals within the density functional formalism.