O 25: Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles II (jointly with TT)

Time: Tuesday 10:30–13:00 Location: HE 101

Topical Talk O 25.1 Tue 10:30 HE 101

Iron Pnicitdes and Chalchogenides: a New Class of Strongly Correlated Electron Systems. — •Gabriel Kotliar — Rutgers University Piscataway NJ

The discovery of superconductivity in the iron pnictides and chalchogenides took the scientific community by surprise. Since then many tools have been applied to these systems, and many competing physical pictures have been proposed.

In this talk will argue that compounds in this family should be thought as Hund's metals, a new class of strongly correlated materials where the correlations are controlled by the strength of the Hund's rule coupling J rather than by the Hubbard U. While correlations in these materials are strong, their physical properties are strikingly different from that of transition metal oxides.

In support of this picture we will present several LDA+DMFT studies for various observables stressing the role of various spectroscopies such as optical conductivity, photoemission and inelastic neutron scattering.

O 25.2 Tue 11:00 HE 101

Dynamical screening of the large local magnetic moment in Fe-based superconductors — •Alessandro Toschi[1], Ryotaro Arita[2], Philipp Hansmann[1,3], Shiro Sakai[1,3], Giorgio Sangiovanni[1], and Karsten Held[1] — [1]Institute of Solid State Physics, Vienna University of Technology (Austria) — [2]Department of Applied Physics, University of Tokyo (Japan) — [3]École Polytechnique, Palaiseau Cedex (France)

Electronic correlation plays a subtle role in Fe-based superconductors. In fact, due to the presence of several moderately correlated bands close to the Fermi level, one observes the formation of a large local magnetic moment driven by the Hund's exchange interaction, which takes place, however, in a mainly metallic background ("Hund's metal"[1]). This physical scenario, as it is shown by our LDA+DMFT calculations[2,3], provides the key to understand the discrepancies observed between experimental estimates of the magnetic moment in the magnetically ordered phase and those obtained via standard LSDA calculations. The magnitude of the discrepancy observed in different compounds would be hence related to the efficacy of the metallic screening, which is decreasing when going from the 1111 (e.g., LaFeAsO) to the 122 class, and eventually to the 11 materials (e.g., FeTe).

[1] K. Haule and G. Kotliar, New J. Phys. **11**, 025021 (2009).

[2] P. Hansmann, R. Arita, A. Toschi, S. Sakai, G. Sangiovanni, and K. Held, Phys. Rev. Lett. **104**, 197002 (2010).

[3] A. Toschi, R. Arita, P. Hansmann, G. Sangiovanni, and K. Held, *in preparation.*

O 25.3 Tue 11:15 HE 101

Iron under extreme conditions: the impact of electronic correlations — •Leonid Pourovskii — CPHT-Ecole Polytechnique, Palaiseau, France — IFM, Linköping university, Linköping, Sweden

We have applied a fully self-consistent full-potential ab initio dynamical mean-filed theory approach to study the impact of electronic correlations on electronic, elastic, and magnetic properties of iron at both moderate and high pressures and temperatures. Our simulations have established the existence of an electronic topological transition in the hcp phase of iron at pressures of about 30-40 GPa, with new hole pockets appearing in the Fermi surface with decreasing volume and leading to anomalies in the Debye sound velocity, lattice parameters c/a ratio and Mössbauer central shift. These anomalies are indeed observed in our experiments. With our calculations extended to pressures and temperatures expected for the Earth deep core we find that the fcc and hcp phases remain in the Fermi liquid regime, while the bcc phase is an incoherent *bad* metal as evidenced by a significant non-Fermi liquid life-time broadening of low-energy electronic states and a large entropic contribution to the electronic free energy. Our calculations also suggest that all three likely crystal structure of iron and iron-rich alloys in the Earth inner core, the hcp, the face centered cubic (fcc), and the body centered cubic (bcc), have sufficiently high magnetic susceptibility to stabilize the geodynamo. The strongest effect is predicted for the bcc Fe, which at the Earth core conditions is still characterized by a Curie-Weiss behavior of the magnetic susceptibility corresponding to a local magnetic moment 1.5 Bohr magnetons.

O 25.4 Tue 11:30 HE 101

Local Density Approximation for Gutzwiller wavefunctions. A SIESTA implementation and a case study: double-exchange magnetism in bulk iron. — •Giovanni Borghi[1], Michele Fabrizio[2,3], and Erio Tosatti[2,3] — [1]Theory and Simulation of Materials, EPFL, Lausanne, Switzerland — [2]SISSA, Trieste, Italy — [3]ICTP, Trieste, Italy

By means of the constrained-search formulation of Density Functional Theory [1], the Kohn-Sham auxiliary system of non-interacting electrons can be generalized to a system of particles that are coupled through local Hubbard-type interactions, and whose ground-state wavefunction is computed within Gutzwiller Variational Method. The resulting Gutzwiller Density Functional is a natural extension of DFT+U functionals, with an additional set of many body parameters that have to be optimized together with the density. Among these, a band-mass renormalization parameter à la Landau accounts for the reduced mobility of correlated particles and their suppressed kinetic energy. We show how the increased flexibility of the Gutzwiller Density Functional can be exploited to better understand the origin of magnetism in transition metals. A comparison of total energies of the paramagnetic and ferromagnetic phases of iron suggests the double-exchange rather than the Stoner mechanism as an explanation of magnetic ordering in this system [2].

[1] M. Levy, Proc. Natl. Acad. Sci. USA **76**, 6062 (1979); E. Lieb, Int. J. Quantum Chem. **24**, 243 (1983).

[2] GB, M. Fabrizio and E. Tosatti, *in preparation.*

O 25.5 Tue 11:45 HE 101

***T*-matrix approach for electron-magnon interactions in ferromagnetic materials** — •Mathias C.T.D. Müller, Christoph Friedrich, Ersoy Sasioglu, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recent ARPES experiments [1,2] indicate that the scattering between electrons and magnons taking place in systems with localized d and f orbitals leads to a pronounced renormalization of the electron band dispersion, creating a *kink* near the Fermi energy very similar to the renormalization due to electron-phonon coupling. In order to describe this renormalization from first principles we use the T-matrix formalism, which describes the correlated motion of an electron-hole pair of opposite spins in terms of ladder diagrams. The multiple scattering gives rise to collective spin excitations [3]. Through emitting and absorption of these magnons, the energy of an electron propagating through a spin-polarized system gets renormalized. Our implementation of the corresponding self-energy correction $\Sigma = -iGT$ is based on the all-electron full-potential linearized augmented-plane-wave (FLAPW) method `FLEUR` [4] combined with Wannier functions [5]. We present first results for elementary ferromagnets.

[1] J. Schäfer *et al.*, Phys. Rev. Lett. **92**, 097205 (2004).

[2] A. Hofmann *et al.*, Phys. Rev. Lett. **102**, 187204 (2009).

[3] E. Şaşıoğlu *et al.*, Phys. Rev. B **81**, 054434 (2010).

[4] www.flapw.de

[5] F. Freimuth *et al.*, Phys. Rev. B **78**, 035120 (2008).

O 25.6 Tue 12:00 HE 101

The magnetism in $LaCoO_3$ from the perspective of the dynamical mean field theory. — •Vlastimil Křápek and Jan Kuneš — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, 16253 Praha 6, Czech Republic

Despite numerous studies the character of the high-temperature magnetism in insulating $LaCoO_3$ is still controversial. Two candidates for the origin of the high-temperature Curie-Weiss response have been considered in literature: the intermediate spin state (IS, S=1) [1] and the high spin state (HS, S=2) [2]. We use the dynamical mean field approximation combined with the local density approximation (LDA+DMFT) to study $LaCoO_3$. We discuss the meaning of IS and HS states in the presence of change fluctuations due to the covalency Co-O bonds and conclude that HS is the dominant magnetic state for all realistic interaction parameters.

[1] M. A. Korotin *et al.*, Phys. Rev. B **54**, 5309 (1996).
[2] P. M. Raccah and J. B. Goodenough, Phys. Rev. **155**, 932 (1967).

O 25.7 Tue 12:15 HE 101

Pressure driven half-metallic ferromagnetism and magnetic moment collapse in $LaMnO_3$: a hybrid functional study — •Jiangang He and Cesare Franchini — University of Vienna, Faculty of Physics and Center for Computational Materials Science, A-1090 Vienna, Austria

The application of hydrostatic pressure to the antiferromagnetic and insulating e_g perovskite $LaMnO_3$ induces an electronic structure transition towards a metallic state at ≈ 34 GPa, and a progressive quenching of the underlying Jahn-Teller structural distortions [1,2]. By means of the Heyd, Scuseria, and Ernzerhof (HSE) screened hybrid functional approach we outline the evolution of the structural, electronic, and magnetic properties of $LaMnO_3$ in the pressure range $0-140$ GPa. Beside providing an atomistic understanding of the observed insulator-to-metal transition we predict the formation of a transport half-metal ferromagnetic cubic phase at elevated pressure (>80 GPa), associated with a high-spin ($S=2$, 3.7 μ_B) to low-spin ($S=1$, 1.7 μ_B) magnetic moment collapse, and characterized by a significantly large spin polarization ($I \approx 80-90\%$). Our results open up the possibility of realizing colossal magnetoresistance behaviours in a stoichiometric manganite.

References:

[1] I. Loa *et al.* Phys. Rev. Lett. **87**, 125501 (2001);
M. Baldini *et al.* Phys. Rev. Lett. **106**, 066402 (2011).
[2] G. Trimarchi and N. Binggeli, Phys. Rev. B **71**, 035101 (2005);
A. Yamasaki *et al.* Phys. Rev. Lett. **96**, 166401 (2006).

O 25.8 Tue 12:30 HE 101

Electronic properties of RbO_2 from DFT+DMFT calculations — •Roman Kovacik and Claude Ederer — School of Physics, Trinity College Dublin, Ireland

Recently, p-electron magnetism has received great attention as alternative option for spintronic applications. The "p-magnetism" is often defect-induced and systematic studies are hampered by poor reproducibility and wide spread in experimental data. It is therefore desirable to study intrinsic p-magnetism in pure bulk materials. We present results of a combined density functional theory + dynamical mean field theory (DFT+DMFT) study for RbO_2, an insulating antiferromagnet where magnetic properties arise from partially filled oxygen p orbitals. For the high-symmetry tetragonal structure, we calculate the Hamiltonian in the basis of maximally localized Wannier functions [1] with antibonding π^* character, which is then solved within DMFT using a continuous-time quantum Monte Carlo solver [2]. We construct a metal-insulator phase diagram as function of temperature and Hubbard interaction parameters U and J. For realistic values of U and J, we find that RbO_2 is a paramagnetic insulator at room temperature. We also find indications for orbital order at low temperatures ($T \approx 30$ K) in agreement with our previous DFT study [3]. Furthermore, we discuss differences between the realistic Hamiltonian and the one based on the semicircle density of states.

[1] I. Souza, N. Marzari, D. Vanderbilt, Phys. Rev. B 65, 035109 (2001).
[2] E. Gull, A. J. Millis, *et al.*, Rev. Mod. Phys. 83, 349 (2011).
[3] R. Kováčik and C. Ederer, Phys. Rev. B 80, 140411(R) (2009).

O 25.9 Tue 12:45 HE 101

Crystalline and Magnetic Anisotropy of the 3d Transition-Metal Oxides — •Andreas Schrön[1,3], Claudia Rödl[1,2,3], and Friedhelm Bechstedt[1,3] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau, France — [3]ETSF

The 3d transition-metal oxides (TMOs) are subject of debate since many decades due to their extraordinary properties, such as the formation of an antiferromagnetic ordering AFM2 below their Néel temperature. Many studies, both experimental and theoretical, focus only on the investigation of the crystalline anisotropy of MnO and NiO, which is solely driven by exchange striction along the unique symmetry axis in the [111] direction, while the magnetic anisotropy may be explained in terms of magnetic dipole interactions. In the TMOs FeO and CoO, however, orbital ordering and spin-orbit interaction play an additional, yet crucial role for both crystalline and magnetic anisotropy. Investigation of the latter materials is a demanding task both experimentally and theoretically.

We present our density-functional theory (DFT) study of the crystalline and magnetic anisotropy of the 3d TMOs. For the proper treatment of exchange and correlation (XC) we apply the generalized gradient approximation (GGA) to DFT within the parametrization of Perdew, Burke, and Ernzerhof (PBE). The on-site Coulomb interaction is corrected with an effective interaction U according to Dudarev's approximation (GGA+U).