# MA 33: Correlation Theory I

Time: Wednesday 9:30–12:15 Location: HSZ 403

MA 33.1 Wed 9:30 HSZ 403

**Electronic and magnetic state of LMO/STO heterostructures: Effect of local correlation and nonlocal exchange** — •Hrishit Banerjee[1], Oleg Janson[2], Karsten Held[3], Tanusri Saha-Dasgupta[4], and Markus Aichhorn[1] — [1]TU Graz, Austria — [2]IFW Dresden, Germany — [3]TU Wien, Austria. — [4]S. N. Bose National Centre for Basic Sciences, Kolkata, India

Motivated by the puzzling report of a ferromagnetic insulating state in $LaMnO_3$ (LMO)/$SrTiO_3$ (STO) heterostructures, we calculate the electronic and magnetic state of LMO, strained to a STO square substrate. We use 3 different computational approaches: (a) DFT+U, (b) DFT + DMFT, and (c) DFT + HF as a hybrid functional. While the first two approaches include local correlations and exchange at Mn sites, treated in a static and dynamic manner, respectively, the last one takes into account the effect of nonlocal exchange at all sites. We find in all 3 approaches that compressive strain induced by square substrate of STO turns LMO to a ferromagnet with suppressed Jahn-Teller distortion, in agreement with experiment. The hybrid calculations result in a ferromagnetic insulating solution, found to arise from an electronic charge disproportionation. When correlations are included through DMFT, first a paramagnetic insulating and then on inclusion of magnetism, a ferromagnetic insulating state is observed for strained LMO. Our conclusions remain valid when we investigate LMO/STO within the experimental setup of a superlattice geometry using hybrid functionals. DMFT calculations show the presence of a paramagnetic insulating state. Ref.: Phys. Rev. B 100, 115143 (2019)

MA 33.2 Wed 9:45 HSZ 403

**A critical assessment of the Hubbard U correction in the calculation of spin state energetics** — •Antonio Lorenzo Mariano and Roberta Poloni — Univ. Grenoble-Alpes, CNRS, Grenoble-INP, SIMaP, Grenoble 38000, France

During the past few years there has been much effort towards the accurate description of spin-state energetics in Fe(II) molecular complexes using ab initio methods. Within density functional theory, large deviations in the adiabatic energy difference between low spin (LS) and high spin (HS) are found among different families of XC functionals. Semilocal functionals overstabilize LS while Hartree-Fock overstabilizes HS. Global hybrids, metaGGAs and density-corrected approaches have also been suggested. In our work, we provide a critical assessment of the Hubbard U approach in the description of spin-state energetics and explain the origin of the overly destabilized LS state. Comparing LDA+U and PBE+U results against coupled cluster-corrected multireference perturbation theory values, i.e. CASPT2/CC [1], for a large series of molecular complexes, our study further explains that the reasonably good performance of LDA+U reported so far arises from a cancellation of errors [2]. [1] K. Pierloot et al., J. Chem. Theory Comput., 14, 2446-2455 (2018). [2] L. A. Mariano et al., to be submitted.

MA 33.3 Wed 10:00 HSZ 403

**Implementation of the DFT+Hubbard-I method in FLEUR and application to 4$f$ materials** — •Henning Janssen[1], Stefan Blügel[1], Gustav Bihlmayer[1], Alexander B. Shick[2], and Jindřich Kolorenč[2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Physics ASCR, CZ-18221 Prague, Czech Republic

The treatment of systems with strongly correlated electrons from first principles is a topic of big interest, e.g. for the description of the magnetic properties of lanthanides. The Hubbard-I method [1] method embeds a single impurity Anderson model, which describes the correlated orbital, into density functional theory (DFT) calculations and approximates the former by neglecting any interactions with the outside bath, i.e. hybridization with other orbitals. We discuss its implementation in the full potential linearized augmented planewave (FLAPW) method as realized in the FLEUR code [2].

In the course of the implementation, the calculation of local Green's function inside the muffin-tin spheres in the FLAPW framework is performed. Using Andersen's local force theorem Green's functions can also be used to calculate the magnetic properties of Heisenberg-like systems. The calculation of the spin stiffness is performed for bulk cobalt and iron, while the Hubbard-I procedure is applied to the test systems of gadolinium and europium.

[1]: A. B. Shick et al., Phys. Rev. B **80**, 085106 (2009)
[2]: www.juDFT.de

MA 33.4 Wed 10:15 HSZ 403

**Electronic, Magnetic and Topological Properties of Ca1K1Fe4As4** — •Niclas Heinsdorf[1], Dominik Lessnisch[1], Mikel Iraola Iñurrieta[2], Steve Winter[1], Vladislav Borisov[1,3], and Roser Valentí[1] — [1]Institut für theoretische Physik, Goethe Universität, Frankfurt — [2]Donostia International Physics Center, Donostia/San Sebastian — [3]Department of Physics and Astronomy, University of Uppsala

The 1144 family of Fe-based superconductors, such as Ca1K1Fe4As4, respresents one of the most recent additions to high-Tc superconductors. This family shows a very rich phase diagram as a function of doping and pressure, including superconductivity, spin-vortex magnetism and collapsed tetragonal states. In this talk we will discuss the magnetism and topological properties of Ca1K1Fe4As4 through a combination of DFT, analysis of Elementary Band Representations and effective model calculations.

MA 33.5 Wed 10:30 HSZ 403

**Competition of Hund's and spin-orbit couplings in cubic $d^4$ halides** — •Alexander Yaresko[1], Hiroto Takahashi[1,2], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Department of Physics, The University of Tokyo, Bunkyo-ku, Tokyo 133-0022, Japan — [3]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

In transition metal compounds with more than one $d$-electron or hole Hund's coupling $J_{\mathrm{H}}$ and pin-orbit coupling $\xi$ compete. The competition manifests itself in the contrast between the $LS$-coupling and the $jj$-coupling schemes in the large $J_{\mathrm{H}}$ and large $\xi$ limits, respectively. Cubic double-perovskite-like $K_2RuCl_6$ and $K_2OsCl_6$ compounds with $t_{2g}^4$ $Ru^{4+}$ and $Os^{4+}$ at the center of a regular $Cl_6$ octahedron are expected to be non-magnetic $J_{\mathrm{eff}} = 0$ Mott insulators; with the former being closer to the $LS$- and the latter to the $jj$-coupling limit. We performed LDA+U calculations using $J_{\mathrm{H}}$ as a tunable parameter which reveal that a transition from a non-magnetic to magnetic insulating ground state is controlled by the ratio $J_{\mathrm{H}}/\xi$. With realistic parameters of $J_{\mathrm{H}}$, $K_2RuCl_6$ is placed in the $LS$-coupling regime and $K_2OsCl_6$ is at the border between the two schemes.

**15 min. break.**

MA 33.6 Wed 11:00 HSZ 403

**Methods of electron transport in the theory of spin stiffness** — •Ilja Turek[1], Josef Kudrnovsky[2], and Vaclav Drchal[2] — [1]Institute of Physics of Materials, Czech Acad. Sci., Brno, Czech Rep. — [2]Institute of Physics, Czech Acad. Sci., Prague, Czech Rep.

We present an ab initio theory of the spin-wave stiffness for itinerant ferromagnets with pair exchange interactions derived from the magnetic force theorem [1]. The resulting formula involves one-particle Green's functions and effective velocity operators appearing in a recent theory of electron transport [2]. Application of this approach to clean crystals allows one to overcome the problem of nonconvergent lattice summations, as documented by results for pure metals Fe, Co, and Ni. Application to random alloys within the coherent potential approximation, illustrated by results for fcc Ni-Fe and bcc Fe-Al systems, enables one to include the disorder-induced vertex corrections, often neglected in evaluation of the exchange interactions.

[1] A. I. Liechtenstein et al., J. Magn. Magn. Mater. 67 (1987) 65. [2] I. Turek et al., Phys. Rev. B 65 (2002) 125101.

MA 33.7 Wed 11:15 HSZ 403

**Fractional quantum Hall models on lattices** — •Srivatsa Nagara Srinivasa Prasanna — MPIPKS, Dresden

Conformal field theory has recently been applied to derive few-body Hamiltonians whose ground states are lattice versions of fractional quantum Hall states. The exact lattice models involve interactions over long distances, which is difficult to realize in experiments. It seems, however, that such long-range interactions should not be necessary, as

the correlations decay exponentially in the bulk. This poses the question, whether the Hamiltonians can be truncated to contain only local interactions without changing the physics of the ground state. Previous studies have, in a couple of cases with particularly much symmetry, obtained such local Hamiltonians by keeping only a few local terms and numerically optimizing the coefficients. Here, we investigate a different strategy to construct truncated Hamiltonians, which does not rely on optimization, and which can be applied independently of the choice of lattice.

MA 33.8 Wed 11:30 HSZ 403

**Ab-initio calculations of magnetic properties of $Ba_2YIrO_6$** — •Hermann Schnait — TU Graz

The strongly correlated double perovskite $Ba_2YIrO_6$ (electronic configuration $5d^4$) shows unexpected magnetic properties in experiment. We investigate this behaviour using DFT+DMFT techniques including spin-orbit coupling, within the $t_{2g}$ manifold.

As some experiments claim a magnetic ordering temperature of about 3K and CTQMC impurity solvers would not be able to yield results in this regime, a novel MPS-based solver for multi-orbital systems (Fork-Tensor Product States - FTPS) is employed for T=0K calculations. The magnetic moment is measured both at T=0K and at finite temperatures and possible long-range antiferromagnetic ordering is investigated.

MA 33.9 Wed 11:45 HSZ 403

**Non-local Correlation and Interaction Effects on the Phase Diagram of the Kane-Mele-Hubbard Model** — •Markus Richter — TU-Graz, Austria

We use the honeycomb lattice as a playground to investigate the effects of strong correlations, non-local interactions, and spin-orbit coupling, using one orbital per site at half filling.

The model Hamiltonian of our choice is the extended Kane-Mele Hubbard model. This model provides, besides the unordered phase, two ordered phases, namely spin-density waves (SDW) and charge-density waves (CDW), as well as the additional characterization of being topologically trivial or non-trivial.

To analyze the interplay between the different phases we calculate phase diagrams using the different methods (extended) DMFT and TRILEX (triply irreducible local expansion). Unlike (E)DMFT, within TRILEX the self-energy becomes also k-dependent due to local vertex corrections.

MA 33.10 Wed 12:00 HSZ 403

**Theoretical study of the homo-trinuclear magnetic molecule $[Fe_3O(COOCH_3)_6(H_2O)_3]$** — •Rui Shi, Georgios Lefkidis, and Wolfgang Hübner — Department of Physics and Research Center OPTIMAS, Technische Universität Kaiserslautern, Kaiserslautern, Germany

In close collaboration with experiment we study the magnetic properties of the recently synthesized mixed-valence trinuclear iron acetate complex $[Fe_3O(COOCH_3)_6(H_2O)_3]$, which, like similar iron complexes, can boost the design of nanospintronic devices [1].

We optimize the structure geometry using the coupled-cluster method with single and double excitations (CCSD), and compute the electronic excited states with the equation-of-motion coupled-cluster method (EOM-CCSD) and perturbative inclusion of spin-orbit coupling. The infrared (IR) spectrum is numerically calculated through the energy gradient along the normal modes at the CCSD level [2], with an active window for the electronic correlations of 100 molecular orbitals. We find that the correlations substantially improve the vibration frequencies (up to 100 $cm^{-1}$) with respect to the Hartree-Fock resuls. Most notably, we theoretically compute the magnetic circular dichroism spectrum (MCD) and achieve excellent agreement with all five peaks detected in the experimental frequency window.

[1] H. Du, J. Liu, N. Zhang, J. Chang, W. Jin, C. Li, G. Lefkidis, and W. Hübner, Phys. Rev. B **99**, 134430 (2019)

[2] D. M. Becherer, D. Bellaire, F. Dietrich, M. Gerhards, G. Lefkidis, and W. Hübner, Phys. Rev. B **97**, 224404 (2018)