MA 27: Electron Theory of Magnetism and Correlations

Time: Wednesday 9:30–11:30 Location: HSZ 403

MA 27.1 Wed 9:30 HSZ 403

Electronic structure of the non-centrosymmetric antiferromagnetic $AgCrSe_2$ — •Seo-Jin Kim[1], Haijing Zhang[1], Marcus Schmidt[1], Michael Baenitz[1], Gesa Siemann[2], Chiara Bigi[2], Phil D. C. King[2], Vincent Polewczyk[3], Giovanni Vinai[3], and Helge Rosner[1] — [1]MPI CPfS, D-01187 Dresden, Germany — [2]IOM-CNR, Laboratorio TASC, Area Science Park, S.S. 14 km 163.5, Trieste I-34149, Italy — [3]School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom

We present the theoretical studies of the electronic structure and the anomalous Hall effect in $AgCrSe_2$ based on density functional theory together with experimental results. $AgCrSe_2$ is a layered triangular lattice system that lacks inversion symmetry. It exhibits a cycloidal coupling in the $CrSe_2$ layer with a small angle and an antiferromagnetic coupling between adjacent layers with a small canting along c-axis. The comparison of the Cr partial DOS determined from the photoemission measurements and the magnetic LDA+U calculations with a value of U = 0.75 eV shows a good agreement. This reveals that this compound is rather weakly correlated due to a strong hybridization with the ligands. The Se 4p states are dominating near the Fermi energy, resulting in a sizable band split of the order of 300 meV induced by the SOC. This system shows an unconventional anomalous Hall effect. The anomalous Hall conductivity is calculated based on the Berry curvature using an effective model constructed by the Wannierisation. The calculated σ_{xy} shows a good agreement to the experiments.

MA 27.2 Wed 9:45 HSZ 403

Geometrical dynamics of magnetic moments coupled to a correlated antiferromagnet — •David Alan Krüger, Nicolas Lenzing, and Michael Potthoff — Department of Physics, University of Hamburg, Hamburg, Germany

The geometrical spin torque represents an indirect interaction of magnetic moments, which are weakly exchange coupled to a system of itinerant electrons. It originates from a finite spin-Berry curvature, it modifies and adds to the conventional indirect RKKY exchange, and it leads to an anomalous, non-Hamiltonian dynamics of the magnetic moments. We demonstrate that there is an unprecedentedly strong geometrical spin torque in case of an electron system, where correlations cause antiferromagnetic long-range order. The key observation is that the anomalous torque is strongly boosted by low-energy magnon modes emerging in the two-electron spin-excitation spectrum as a necessary consequence of spontaneous spin-rotation symmetry breaking. As long as single- electron excitations are gapped out, the effect is largely universal, i.e., essentially independent of the details of the electronic structure, but decisively dependent on the lattice dimension. Analogous to the reasoning that leads to the Mermin-Wagner theorem, there is a lower critical dimension at and below which the spin-Berry curvature diverges. Our proposal is supported by numerical results obtained by the random-phase approximation and by Holstein-Primakov spin-wave theory for the Hubbard model in the weak- and in the strong-coupling limit, respectively.

MA 27.3 Wed 10:00 HSZ 403

Exploring electron correlation effects in the electronic structure and spin transport properties of transition metal multilayers — •Andrea Droghetti[1], Miloš Radonjić[2], Declan Nell[1], Liviu Chioncel[3], and Ivan Rungger[4] — [1]Trinity College Dublin (Ireland) — [2]University of Belgrade (Serbia) — [3]University of Augsburg (Germany) — [4]National Physical Laboratory (UK)

Magnetic thin film heterostructures, which are the material platforms for spintronic devices, are quite correlated systems. However, to date, most theoretical studies dedicated to their electronic and spin transport properties, rely on effective single-particle pictures. To go beyond these limitations, we present a computational approach, which combines Density Functional and Dynamical Mean Field Theory, for layered systems, using a multi-orbital perturbative solver for the many-body problem [1]. Calculations accurately describe the spin splitting of 3d states and the appearance of satellite features at transition metal surfaces and interfaces, where electron correlations can get drastically enhanced [2]. Furthermore, when combined with quantum transport schemes [3], our method allows for the simulation of spintronic devices thus addressing how electron correlations affect the giant and tunnel magnetoresistance [4].

[1] A. Droghetti, M.M. Radonjić, A. Halder, I. Rungger, and L. Chioncel, Phys. Rev. B 105, 115129 (2022). [2] D.M. Janas, A. Droghetti, et al., Adv. Mater. 2205698 (2022). [3] A. Droghetti, I Rungger, Phys. Rev. B 95, 085131 (2017). [4] A. Droghetti, M.M. Radonjić, L. Chioncel, I. Rungger, Phys. Rev. B 106, 075156 (2022).

MA 27.4 Wed 10:15 HSZ 403

The role of non-local Coulomb interaction on spin models in the Hubbard limit — •Wejdan Beida, Markus Hoffmann, Juba Bouaziz, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA,52425 Jülich Germany

We extend the derivation of model spin Hamiltonians by including the non-local Coulomb interaction in the multi-band Hubbard model. We use Löwdin partitioning as the downfolding method of the dynamical electronic degrees of freedom described in the extended Hubbard model at half filling into low energy spin corner. The ground state of spin systems has been perturbatively corrected up to fourth order in the hopping parameter of the Hubbard model. The role which the non-local Coulomb interaction plays is strengthening the magnetism of the ground state. More importantly, it increases the importance of higher-order spin interactions beyond Heisenberg; Biquadratic, Four-spin, and Three-spin interactions. Generally speaking, this is confirmed by spin lattices with a site total spin in the range 1/2 * S * 3/2. For S = 1/2, we characteristically investigate the effect of next nearest neighbour hopping and inter-site Coulomb interaction on spin models for square and hexagonal lattice geometries.

15 min. break

MA 27.5 Wed 10:45 HSZ 403

Influence of the temperature on the relation between the magnetic hyperfine field and the magnetic moment — •Ondrej Sipr[1,2] and Hubert Ebert[3] — [1]Institute of Physics, Czech Academy of Sciences, Praha — [2]New Technologies Research Centre, University of West Bohemia, Plzeň — [3]Ludwig-Maximilians-Universität München

The magnetic hyperfine field B_{hf} is often used to probe magnetism in alloys, compounds and doped systems in an element-specific way. Accompanying this is the question about the relationship between B_{hf} and the magnetic moment. It was shown before both experimentally and theoretically that the ratio between B_{hf} and the magnetic moment depends on the alloy system and the composition. Here, we apply ab initio calculations to investigate how B_{hf} and its relation to the magnetic moment depend on the temperature.

We find that the contribution of the core electrons to B_{hf} is indeed proportional to the magnetic moment over the whole temperature range, from zero up to the Curie temperature. However, the temperature-dependence of the contribution of the valence electrons is more complicated and as a result of this, the ratio between the total B_{hf} and the magnetic moment significantly varies with the temperature. Based on our theoretical results, we show that probing element-specific magnetism by means of measuring the magnetic hyperfine field and by measuring the x-ray magnetic circular dichroism will lead in general to different pictures.

MA 27.6 Wed 11:00 HSZ 403

Nonlocal correlation effects due to virtual spin-flip processes in itinerant electron ferromagnets — •Sebastian Paischer[1], Mikhail Katsnelson[2], Giovanni Vignale[3], Arthur Ernst[1], and Pawel Buczek[4] — [1]Johannes Kepler University, Linz, Austria — [2]Radboud University, Nijmegen, Netherlands — [3]National University of Singapore, Singapore — [4]Hamburg University of Applied Sciences, Hamburg, Germany

An important type of the many-body effects in itinerant-electron magnets originates from the interaction of electrons with bosonic spin-flip excitations, both coherent (magnons) and incoherent (Stoner particle-hole excitations). While there has been a steady progress in understanding the properties of spin-flip excitations at a model level only little is known about microscopic details of their interactions with the electronic degrees of freedom in specific materials. Over the last

few years we developed a first-principles method to account for the electron-magnon interaction in complex solids. While the method is based upon many body perturbation theory, we approximate the complex quantities from perturbation theory with quantities from time dependent density functional theory. This drastically reduces the numerical burden of the calculations and allows to consider complex materials like half-metallic ferromagnets. In this talk some of the main results and insights from this method will be presented.

MA 27.7 Wed 11:15 HSZ 403

Data-driven estimation of spin models in undoped cuprates — •Denys Y. Kononenko[1], Ulrich K. Rössler[1], Jeroen van den Brink[1,2], and Oleg Janson[1] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Dresden, Germany — [2]Institute for Theoretical Physics, TU Dresden, Dresden, Germany

Undoped cuprates host a wide variety of low-dimensional and frustrated spin models. The typically leading antiferromagnetic contribution to a magnetic exchange can be accurately estimated if the respective transfer integral is known. To date, the computational estimation of the transfer integral involves a well-established but cumbersome computational procedure. We demonstrate how the Gaussian Process Regression (GPR) model, trained on the results of the density functional theory calculations, can be employed to predict the transfer integrals using crystal structure as the only input. The GPR model receives descriptors of the local crystal environment of two copper sites as an input. The descriptors are based on the truncated expansion of the site position functions on the basis of the three-dimensional Zernike functions [1]. In this way, information on the spatial configuration and the chemical composition of the local crystal environment is incorporated into the descriptor. The approach facilitates rapid screening of spin models with desirable features among a broad range of known and unknown cuprates.

[1] M. Novotni and R. Klein, Computer Aided Design 36, 1047 (2004)