MA 39: Correlation Theory II

Time: Wednesday 15:00–16:00 Location: HSZ 403

MA 39.1 Wed 15:00 HSZ 403

Magnetism of the rare-earth elements, have we really understood everything ? — •Olle Eriksson — Uppsala University, Uppsala, Sweden — Örebro University, Örebro, Sweden

The magnetic properties of rare-earth elements will be described in this talk, with focus on how well electronic structure theory is able to reproduce observations. In this presentation, it is described how information from electronic structure calculations can be mapped to a low energy effective spin-Hamiltonian, and the accuracy of this Hamiltonian is tested against known observables like magnon dispersion and ordering temperature. Recent results suggest that the magnetic configuration of light rare-earths is considerably more complex than previously assumed. These complex magnetic structures are analyzed from an electronic structure point of view. It is demonstrated that properties hitherto unknown among any magnetic system, may indeed be observed in the light rare-earths.

MA 39.2 Wed 15:15 HSZ 403

First principles calculations and Monte Carlo simulations of half-metallic $CaCu_3Fe_3Re_2O_{12}$ quadruple perovskite — •Duo Wang[1], Saurabh Ghosh[2], and Biplab Sanyal[1] — [1]Uppsala University, Uppsala, Sweden — [2]SRM University, Chennai, India

Materials that have high spin-polarized conduction electrons at room temperature are very important for spintronic developments. Wentin Chen *et al.* have synthesized the quadruple perovskite $CaCu_3Fe_3Re_2O_{12}$, which shows half-metallic electronic structure, large magnetization and very high Curie temperature (up to 560K). We have performed density functional calculations on the ground state structure ($CaCu^{2+}(\uparrow)_3Fe^{3+}(\uparrow)_2Re^{5+}(\downarrow)_2O_{12}$), and calculated interatomic exchange interactions with the Full-Potential Linear Muffin-Tin Orbital (FP-LMTO) method. We find that both J_{Re-Cu} and J_{Re-Fe} show strong antiferromagnetic coupling along with ferromagnetic coupling between Fe moments. This is consistent with ferrimagnetic nature of A_2FeReO_6 (A=Ca, Sr and Ba, respectively) double perovskite that the high Curie temperature indicate strong antiferromagnetic couplings. We also performed Monte Carlo simulations using the exchange parameters obtained from the FP-LMTO method. The magnetic transition temperature is found to be 295K. Besides that, the size of A-site cation will affect the crystal structure, magnetism, exchange interactions and also magnetic ordering temperature. Calculations to replace A-site atom (Ca) are ongoing.

MA 39.3 Wed 15:30 HSZ 403

Magnetic interactions in the honeycomb Kitaev-Heisenberg systems H3LiIr2O6 and Cu2IrO3 by ab initio quantum chemical methods — •Mohamed Eldeeb[1], Ravi Yadav[1], Satoshi Nishimoto[1,2], Jeroen van den Brink[1,2], and Liviu Hozoi[1] — [1]Institute for Theoretical Solid State Physics, Leibniz IFW Dresden, Helmholtzstr. 20, 01069, Dresden, Germany — [2]Department of Physics, Technical University Dresden, Helmholtzstraße 10, D-01069 Dresden, Germany

The magnetic interactions in honeycomb iridium oxide compounds are studied using quantum chemical wavefunction-based methods. Mapping the results onto the corresponding effective spin model shows the crucial dependence of the anisotropic magnetic couplings, in particular Kitaev exchange, on the precise position of inter-layer species and on additional geometrical factors such as Ir-O-Ir bond angles and Ir-O bond lengths. While the latter define the actual superexchange path between magnetic centers, the former may come into play through strong out-of-plane polarization of ligand 2p orbitals mediating intersite hopping [1,2]. (1)R. Yadav, R. Ray, M. S. Eldeeb, S. Nishimoto, L. Hozoi, and J. van den Brink, Phys. Rev. Lett. 121, 197203 (2018). (2) R. Yadav, M. S. Eldeeb, R. Ray, S. Aswartham, M. I.Sturza, S. Nishimoto, J. van den Brink, and L. Hozoi, Chem. Sci. 10, 1866 (2019).

MA 39.4 Wed 15:45 HSZ 403

Quantum Electrodynamical Bloch Theory with Homogeneous Magnetic Fields — •Vasil Rokaj, Markus Penz, Michael Sentef, Michael Ruggenthaler, and Angel Rubio — Max Planck Institute for the Structure & Dynamics of Matter, Hamburg, Germany

Probing electronic properties of periodic systems by homogeneous magnetic fields has unravelled fundamental new phenomena in condensed matter physics. Much theoretical work has been devoted to describe those systems in different regimes, still a general first principles modeling of such fundamental effects is lacking. Here we propose a solution to the problem of Bloch electrons in a homogeneous magnetic field by including the quantum fluctuations of the photon field. A generalized quantum electrodynamical (QED) Bloch theory from first principles is presented. As an application, we show how the well-known Landau physics is modified by the photon field and that Landau polaritons emerge. Moreover, for a 2D solid in a perpendicular magnetic field, in the limit of vanishing quantum fluctuations, we recover the standard results of solid-state physics: the fractal spectrum of the Hofstadter butterfly. Further generalizations and modifications of the Hofstadter butterfly will be presented for 2D materials like graphene and Moire superlattices which are of current experimental interest.

[1]V.Rokaj et al. Phys. Rev. Lett. 123, 047202 (2019)