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Campus Schenefeld, main building (XHQ) room E1.172

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First-principles modelling of electronic and magnetic excitations in correlated materials

First-principles modelling of electronic and magnetic excitations in correlated materials. In the past decades there has been an enormous progress in developing the realistic electronic structure theory for strongly correlated systems. Most of the modern first-principles studies are based on a combination of density functional theory and dynamical mean field theory (DFT+DMFT) [1]. Within this approach, the DFT is used as a starting point for more sophisticated DMFT calculations for a selected subset of “correlated” orbitals. The approach has proven to be extremely successful and is commonly employed to model the electronic structure of a wide range of d- and f-based correlated materials. In my talk I will show the applications of DFT+DMFT for studying various types of excitation spectra.

First, I will address the calculations of the core-level L-edge x-ray absorption spectra (XAS) in TM oxides. We have adopted the idea proposed by Haverkort et al [2] and implemented it in the language of DFT+DMFT [3]. We applied this method to TM monoxides and obtained the spectra, which are in excellent agreement with experiment. We also investigated the importance of explicit account of the core hole, which is usually neglected. Our results suggest that its presence enhances the Coulomb repulsion between the TM d-states and tends to suppress the TM-oxygen hybridisation. The limitations and further developments of the method will be discussed.

In the second part of my talk I will discuss the modelling of the magnetic excitation spectra. Magnon excitations are non-local and are therefore not directly accessible within DMFT. Thus we have to employ a so-called two-step approach. We first map the system on a Heisenberg model and extract the effective exchange parameters J_{ij} 's from DFT+DMFT, following Ref.[4]. Then the atomistic spin dynamics simulations are employed to simulate magnon spectra and predict the magnetic ordering temperatures. The J_{ij} ' in real materials have a complicated nature and depend on how the correlations taken into account [5]. I will show how the decomposition of the exchange parameters in terms of their orbital contributions can provide a useful insight into the essence of magnetism in a material. In particular, we found an intrinsic competition between ferromagnetic and antiferromagnetic interactions between different orbitals in elemental Mn and Fe [6]. Moreover, I will demonstrate that iron is a unique example where one can even distinguish RKKY, double- and super-exchange contributions to the magnetic couplings [7].

References:

- [1] G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianetti, Rev.Mod. Phys., 78, 865 (2006)
- [2] M. W. Haverkort, M. Zwierzycki, and O. K. Andersen, Phys. Rev. B 85, 165113 (2012)
- [3] J. Lüder et al, arXiv: 1706.08168
- [4] M.I. Katsnelson and A.I. Lichtenstein, Phys. Rev. B 61 8906 (2000)
- [5] YK et al, Phys. Rev. B 91, 125133 (2015)
- [6] R. Cardias, et al, Sci. Rep. 7, 4058 (2017)
- [7] YK et al, Phys. Rev. Lett. 116, 217202 (2016)

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