Effective inter-site exchange interactions from DFT+DMFT

Yaroslav Kvashnin, Igor Di Marco, Oscar Grånäs, Corina Etz, and Olle Eriksson

Uppsala University, Department of Physics and Astronomy, Lägerhyddsvägen 2, SE-75120 Uppsala, Sweden

The inter-site exchange couplings (J's) is one of the main quantities of magnetic materials. They define the Curie temperature, such an important property of a compound for its technological application. An ability to predict and tweak the J-parameters in various materials would be an essential step towards the design of new permanent magnets. Therefore, a great effort is made in the field of computational modelling. However, this task becomes even more challenging due to the fact that many of suitable compounds exhibit strong correlation effects.

In this talk I will present our recent implementation of the method for extracting exchange parameters in strongly correlated systems from first-principles calculations. We model the electronic structure with the help of the full-potential linear muffin-tin orbital code, developed in Uppsala [1]. The effects of electron correlations are studied within the same framework by means of charge self-consistent density functional theory + dynamical mean field theory (CSC DFT+DMFT) method [2]. In order to calculate the effective exchange parameters, we employ the linear-response-like approach by Lichtenstein *et al.* [3]. Combined all together, these methods allow us to investigate how J's are affected by electron correlations at finite temperature.

In the last part of my presentation I will show some particular applications of the method. A special attention will be given to the case of $SrRuO_3$. The impact of correlation effects and structural changes on the J-parameters in this system will be discussed.

[1] J. M. Wills, M. Alouani, P. Andersson, A. Delin, O. Eriksson, and O. Grechnev, Springer Series in Solid-State Sciences pp. 1–195 (2010).

[2] O. Granas, I. Di Marco, P. Thunstrom, L. Nordstrom, O. Eriksson, T. Bjorkman, and J. M. Wills, Computational Materials Science 55, 295 (2012).

[3] A. I. Liechtenstein et al., J. Magn. Magn. Mater., 67, 65 (1987) ; M. I. Katsnelson and A. I. Liechtenstein, J. Phys. Condens. Matter, 16, 7439 (2004).