MAR10-2009-001761

Abstract for an Invited Paper
for the MAR10 Meeting of
the American Physical Society

Prediction of d^0 magnetism in self-interaction corrected density functional theory

CHAITANYA DAS PEMMARAJU, Trinity College Dublin

Over the past couple of years, the phenomenon of "d^0 magnetism" has greatly intrigued the magnetism community [1]. Unlike conventional magnetic materials, "d^0 magnets" lack any magnetic ions with open d or f shells but surprisingly, exhibit signatures of ferromagnetism often with a Curie temperature exceeding 300 K. Current research in the field is geared towards trying to understand the mechanism underlying this observed ferromagnetism which is difficult to explain within the conventional m-J paradigm [1]. The most widely studied class of d^0 materials are un-doped and light element doped wide gap Oxides such as HfO2, MgO, ZnO, TiO2 all of which have been put forward as possible d0 ferromagnets. General experimental trends suggest that the magnetism is a feature of highly defective samples leading to the expectation that the phenomenon must be defect related. In particular, based on density functional theory (DFT) calculations acceptor defects formed from the O-2p states in these Oxides have been proposed as being responsible for the ferromagnetism [2,3]. However. predicting magnetism originating from 2p orbitals is a delicate problem, which depends on the subtle interplay between covalency and Hund's coupling. DFT calculations based on semi-local functionals such as the local spin-density approximation (LSDA) can lead to qualitative failures on several fronts. On one hand the excessive delocalization of spin-polarized holes leads to half-metallic ground states and the expectation of room-temperature ferromagnetism. On the other hand, in some cases a magnetic ground state may not be predicted at all as the Hund's coupling might be under estimated. Furthermore, polaronic distortions which are often a feature of acceptor defects in Oxides are not predicted [4,5]. In this presentation, we argue that the self interaction error (SIE) inherent to semi-local functionals is responsible for the failures of LSDA and demonstrate through various examples that beyond-LSDA approaches that are either self-interaction free or effectively correct for it overcome such failures to produce a more accurate description of acceptor defects in Oxides. Typically, correcting for the SIE, leads to an enhanced localization of the holes responsible for the magnetism. Additionally, the ground state becomes insulating driven by polaronic distortions around the defect site and the magnetic coupling between the impurities becomes weak [4,5,6].

[1] J.M.D. Coey, Solid State Sci., **7**, 660 (2005).
[2] I.S. Elfimov et al, PRL **89**, 216403 (2002).
[3] C. D. Pemmaraju and S. Sanvito, PRL **94**,217205 (2005)
[4] A. Droghetti et al, PRB **78**, 140404(R) (2008)
[5] J.A. Chan et al, PRL **103**, 016404, (2009).
[6] V. Pardo et al, PRB **78**, 134427 (2008)