Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Defect-induced magnetism in oxides ANDREA DROGHETTI, SRI CHAITANYA DAS PEMMARAJU, STEFANO SANVITO, Trinity College Dublin — The so called "d^0 magnets" are a class of materials which, lacking any magnetic ions with open d or f shells, should in principle not be magnetic, but nevertheless exhibit signatures of room temperature ferromagnetism. The most widely studied class of d^0 magnets is that of medium to wide gap oxides. Since ferromagnetism is generally observed in highly defective samples, it is expected that the magnetism must be somehow defect-related. However, at the present, there is no clear explanation of the experimental observations. We then present the results of a detailed research which combines Density Functional Theory (DFT) with model Hamiltonian calculations. In particular we consider whether ferromagnetism might be due to carrier-mediated long-range coupling between magnetic moments residing on cation vacancies or to a Stoner-like splitting of an impurity band in defect-rich regions of the samples.

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Date submitted: 18 Nov 2009 Electronic form version 1.4