

Abstract Submitted  
for the MAR05 Meeting of  
The American Physical Society

**Origin of ferromagnetism in transition metal doped TiO<sub>2</sub>** REBECCA JANISCH, Materials Department, University of California Santa Barbara, NICOLA A. SPALDIN, Materials Department, University of California Santa Barbara — Reports of robust room-temperature ferromagnetism in oxide-based dilute magnetic semiconductors, such as Co-doped TiO<sub>2</sub> and ZnO, make these materials promising candidates for device applications. However, the origin of this robust ferromagnetism and the factors that influence its strength have not yet been fully understood. One model, proposed by Venkatesan and Coey, suggests that the observed ferromagnetism in doped ZnO and SnO<sub>2</sub> is mediated via an electron trapped in a bridging oxygen vacancy [1,2]. On the other hand there is also evidence, e.g. in the case of Co-doped TiO<sub>2</sub>, that free carriers play a role in mediating the magnetic interaction (e.g.[3]). To test the validity of the different models for the TiO<sub>2</sub>-based dilute magnetic semiconductors, and to modify them where necessary, we study transition metal doped TiO<sub>2</sub> in the anatase structure by means of ab-initio density-functional band-structure calculations. We analyse the interaction of the transition metal dopants with the electronic states of the host as a function of the distribution and concentration of the impurity atoms. Finally we determine the influence of point and extended defects on the magnetic interactions.

[1] D.M.C. Coey et al., J. Appl. Phys. Lett. **84**, 1332 (2004). [2] M. Venkatesan et al., cond-mat/0406719. [3] H. Toyosaki et al., Nature **3**, 221 (2004).

Rebecca Janisch  
Materials Department, University of California Santa Barbara

Date submitted: 29 Nov 2004

Electronic form version 1.4