Abstract Submitted for the MAR10 Meeting of The American Physical Society

Ferromagnetism in N doped ZnO and MgO MICHAEL SHAUGH-NESSY, UC Davis, Lawrence Livermore National Laboratory, L.H. YANG, Lawrence Livermore National Laboratory, C.Y. FONG, UC Davis — We investigate single and multiple dopings of N in $\text{ZnO}_{1-x} \text{N}_x$ and in $\text{MgO}_{1-x} \text{N}_x$ using a first principles density functional theory supercell method for x< 10%. We find evidence for ferromagnetism and propose a mechanism mediating the interaction. The magnetic coupling between the local moments on the N defects is studied as a function of the distance between N atoms and the role of hole and carrier co-doping is investigated. An RKKY-type interaction is found to mediate coupling, leading to both ferromagnetic and antiferromagnetic couplings for different doping configurations.

Michael Shaughnessy UC Davis, Lawrence Livermore National Laboratory

Date submitted: 19 Nov 2009 Electronic form version 1.4