Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Ferromagnetism in GaN:Gd: A density functional theory study[1]
LEI LIU, LBNL, UCB, PETER YU, UCB, LBNL, Z.X. MA, LBNL, SAM MAO, LBNL, UCB — First principle calculations of the electronic structure and magnetic interaction of GaN:Gd have been performed within the Generalized Gradient Approximation (GGA) of the density functional theory (DFT) with the on-site Coulomb energy U taken into account (also referred to as GGA+U). The ferromagnetic $p-d$ coupling is found to be over two orders of magnitude larger than the$s-d$ exchange coupling. The experimental colossal magnetic moments and room temperature ferromagnetism in GaN:Gd reported recently are explained by the interaction of Gd $4f$ spins via $p-d$ coupling involving holes introduced by intrinsic defects such as Ga vacancies.

[1]Supported by the U.S. Department of Energy, NNSA/NA-22, under Contract No. DE-AC02-05CH11231.

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Date submitted: 27 Nov 2007 Electronic form version 1.4