Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First principles calculations for Gd doped GaN CHANDRIMA MITRA, WALTER LAMBRECHT, Case Western Reserve University — Gd doped GaN has been reported by Dhar et al. to have magnetic moments of order a few 1000 μ_B per Gd in the very dilute limit of 10^{15} Gd/cm^3 and to show above room temperature ferromagnetism. Here we present first principle electronic structure calculations to study the spin splitting of the conduction band with varying concentration of Gd in GaN. Our calculations show that the spin splitting varies linearly with the concentration of Gd which suggests an almost zero splitting if one were to extrapolate to the 1 ppm dilute concentration of Gd. Thus the large magnetic moments cannot be explained simply by assuming donor electrons (for example from oxygen) will fill the spin-split conduction band. The spin polarization of the Ga and N atoms around Gd atom in a supercell of 1.5% Gd were found to be small and to become negligible beyond second nearest neighbors. In these, studies, we either added oxygen or Si as co-dopants or a background charge to fill the spin-split conduction band. This indicates that the proposed model of Dhar of polarization of the host is not supported by our calculations. The magnetic exchange interaction parameter, for nearest neighbour Gd atoms have also been calculated by mapping the energy differences between the ferromagnetic and antiferromagnetic arrangement onto the Heisenberg's model. Effects of strain, supercell size and shape, and other dopants on the exchange interactions were investigated.

Chandrima Mitra
Case Western Reserve University

Date submitted: 20 Nov 2007 Electronic form version 1.4