Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Digital magnetic heterostructures based on GaN LUIZ G. FERREIRA, Universidade de São Paulo, Brazil, MARCELO MARQUES, JOÃO P. T. SANTOS, LARA K. TELES, Instituto Tecnologico de Aeronautica, Brazil — Delta doped heterostructures based on GaN are possible wide band gap spintronic material with high temperature ferromagnetic transition [Hory et al, Physica B 324, 142 (2002); Reed et al, Appl. Phys. Lett. 79, 3473 (2001)]. They are formed by a thin magnetic layer or submonolayer, embedded into thick semiconductor layers [Marques et al, Phys. Rev. B 73, 224409 (2006)]. In this work we studied digital magnetic heterostructures with isolated magnetic monolayers of V, Cr, Mn, Fe, Co, Ni, or Cu embedded in GaN. We performed first-principles calculations within the density functional theory with self-energy, to account for excitation energies [Ferreira et al, Phys. Rev. B 78, 125116 (2008)]. The technique allowed us to calculate the GaN band gap as $E_{gap}^{calculated} = 3.53eV$ with no adjustable parameters. GaN:V and GaN:Cr do have ferromagnetic ground states with high Curie temperatures, as predicted by a mean-field approximation. GaN:Cr presents a 2D half-metallic ground state with 100% spin polarization. GaN:V has an unusual ground state, with a $2.0\mu_B$ magnetic moment, no states at the Fermi energy, a minority spin gap of 3.0eV, and a majority spin gap of only 0.3eV.

Luiz G. Ferreira
Universidade de São Paulo

Date submitted: 18 Nov 2010 Electronic form version 1.4