Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Mg-doped GaN nanostructures: Energetics, magnetism and H2 adsorption QIAN WANG, Virginia Commonwealth University, QIANG SUN, Peking University and Virginia Commonwealth University, PURU JENA, Virginia Commonwealth University — It has been shown that p-type GaN can greatly improve the performance of GaN-based devices. Mg is a suitable candidate dopant for p-type GaN. Since the ionic radius of Mg is comparable with that of Ga, Mg doping can be expected to eliminate self-compensation effects. Thus, synthesis of Mg-doped p-type GaN for fabrication of optoelectronic devices has been hotly pursued. Using density functional theory and generalized gradient approximation for exchange and correlation potential we show that Mg doped GaN nanocage and nanotube can be magnetic with Mg contributed spins distributed over the neighboring N sites. Mg atoms show no tendency for clustering and due to the positive charge residing on them; they can trap hydrogen in molecular form via the charge polarization mechanism. The binding energies of hydrogen lie in the range of 0.1∼0.2 eV/H2 which are ideal for storage applications under ambient thermodynamic conditions.

Qian Wang
Virginia Commonwealth University

Date submitted: 19 Nov 2008 Electronic form version 1.4