

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Structures and magnetic properties of Cr-doped GaN nanotubes

QIAN WANG, QIANG SUN, PURU JENA, VCU, YOSHIYUKI KAWAZOE, IMS, Japan, VCU TEAM, IMS JAPAN COLLABORATION — The electronic and magnetic properties of Cr-doped GaN nanotubes are investigated theoretically from first principles using the generalized gradient approximation (GGA) as well as LSDA+U method. We have shown that GaN single wall nanotube, which was generated from GaN wurtzite crystal undergoes large structural relaxation and resemble the structure of carbon (9,0) single wall nanotubes. In addition, it is stable at room temperature. Cr-doped GaN single wall and multi-wall nanotubes are ferromagnetic with each Cr atom carrying a magnetic moment of about $2.67 \mu_B$. This ferromagnetic coupling is mediated by the neighboring N atoms which are weakly polarized and carry a magnetic moment of $-0.18 \mu_B$. These results are not sensitive to the tube diameter, Cr concentration, and the level of correlation. Thus, Cr doped GaN nanotubes may be a robust system for applications in spintronics.

Anil Kandalam
VCU

Date submitted: 01 Dec 2005

Electronic form version 1.4