Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Spin-polarized states in zigzag-edge graphene nanostrips[1] JOHN W. MINTMIRE, JUNWEN LI, Oklahoma State University, DANIEL GUNLYCKE, CARTER T. WHITE, Naval Research Laboratory — Zigzag-edge graphene nanostrips (GNSs) are known to exhibit localized edge states in the vicinity of the Fermi level. It has previously been reported that these edge states are ferrimagnetic. We present a study based on first-principle DFT and Hubbard model calculations that confirm the ferrimagnetic nature of the edge states. By comparing the results, we have estimated the Hubbard U to be approximately 2.7 eV. Energy dispersions, spin polarizations, and total energies are calculated for various widths of the nanostrips. In both our approaches, we find that the ferrimagnetic states have lower energy than the spin-restricted solution.

[1]This work was supported by the NRC, ONR, and DoD HPCMO CHSSI program.

Daniel Gunlycke
Naval Research Laboratory

Date submitted: 20 Nov 2006 Electronic form version 1.4