Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First-principles calculations of zigzag-edge graphene nanostrips with different edge species[1] JOHN W. MINTMIRE, Oklahoma State University, DANIEL GUNLYCKE, Naval Research Laboratory, JUNWEN LI, Oklahoma State University, CARTER T. WHITE, Naval Research Laboratory — First-principles calculations have suggested that zigzag-edge graphene nanostrips terminated with hydrogen atoms have edge states which exhibit magnetic behavior. However, it is not clear that zigzag-edge graphene nanostrips terminated with other atoms or functional groups also show similar magnetic behavior. Our local-spin-density calculations suggest that some zigzag-edge nanostrips, including oxygen-terminated nanostrips, have no magnetic edges. One reason could be that there is charge transfer at the edges which effectively dopes the pi-orbital network, causing the spin polarization to collapse.

[1]This work was supported by the NRC and ONR through NRL, and at OSU by the DOE EPSCoR program.

John Mintmire
Oklahoma State University

Date submitted: 27 Nov 2007 Electronic form version 1.4