Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Ab-initio Calculation of the Magnetic Properties of BN Nanoribbon[1] JEFF RUFINUS, Widener University, Science Division, Chester, PA 19013 — Recently, the search for new spintronics materials has also included graphene-based materials due to the theoretical prediction that this type of material may show the half-metallic property. Here, we present the results of a density functional theory within a generalized gradient approximation study of narrow Boron Nitride nanoribbon (BNNR). The objective of this study is to determine whether this type of material will be ferromagnetic (FM), antiferromagnetic (AFM), or ferrimagnetic. Our results show that the narrow zigzag shaped BNNR prefers antiferromagnetic state. The energy difference among the three states (FM, AFM, ferrimagnetic), however, is very small. Increasing the width of BNNR, was predicted to cause the stabilization of FM state instead of the AFM state.

[1]Work supported by Widener University grants. Computational time from PSC and OSCER-OU is acknowledged.

Jeff Rufinus
Widener University, Science Division, Chester, PA 19013

Date submitted: 11 Nov 2011 Electronic form version 1.4