Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

First principles study of trilayers of graphene-BN-graphene[1] XIAOLIANG ZHONG, RODRIGO AMORIM, RAVINDRA PANDEY, Michigan Technological University, SHASHI KARNA, US Army Research Laboratory, Weapons and Materials Research Directorate, ATTN: RDRL-WM — The stability, electronic structure and electronic transport properties of graphene-BN-graphene (C-BN-C) trilayers are studied in the framework of density functional theory. Different stacking formats, i.e., AAA, ABA and ABC stackings are considered. The ABA stacking is found to be most energetically favorable, followed by ABC and AAA stackings. The interlayer spacing of trilayers are close to those of corresponding C-BN bilayers, while the intralayer bond length can be regarded as the weighted mean of constituent layers. All considered configurations are found to be metallic, independent of stacking formats. When an external electric field is applied perpendicularly, electronic band structures undergo stacking-dependent variations. While both AAA and ABA stackings show good tunability of energy gap, ABC stacking shows less flexibility of gap tuning. We will also present the results of the electronic transport properties which are modeled by sandwiching trilayers between gold contact electrodes.

[1]The work at Michigan Technological University was performed under support by the Army Research Laboratory through Contract No. W911NF-09-2-0026-133417.

Xiaoliang Zhong
Michigan Technological University

Date submitted: 07 Nov 2011 Electronic form version 1.4