Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Determination of superexchange correlations in magnetically substituted graphene[1] C.B. CROOK, C. CONSTANTIN, Department of Physics and Astronomy, James Madison University, T. AHMED, Theoretical Divison, Los Alamos National Laboratory, J.-X. ZHU, Theoretical Divison and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, A.V. BALATSKY, Institute for Materials Science, Los Alamos National Laboratory, J.T. HARALDSEN, Department of Physics and Astronomy, James Madison University — We investigate the electronic and magnetic properties between two homogeneous magnetic impurities (vanadium, chromium, or manganese) in a 128-atom graphene superlattice. With varying the impurity distance, we calculate these properties using a first principles approach. For each configuration, we determine the electronic bandstructure and density of states, along with the Mullikan populations for each atom. Furthermore, we calculate the exchange parameter between the two magnetic ions through the analysis of the change in total energy for different magnetic configurations. We found that the magnetic impurities induce a mangetic moment in the graphene superlattice, helping to meditate the superexchange between the impurities. Depending on the choice of ion used, the interactions between the two ions can exhibit either a ferromagnetic or an antiferromagnetic behavior. These correlations indicate an RKKY-like behavior in the system.

[1]We acknowledge support from the Tickle Fellowship Program, Center for Integrated Nanotechnologies User Program, and Institute for Materials Science

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Date submitted: 09 Nov 2014 Electronic form version 1.4