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Understanding Magnetic Trimer Interactions in (Cr,Mn)-Substituted Graphene[1] JASON T. HARALDSEN, Department of Physics, University of North Florida, CHARLES B. CROOK, GREGORY HOUCHINS, Department of Physics and Astronomy, James Madison University, JIAN-XIN ZHU, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, COSTEL CONSTANTIN, Department of Physics and Astronomy, James Madison University, ALEXANDER V. BALATSKY, Institute for Materials Science, Los Alamos National Laboratory — We investigate the magnetic interactions within a graphene superlattice produced by three directly substituted transition-metal atoms (specifically chromium and manganese). Using a first principles approach, we calculate the electronic and magnetic properties for this system assuming an equilateral trimer configuration with varying atomic separations. Through an examination of the electronic band structure, density of states, and Millikan populations (magnetic moment) for each atom, we find that the presence of magnetic impurities establishes a distinct magnetic moment in the graphene lattice, where the interactions are dependent on the spatial and magnetic characteristic between the magnetic atoms and the carbon atoms, which leads to either ferromagnetic or antiferromagnetic behavior. Furthermore, we use magnetization mapping to show that the substituted atoms induce an overall magnetic moment in the graphene lattice, which may help guide the discussion on spintronic graphene.

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