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Understanding the optical and electronic properties of Ga-doped graphene[1] N.C. CREANGE, C. CONSTANTIN, Department of Physics and Astronomy, James Madison University, J.-X. ZHU, Theoretical Division 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 simulate the optical and electrical responses in gallium-doped graphene, using density functional theory with a local density approximation. We show the effects of impurity doping (0-3.91%) in the graphene sheet and for each doping percentage the change in electron density, refractive index, and optical conductivity are reported. Here, gallium atoms are placed randomly (using a 5-point average) throughout a 128-atom sheet of graphene. These calculations demonstrate the effects of hole doping due to direct atomic substitution, where we find a disruption in the electron density for small doping levels, which is due to impurity scattering of the electrons. However, there seems to be a doping percentage, above which we have calculated, at which the system transitions to produce metallic or semi-metallic behavior. These calculations are compared to a purely theoretical 100% Ga sheet for comparison of conductivity. Furthermore, we examine the change in the electronic band structure and density of states, where the introduction of gallium electronic bands produces a shift in the electron bands and dissolves the characteristic Dirac cone within graphene.

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