Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Possible bandgap opening in graphene due to deposited Au nanoparticles: First-principles calculations RONALDO J.C. BATISTA, SABRINA S. CARARA, HELIO CHACHAM, Universidade Federal de Minas Gerais, Brazil — We perform first-principles calculations to investigate electronic and structural properties of graphene with a layer of deposited Au nanoparticles. We consider Au_{38} nanoparticles that can be either covered with methylthiol molecules, or not. We also consider that the nanoparticles are arranged in a hexagonal lattice, and we focus on the effect of net charge, applied electric fields, and molecular coverage on the electronic structure of the graphene+nanoparticles system. We find that covered nanoparticles interact weakly with graphene, and that the main effect of the nanoparticles on the electronic structure of graphene is a doping effect that can be modified with the application of an electric field perpendicular to the graphene plane. The system is always metallic, without the opening of a bandgap, even if the nanoparticles are charged: neither the Coulomb potential nor the weak nanoparticle-graphene interaction is able to break the graphene sublattice symmetry. In contrast, in the case of deposited bare (non-covered) Au nanoparticles, there is a relatively strong interaction between low-coordinated Au atoms and graphene carbon atoms beneath. This leads to a symmetry breaking of the graphene sublattices and to the opening of a small bandgap of a few tens of meV.

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Date submitted: 29 Nov 2007 Electronic form version 1.4