

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Ab initio Study of the Interactions between Single Vacancies in Graphene¹ MAHMOUD HAMMOURI, IGOR VASILIEV, New Mexico State University — Graphene is a promising material for nanoelectronic and spintronic applications. The introduction of point defects such as vacancies can turn graphene into a magnetic material. We present a first-principles computational study of the interactions between single vacancies in graphene. The total energies, lattice deformation energies, and spin magnetic moments of the interacting vacancies are calculated using the SIESTA density functional electronic structure code combined with the generalized gradient approximation for the exchange correlation functional. We discuss the variation of the total energy and the total magnetic moment of defective graphene as a function of the separation distance between vacancies. Our calculations show that the magnetic moment of graphene disappears when the vacancies are located within a certain distance from each other.

¹Supported by NSF CHE-1112388 and NMSU Graduate School

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Date submitted: 07 Nov 2012

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