Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Ab Initio Study of the Interactions between Dopant Atoms and Point Defects in Graphene[1] TAREK TAWALBEH, IGOR VASILIEV, New Mexico State University — We apply a first-principles computational method based on density functional theory to study the interaction of substitutional boron and nitrogen atoms with Stone-Wales defects and vacancies in graphene. Our calculations are carried out using a pseudopotential technique combined with the generalized gradient approximation for the exchange-correlation functional implemented in the SIESTA electronic structure package. Graphene sheets are modeled by periodic supercells containing up to 160 atoms. The equilibrium geometries, total energies, electronic structures, and densities of states of doped and defective graphene sheets are examined as a function of the separation distance between dopant atoms and point defects in graphene. The results of our study demonstrate the presence of attractive interaction between dopant atoms and point defects in graphene. The interaction energy decreases rapidly with increasing the dopant-defect separation distance.

[1]Supported by NSF CHE-1112388.

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Date submitted: 10 Nov 2011 Electronic form version 1.4