

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

First-Principles Study of Nucleic Acid Bases Physisorbed on Graphene S. GOWTHAM, R. H. SCHEICHER, Department of Physics and Multi-Scale Technology Institute, Michigan Technological University, Houghton, MI 49931, RAJEEV AHUJA, Department of Physics, Uppsala University, Sweden; Department of Materials Science and Engineering, Royal Institute of Technology, Sweden, RAVINDRA PANDEY, Department of Physics and Multi-Scale Technology Institute, Michigan Technological University, Houghton, MI 49931, SHASHI P. KARNA, US Army Research Laboratory, Weapons and Materials Research Directorate, ATTN: AMSRD-ARL-WM, Aberdeen Proving Ground, MD 21005-5069 — We report the results of our investigation on the interaction of nucleic acid bases with graphene, carried out within the density functional theory framework, with additional calculations utilizing Hartree–Fock plus second–order Møller–Plesset perturbation theory. The calculated binding energy of the five nucleobases shows the following hierarchy: $G > T \approx C \approx A > U$, though the equilibrium configuration consists of nearly the same separation between the sheet and the bases considered. The stabilizing factor in the interaction between the nucleobases and the graphene sheet appears to be dominated by the molecular polarizability that induces a weakly attractive dispersion force between them. The present study is a first step toward understanding why different DNA sequences interact differently with CNTs, as observed experimentally.

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Date submitted: 20 Nov 2006

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