

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Non-covalent functionalization of single wall carbon nanotubes and graphene by a conjugated polymer¹ JILILI JIWUER, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia, AYJAMAL ABDURAHMAN, ÖGÜZ GÜLSEREN, Department of Physics, Bilkent University, 06800 Ankara, Turkey, UDO SCHWINGENSCHLÖGL, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia — We report first-principles calculations on the binding of poly[(9,9-bis-(6-bromohexylfluorene-2,7-diyl)-co-(benzene-1,4-diyl)] to a (8,0) single wall carbon nanotube (SWCNT) and to graphene. Considering different relative orientations of the subsystems, we find for the generalized gradient approximation (GGA) a non-binding state, whereas the local density approximation (LDA) predicts reasonable binding energies. The results coincide after inclusion of van der Waals (vdW) corrections, which demonstrates a weak interaction between the polymer and SWCNT/graphene, mostly of van der Waals type. Accordingly, the density of states shows essentially no hybridization. The physisorption mechanism explains recent experimental observations and suggests that the conjugated polymer can be used for non-covalent functionalization. (Reference: Appl. Phys. Lett. 105, 013103, 2014)

¹Research reported in this publication was supported by the King Abdullah University of Science and Technology (KAUST).

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Date submitted: 14 Oct 2014

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