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First-Principles Investigation of Polymer Binding to Graphene and Carbon Nanotubes[1] OGUZ GULSEREN, AYJAMAL ABDURAHMAN, Bilkent University — The interactions between a polymer (Poly[(phenylene)-co-(9,9-bis-(6-bromohexyl)uorene)]) and graphene and carbon nanotubes are investigated by using pseudopotential planewave calculations based on density functional theory (DFT). In the quest of searching the most favorable binding configurations, the monomer under investigation is placed at different orientations on graphene. In order to obtain further insight into the binding interactions of polymer-graphene system, we also calculated the binding energy for the structure in which the polymer is attached to graphene sheet via atomic oxygen. Considering the graphene impurity, we have also further investigated the polymer approaching from the chain side onto graphene with a vacancy. However, our results demonstrated that the interaction between the (Poly[(phenylene)-co-(9,9-bis-(6-bromohexyl) uorene)]) polymer and graphene is weak, mostly dispersive, but this interaction is slightly stronger when the graphene has structural defects, like vacancies. The implications of these results to the polymer and carbon nanotube interactions also are discussed.

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Oguz Gulseren
Bilkent University

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