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Adsorption of Aromatic Compounds on Carbon Nanotubes LILIA

WOODS, University of South Florida, ȘTEFAN BĂDESCU, Naval Research Laboratory, TOM REINECKE¹ — The functionalization of carbon nanotubes (CNTs) by molecular adsorption is of scientific interest and also of importance in potential applications as sensors. We have studied theoretically the interactions between CNTs and organic aromatic molecules that are derived from benzene by addition of different functional groups (e.g. CH_3 , OH , NO_2). We perform density functional *ab initio* calculations based on the plane-wave supercell method using the generalized gradient approximation. We explore the possible configurations of bonding to both zigzag and armchair CNTs. Two types of minimum energy configurations are distinguished: i) those where the benzene ring is parallel to the CNT surface and the coupling is dominated by $\pi - \pi$ interactions; ii) those where the functional groups of the molecules arrange normal to the CNT surface and bind stronger to the CNT. We discuss quantities related to experimental observables, such as adsorption energy, bonding, and changes induced on the CNT electronic structure.

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