

Abstract Submitted
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Interaction of water and methanol with graphene, C60 and (10,10) nanotube¹ VIJAY KUMAR, Dr. Vijay Kumar Foundation, Gurgaon, India, M. AMAR, Wright State Univ., J.F. MAGUIRE, Air Force Research Laboratory, Y. KAWAZOE, IMR, Tohoku Univ. Sendai, Japan — We study interaction of water and methanol molecules with graphene, C60 and (10,10) carbon nanotube using plane wave pseudopotential method and GGA. The interaction energies, ΔE , of H₂O and CH₃OH molecules on a (10,10) SWCNT, C60 and a graphene sheet are quite small (a few tens of meV) and are weakly dependent on the orientation of the molecules. The different electronic structures of graphene, nanotubes, and C60 lead to the differences. For (10,10) nanotube ΔE of water (39 meV) is favorable outside the nanotube and it increases for a water dimer. For methanol ΔE outside as well as inside the nanotube is nearly the same (40 meV). A competition between molecules-molecule and molecule-nanotube wall interaction could, however, lead to interesting molecular ordering behavior. ΔE of water on C60 is significantly smaller presumably due to its large HOMO-LUMO gap but for a graphene sheet the band gap vanishes and ΔE has an intermediate value between C60 and (10,10) nanotube. For methanol on graphene sheet ΔE increases to 60 meV due to more significant overlap of the molecular orbitals with those of the graphene sheet.

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