Abstract Submitted
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Ab Initio Study of Covalently Functionalized Graphene and Carbon Nanotubes[1] SANJIV JHA, MAHMOUD HAMMOURI, IGOR VASILIEV, New Mexico State Univ, IGOR MAGEDOV[2], LILIYA FROLOVA, NIKOLAI KALUGIN, New Mexico Tech — The electronic and structural properties of carbon nanomaterials can be affected by chemical functionalization. We apply *ab initio* computational methods based on density functional theory to study the properties of graphene and single-walled carbon nanotubes functionalized with benzyne. Our calculations are carried out using the SIESTA electronic structure code combined with the generalized gradient approximation for the exchange correlation functional. The calculated binding energies, densities of states, and band structures of functionalized graphene and carbon nanotubes are analyzed in comparison with the available experimental data. The surfaces of carbon nanotubes are found to be significantly more reactive toward benzyne molecules than the surface of graphene. The strength of interaction between benzyne and carbon nanotubes is affected by the curvature of the nanotube sidewall. The binding energies of benzyne molecules attached to both semiconducting zigzag and metallic armchair nanotubes increase with decreasing the nanotube diameter.

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