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First-principles study on the structural and electronic properties of graphene upon benzene and naphthalene adsorption

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ABSTRACT

Within the framework of the local density approximation (LDA) of the density functional theory (DFT) and the pseudopotential method, we have carried out *ab initio* calculations to investigate the structural and electronic properties of graphene upon the adsorption of benzene and naphthalene molecules. Our total-energy calculations suggest that, for both benzene and naphthalene adsorbed on graphene, the stack configuration is the most stable structure. The corresponding adsorption energies at different sites are estimated for both molecular adsorbates. The equilibrium parameters and the electronic band structure for the stable geometries have been calculated and compared with the available findings.