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Original Article

Adsorption of some Nitrophenols onto Graphene and Functionalized Graphene Sheets: Quantum Mechanics Calculations, Monte Carlo, and Molecular Dynamics Simulations

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ABSTRACT

Adsorption of some nitrophenols as significant environmental pollutants was investigated on pristine graphene and functionalized graphene sheets with O–H···F groups via quantum mechanical calculations, molecular dynamics, and Monte Carlo simulations. Energy data, structural parameters, electronic properties, electron charge densities, molecular electrostatic potential maps, charge transfer, density of states plots, non-covalent interactions, and adsorption isotherms were surveyed to get the possibilities of the selected adsorbents for the adsorption of nitrophenols. Molecular dynamics simulations disclosed that the hydrogen bonding and van der Waals interactions effectively assist to stability of the adsorbate-adsorbent pairs. Average binding energy of the pairs includes nitrophenols in closed and open form with adsorbents is 21.45 and 38.19 kcal mol^{-1}, respectively. Also, sum of electron charge density values at bond critical points that formed between nitrophenols in closed and open form with adsorbents is 42.03 and 43.54 au, respectively. The aromaticity of the central rings of the graphene and functionalized graphene is 0.0487 and 0.0482 au, respectively. Decrease of aromaticity at central rings of both adsorbates and adsorbents is followed by increase of binding energy values of the pairs. Energy decomposition analysis indicate that average electrostatic energy of the pairs include nitrophenols in closed and open form with adsorbents is -14.08 and -14.32 kcal mol^{-1}, respectively. Results suggested that the pristine graphene and functionalized graphene would be suitable adsorbents for adsorption of nitrophenols.

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