A DENSITY FUNCTIONAL STUDY OF THE ADSORPTION OF CARBON DIOXIDE MOLECULE ON GRAPHENE

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S u m m a r y

The physisorption of a CO_2 molecule on a graphene sheet using *ab initio* density functional theory is investigated. The geometrical structure of graphene, including various parameters viz. the bond lengths and bond angles are calculated for a graphene sheet under the adsorption of a CO_2 gas. Additionally, the density of states of a graphene sheet is calculated with & without adsorption of CO_2 molecules. It is observed that the CO_2 molecule is adsorbed on the graphene sheet with the adsorption energy of about 61.7 meV or less. The HOMO-LUMO energy levels of the graphene sheet before and after the adsorption of a CO_2 molecule remain unaltered. Therefore, the graphene sheet cannot detect a CO_2 molecule owing to their weak interaction.