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INSERTION OF ATOMS AND FULLERENES INTO LAYERS OF GRAPHENE STRUCTURES

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Abstract. In this paper, we use a continuum approach together with the Lennard-Jones potential to determine the potential energy for an atom and a C_{60} fullerene interacting with a single-layer graphene sheet. We also consider the interactions involving double-layer graphene structures. In order to explore the possibility of using double-layer graphene structures as a nano-carrier for targeted drug delivery, we investigate the molecular insertion of a carbon atom and a C_{60} molecule into the space between the graphene layers. We find that an atom and the outer surface of the fullerene prefer to be approximately 3.4 and 2.95 Å away from a single-layer graphene, which is consistent with the literature. Further, we find that the minimum distances between the two layers of the graphene structure for an atom and a C_{60} molecule to be accepted into the interspace are 6.2 and 12.2 Å, respectively. However, we find that when the distances between the layers equal to 6.8 and 13 Å for the atom and the C_{60} molecule, respectively, the total interaction energy is minimum and therefore the system is most stable. When the inter-layer distance is greater than 6.8 and 13 Å for the atom and the fullerene C_{60}, even though the atom and the fullerene C_{60} will be accepted into the inter-layer spacing, the system is not stable as the energy is higher. Knowledge of the size of the inter-layer spacing may be particularly useful for the design of the double-layer graphene structures for drug delivery applications.

Keywords. Graphene, Fullerene, van der Waals interaction, Lennard-Jones potential, Potential energy

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