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Drug release using nanoparticles in the cancer cells on 2-D materials in order to target drug delivery: A numerical simulation via molecular dynamics method

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Abstract

The application of nanotechnology promises to solve many common limitations in medicine. Drug release using nanoparticles in cancer cells can reduce many harmful effects caused by the transfer of drugs into the body. Release systems improve drug efficiency by controlling drug release parameters. In this regard, in this work, it has been tried to investigate functionalized graphene as a suitable nanocarrier for the drug doxorubicin by using the ability of molecular dynamics simulation to investigate intermolecular interactions. According to the results obtained from energy analysis, Gibbs free energy, hydrogen bond, radius of gyration and RDF, graphene, which was modified with the help of amine functional group, is known as the best two-dimensional nanocarrier for the transfer of doxorubicin to cancer cells. The simulations performed in this work can pave the way for laboratory studies of drug transfer using two-dimensional nanostructures.