

Investigating the adsorption of Dexamethasone on Silver (Ag) (111) Surface: A DFT-D Study.

Investigating the way in which therapeutic drugs interact with engineered nanoparticles (ENPs) is crucial for understanding the fate and behaviour of engineered nanoparticles in the human body. After the outbreak of COVID-19, drugs such as dexamethasone and hydroxychloroquine were suggested as viable candidates to combat the adverse effects of the disease. In this study, dispersion-corrected density functional theory (DFT-D) was employed to elucidate the interaction of dexamethasone with Ag (111) surface. To mimic a realistic biological environment, water as a solvent was used within the conductor-like screening model (COSMO) framework. The adsorption energy dexamethasone on the Ag (111) surface was -15.3481743 kcal/mol and the equilibrium distance between the surface, and hydroxychloroquine being 18 Angstrom. The drug exhibited a high adsorption potential on the Ag (111) surface, indicating stronger surface interaction with Ag. The results illustrated that the chosen drug interacts with the surface and is favourable on Ag (111) surface in terms of adsorption energy, solvation energy, isosurface of charge deformation difference, total and partial density of states, and thus its applicability as a drug carrier. Charge transfer, which was one of the calculated descriptors of electrophilicity (χ), agreed that this process would happen between the drug and Ag (111) surface.

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