Molecular Dynamics Simulations of Chlortetracycline Antibiotic Adsorption from Water using Iron Oxide Nanoparticle

In this study, iron oxide nanoparticle ($\text{Fe}_3\text{O}_4$ NP) is used to adsorb chlortetracycline (CTC) as a common pollutant antibiotic from aqueous media. The adsorption behavior of CTC on $\text{Fe}_3\text{O}_4$ nanoparticle is studied by applying molecular dynamics simulation. In order to describe the adsorption behavior, adsorption energy, radial distribution function (RDF) and hydrogen bond analyses are calculated. Results show that CTC interacts with NP from its hydroxyland amine functional groups by formation the hydrogen bonds. Due to this new hydrogen bond formation, the average number of hydrogen bonds between CTC and water molecules decreases. Also, calculated adsorption energy show an acceptable value which confirms the strong interactions between CTC and NP surface.

Keywords: Iron Oxide Nanoparticle; Chlortetracycline; Antibiotic; Molecular Dynamics Simulations; Adsorption

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