

عنوان مقاله:

SIMULATION OF TETRACYCLINE ONTO GRAPHENE NANO SHEET

محل انتشار:

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نویسندگان:

Gholamreza Soliemani - *Islamic Azad University Central Tehran Brach Physics Department Iran, Islamic Republic of*

Ehsan Ezzatpour Ghadim - *Research and Young Elite Club, Islamic Azad University, Central Tehran Branch, Tehran, Iran. Iran, Islamic Republic of*

Salimeh Kimiagar - *Islamic Azad University Central Tehran Brach Physics Department Iran, Islamic Republic of*

خلاصه مقاله:

Tetracycline (TC) is a broad spectrum of antibiotic which is used to cure infectious diseases and cancer. It can cause harmful side effects due to its high absorption in all organs. On the other hand graphene is appropriate to carry drug and release it to special target, organ or cell. It may decrease the side effects of the drug dramatically by using low dosage of medicine. Graphene oxide (GO) is able to adsorb the molecule of TC via π - π stacking. Base on this mechanism, simulation of TC molecule onto graphene nano sheets was adjusted. Study of force in the z direction illustrated that TC is closed to graphene via carbon (C λ) phenolic ring then it rotates and is again closed to the .graphene from amino group side. This case is adsorption equilibrium and total energy of the system is $-6.800eV$

کلمات کلیدی:

Tetracycline, simulation, Graphene oxide, Equilibrium Adsorption

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