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Investigation of the interaction of 5-fluorouracil anticancer drug connected to the pristine, titanium doped boron phosphide nanocage ($B_{12}P_{12}$) with adenine nucleobases: by density functional theory

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Abstract

The aims of this work, is to investigate the adsorption of 5-Fluorouracil drug connected to the pristine, Titanium doped boron phosphide nanocage ($B_{12}P_{12}$) with adenine nucleobases by using density functional theory (DFT). For this means at the first step, we considered different configurations for adsorbing (5-FU) on the surface of nanocluster and adenine, and then all considered models are optimized at the WB97XD/Lanl2DZ level of theory by Gaussian (09) software. From optimized structures, geometrical parameters involve bond length and bond angle, thermodynamic, atom in molecule (AIM), reduced density gradient (RDG), Uv-visible spectrum, HOMO-LUMO orbitals, density of states (DOS), and quantum parameters are calculated and all results are analyzed. The calculated results reveal that in the Ti doped $B_{12}P_{12}$ nano cage, the gap energy and global hardness of system decrease significantly, and so the conductivity and reactivity of system increase from original state. This property is favorable for making sensitive sensor for this drug. The adsorption energy and enthalpy values for all studied models are negative, which indicate that the absorption process and their thermodynamic stability are favorable. The RDG and AIM results confirm that the adsorption of 5-FU drug connected to the nanocage with adenine is non-covalent type. The computational results demonstrate that the pristine and Ti–doped $B_{12}P_{12}$ can be used as a suitable candidate for fabricating detector and absorber for 5-FU drug.

Keywords: 5-fluorouracil, boron phosphide nanocage, adenine, density function theory, titanium, quantum parameter.

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