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# Application of Zinc oxide nanostructures as a promising nanocarriers for 5-ALA in drug delivery system based on DFT-MD simulations

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We have examined the interactions between 5-aminolevulinic acid (ALA) drug and ZnO nanostructures using DFT method. In the context of the dispersion corrected PBE technic, the energetics, charge transfer, electronic structure and equilibrium geometries have been estimated. The ZnO nanostructures showed promising performance in the ALA drug functionalization, taking into account the interaction energy values. The band gap is almost remained unchanged for both of the substrates under consideration after ALA adsorption, and the semiconductor properties of the substrates are preserved, according to the analyzed DOSs spectra. The interaction nature of ALA-ZnO nanostructures according to the QTAIM analysis was found as polar attraction with partial covalent bonding between O and Zn. Our DFT based MD simulation results reveal that, in the aqueous solution, ALA moves toward the interior sidewall of ZnO nanostructures and binds to the Zn atom through its O and N atoms and the hydroxyl H atom was dissociated and bind to the O atom of ZnO surface.

***Keywords:*** Drug delivery; Zinc oxide nanostructure; Adsorption; DFT; Molecular dynamic simulation.

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