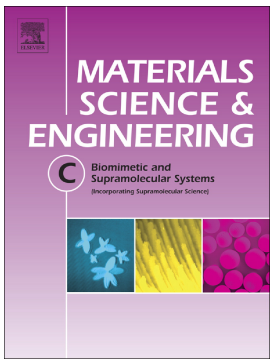

Serine adsorption through different functionalities on the B12N12 and Pt-B12N12 nanocages

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Serine adsorption through different functionalities on the $B_{12}N_{12}$ and Pt-$B_{12}N_{12}$ nanocages

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Abstract

The present work reports the adsorption of serine in the neutral and zwitterionic forms on the pure and Pt-decorated $B_{12}N_{12}$ fullerenes by means of density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations. The binding energy of serine over the fullerene has been studied through its hydroxyl (-OH), carboxyl (-COOH), and amine (-NH_2) functional groups. Based on our analysis, the binding energy of serine in zwitterionic form (**F:** -1.52 eV) on $B_{12}N_{12}$ fullerene is less stable than that of the neutral form (**C:** -1.61 eV) using the M06-2X functional. Our results indicated that the most stable chemisorption state for serine is through its amine group (**I:** -2.49 eV) interacting with the Pt-decorated $B_{12}N_{12}$ fullerene in comparison with the carbonyl group (**J:** -1.92 eV). The conductivity of the $B_{12}N_{12}$ and Pt-decorated $B_{12}N_{12}$ fullerenes is influenced by the energy band gap variation when serine is adsorbed upon the outer surface of fullerenes.