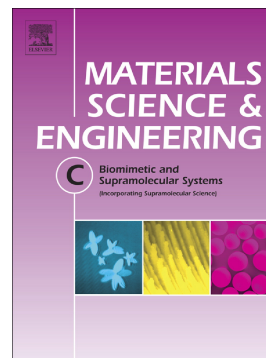


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Serine adsorption through different functionalities on the B₁₂N₁₂ and Pt-B₁₂N₁₂ nanocages

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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 B₁₂N₁₂ 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 (-NH₂) functional groups. Based on our analysis, the binding energy of serine in zwitterionic form (**F**: -1.52 eV) on B₁₂N₁₂ 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 B₁₂N₁₂ fullerene in comparison with the carbonyl group (**J**: -1.92 eV). The conductivity of the B₁₂N₁₂ and Pt-decorated B₁₂N₁₂ fullerenes is influenced by the energy band gap variation when serine is adsorbed upon the outer surface of fullerenes.

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