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Original Research Article

TATB Interaction with Carbon Nanocone and Nanocone Sheet: A Comprehensive Computational Study

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ABSTRACT

In this study 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) interaction with carbon nanocone(NC) and nanocone Sheet (NCS) was evaluated by density functional theory. The calculated thermodynamic parameters including Gibbs free energy changes and Enthalpy alterations showed the interaction of TATB with the both nanostructures are exothermic, spontaneous, experimentally possible and irreversible. The specific heat capacity values proved the heat sensitivity of TATB decline after its adsorption on the surface of carbon nanocone and nanocone sheet. The effect of temperature on this process was also investigated and the results indicated 300 K is the optimum temperature for the interaction of TATB with the nanostructures. The frontier molecular orbital analysis was also employed and the findings indicated the reactivity and energetic traits of TATB have enhanced significantly after its interaction with carbon nanocone and nanocone sheet. Indeed, both of the nanostructures cause a substantial improvement in energetic features and a tangible decrease in the heat sensitivity.

Keywords: TATB, Carbon nanocone, Nanocone Sheet, DFT, Explosives

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