عنوان مقاله:

Adsorption of Tetryl on the Surface of B12N12: A Comprehensive DFT Study

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خلاصه مقاله:

In this study, the adsorption of tetryl on the surface of boron nitride cage was evaluated by density functional theory. For this purpose, the structures of tetryl, B12N12, and the tetryl-B12N12 complexes were geometrically optimized. Then, IR and frontier molecular orbital calculations were performed on them. The calculated adsorption energies, Gibbs free energy changes (ΔGad), adsorption enthalpy changes (ΔHad) and thermodynamic equilibrium constants (Kth) revealed that the adsorption process of both explosives is experimentally feasible, spontaneous, exothermic and non-equilibrium. The specific heat capacity values (CV) showed that the heat sensitivity has been significantly reduced in the tetryl complexes with B12N12. The N-O and C-N bond lengths and the density values demonstrated that tetryl-derived products with boron nitride cage have higher explosive velocity and blasting pressure in comparison to the pure blasting materials without B12N12. The frontier molecular orbital parameters such as band gap, chemical hardness, electrophilicity, chemical potential and charge capacity were also studied and the results proved that boron nitride cage is an ideal electroactive sensing material in order to fabricate novel sensors for the determination of tetryl.

کلمات کلیدی:

Boron nitride cage, Density functional theory, Adsorption, Tetryl, Detection