Research Article

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The Be atom doping: An effective way to improve the Li-atom adsorption in boron rich nanoflake of B_{24}

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ABSTRACT

Based on the density functional techniques, we have carried out the doping Be atom to the B_{24} molecule, nBe@B_{24} (n = 1 and 2), which follows through addition of the Li atom to the most stable nBe@B_{24} (n = 1 and 2) molecules. The calculated results show that the doping Be atom causes to the severe deformation of the B_{24} molecule along with big values of vertical ionization energy for the nBe@B_{24} (n = 1 and 2) molecules. Moreover, the range -2.65 eV ~ -4.49 eV for the adsorption energy per Be atom confirms unique thermodynamic stability of the nBe@B_{24} (n = 1 and 2) molecules. Note that the dominant thermodynamic and chemical stability among all the nBe@B_{24} (n = 1 and 2) molecules belongs to the cage configuration of the B_{24} molecule. The positive charges of the Be atoms, 0.60 e ~ 0.97 e, the lack of the Be-Be interaction and high chemical flexibility of the B atoms have been observed in the nBe@B_{24} (n = 1 and 2) molecules based on the natural bond orbital (NBO) and the atoms in molecules (AIM) analysis. The value of first hyperpolarizability, β_{total}, in the nBe@B_{24} (n = 1 and 2) molecules depends severely on both the number of the Be atoms and the backbone configuration. Moreover, addition of Li atom presents the existence of the Be atom(s) increases the adsorption energy of the Li atom in the B_{24} molecule.

1. Introduction

The boron atom (B) has high chemical flexibility compared with another atoms. This means that the B atoms can be used as electron donor or electron acceptor. In atomic doping the boron rich materials, the role of the B atoms (electron donor or electron acceptor) depends on the kind of dopant. Indeed, this exclusive feature has motived researchers to carry out many theoretical and experimental studies on the boron rich materials [1-13].

The calculated results on the B_n (n=3-19) materials [14-22] reflect that the two-dimensional configurations of the boron rich materials are superior geometries compared with those of three-dimensional based on energy. Additionally, the three-dimensional configuration of the B_{20} molecule, known as double-ring molecule, is more stable than the configurations of its two-dimensional [23, 24]. On the other words, the B_{20} molecule can be introduced as transition state from two-dimensional configurations to ones of three-dimensional in the B_n materials [23, 24]. Boustani et al. [25] searched the possible configurations of the B_{24} molecule. According to the obtained results, the most possible configurations can be incorporated in four different categories of the ring, tube, convex (and quasiplanar) and cage. The ring category includes two different configurations of the monocyclic-ring and the double-ring. Note that double-ring B_{24} molecule is much more stable than the monocyclic-ring of the B_{24} molecule. In the tube category, Boustani et al. [25] reported three tubes with the different number of the B atoms in each ring of tube. The results present that the tube geometry with the three planar rings containing eight B atoms in each ring is dominant configuration for the tube category. In the cage category, Boustani et al. introduced the cage-II which contains the fusion of two icosahedra B_{12} molecules as the most stable

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