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Insight into $Y@X_2B_8$ (Y= Li, CO_2 and Li-CO_2, X = Be, B and C) nanostructures: A computational study

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ABSTRACT

The doping of the Li atom and CO_2 molecule to the X_2B_8 (X = Be, B and C) backbones have been carried out on the potential energy surface to provide clear vision on the structural and electronic features of the $Y@X_2B_8$ (Y = Li, CO_2 and Li&CO_2, X = Be, B and C) systems. Our results show that the adsorption energies of the Li atom in the $Li@X_2B_8$ systems (-1.52 eV ~ -3.05 eV) are much bigger than those of the CO_2 molecule in the $CO_2@X_2B_8$ systems (-0.10 eV ~ -0.89 eV). Moreover, the B_2B_8 and the Be_2B_8 can be selected as prefer backbones for the adsorption of Li atom and the CO_2 molecule, respectively. Finally, bigger adsorption energy of the $Li\&CO_2@Be_2B_8$ system (-1.06 eV) compared with that of the $CO_2@Be_2B_8$ system (-0.89 eV) presents that the Li atom doping in the Be_2B_8 backbone increases adsorption energy of the CO_2 molecule. Similar result has been not found for the B_2B_8 and the C_2B_8 backbones.

1. Introduction

Boron is one of the very interesting elements in the periodic Table. Pure boron molecules are intermediate compounds between the materials with purely nonmetallic and metallic characteristics. This feature results into high chemical flexibility of boron rich molecules and it motives many researchers to search the ground-state geometries of boron rich molecules and reveal their unique characteristics [1-8].

The organized investigation has been carried out by Boustani [9] on possible structural geometries of the B_n (n = 2−14) molecules. The results show that the B_{10} molecule can have three different configurations of the convex B_{10} (C_{2v}), the quasiplanar B_{10} (C_{2h}) and the nonplanar B_{10} (C_s) on the singlet potential energy surface (PES). Moreover, the quasiplanar B_{10} (C_{2h}) molecule contains two different fragments in its structural geometry and is more stable than two other configurations. The quasiplanar B_{10} (C_{2h}) molecule has the planar ring with eight B-atoms along with two central B atoms which locate up and under planar ring. Note that the central B atoms of the B_{10} (C_{2h}) molecule have strong chemical bonds with those of planar ring. [9] It is necessary to say that the replacement of two central B atoms of the quasiplanar B_{10} (C_{2h}) molecule with either two more electropositive atoms of the Be, denoted as the nonplanar Be_2B_8 (D_{8h}) molecule, or two more electronegative atoms of the C, denoted as the planar C_2B_8 (D_{2h}) molecule, has been carried out by Frenking et al. [10-11] The C_2B_8 (D_{2h}) molecule has been found to be the planar molecule [10]. This means that the replacement of two central B atoms of the quasiplanar B_{10} (C_{2h}) molecule with those of C atoms causes to incorporation of the central C_2 unit in the sheet of the planar C_2B_8 (D_{2h}) molecule. In the planar C_2B_8 (D_{2h}) molecule, the strong chemical bonds can be observed between the central C_2 unit and the peripheral B atoms [10]. Different from the planar C_2B_8 (D_{2h}) molecule, the replacement of the central B_2 unit of the quasiplanar B_{10} (C_{2h}) molecule with two Be atoms causes to form the nonplanar Be_2B_8 (D_{8h}) molecule [11] which contains the symmetric ring through eight B atoms in which two Be atoms are vertical to the B atoms ring. The stability factor of the nonplanar Be_2B_8 (D_{8h}) molecule is the strong chemical bonds between Be and B atoms. These B−Be bonds act such as the wheel spokes and cause to unusual short Be−Be distance. In spite of very short Be−Be distance, no bond critical point (BCP) has been

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