Hydrogen hosting on aluminum-doped boron clusters: Density functional theory

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Hydrogen hosting on aluminum-doped boron clusters: density functional theory

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Synopsis The geometries, stabilities, and energetics of aluminum doped boron clusters, up to 13-atom, and their various hydrogenated complexes have been investigated via the density functional theory (DFT). The geometry optimizations have been carried out by using B3LYP functional and 6-311++G** basis set. Up to 5-atom clusters arrangements of the atoms, in the most stable structures, have two-dimensional forms. From 6- to 13-atom clusters three-dimensional forms are favored by the lowest energy structures. Hydrogen hosting effects the structures of AlB_n clusters. Adding an Al atom to the cage B_{12} leads structural changes but hydrogenated boron, $B_{12}H_{12}$ can resist to Al effect.

There have been increasing interests to study boron clusters [1] and any boron containing metal complexes [2] due to the possibility for new nano-structured material constructions. The hydrides of boron and metal-boron are also important to investigate their suitability for hydrogen storages [3,4].

In this work the results of the structural and energetic stabilities for AlB_n clusters, up to n=12, and their various hydrides are presented. DFT/B3LYP/6-311++G** theory was used in Gaussian 03 program package [5] for all optimizations. Structural arrangements of the atoms in the most stable structures found here are in two-dimensional up to 5-atom clusters and three-dimensional forms from 6- to 13-atom clusters for the lowest multiplicities (singlet and doublet).

Hydrogen adding to the studied AlB_n clusters changes their stable structures. Mainly, hydrogen atoms prefer to stay closer to boron atoms in the complexes. Moreover, some of the selected Al-doped cage boron clusters are investigated here. For instance, adding an Al atom changes the structural morphology of the cage B_{12} but hydrogenated boron, $B_{12}H_{12}$ can resist to the effect of the doped Al (Fig. 1).

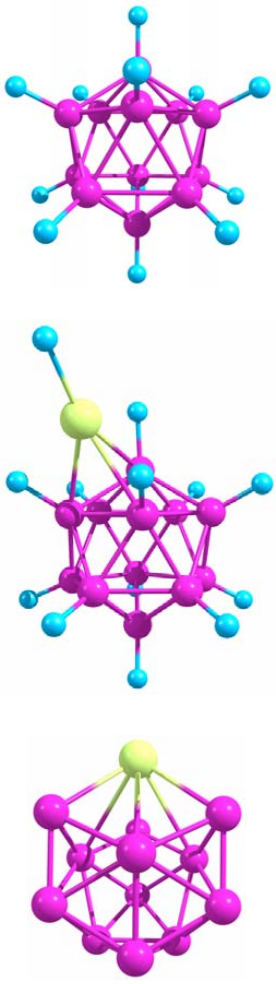

Fig. 1. Al-doped structures of $B_{12}H_{12}$, $AlB_{12}H_{13}$, AlB_{12}

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