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DFT study on the structure and stability of $Al_{13}B_n^{\pm m}$ clusters

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Abstract: $Al_{13}B_n^{\pm m}$ clusters were studied by the DFT-UB3LYP/6-311+G(d) method. The variations of structural and electronic properties with the changes of n and m were probed. For the $Al_{13}B_n^{\pm m}$ clusters, the geometry of their stable structures have a high symmetry when $n \leq 2$, such as $Al_{13}B$ (C_{2v}), $Al_{13}B^+$ (C_{2v}) and $Al_{13}B_2^+$ (D_{4h}). The differences of the Al–B bond lengths between the most stable $Al_{13}B_n^{\pm m}$ clusters are within 0.066 Å, and the energy differences between the isomers (ΔE) are within 1.000 eV for most clusters. The stability sequence of the clusters could be influenced by charges. Most of the lowest-energy structures of $Al_{13}B_n^{\pm m}$ clusters contain the B_2 moiety when $n \geq 3$. Overall, the average binding energy of neutral clusters is larger than that of the corresponding anionic clusters, but smaller than that of the cationic clusters. The neutral clusters possess higher stability when $n = 3$ and 5, while $Al_{13}B_3^+$ and $Al_{13}B_5^+$ clusters are less stable than their neighbors are. Both the fragmentation energy and second order energy difference indicate that some clusters are more stable than their corresponding differently charged species of the same size.

Keywords: symmetry; charges; isomers; electronic properties; lowest-energy; bond lengths.

INTRODUCTION

During the last decades, based on single element clusters, more and more researchers have conducted studies on doped clusters. Clusters of spatial scales in the range of a few angstroms to several hundred angstroms could be considered as the material structure of intermediate level among atoms, molecules and macroscopic solids. They represent the initial state of condensed matter. The study of doped clusters helps in the understanding of solid growth from microscopic particles to blocks, and consummates the cohesion atomic theory. Due to their

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tiny size, clusters not only have unique physical and chemical properties in the terms of geometry and electronic properties,[1–5] but also have potential applications in catalysis,[6,7] hydrogen storage,[8,9] *etc.*

The Al_{13}^{-} cluster has a high electron affinity (3.62 eV) that is very close to the electron affinity of chlorine (3.70 eV), thus the Al_{13}^{-} cluster could be considered as a "super halogen".[10,11] Moreover, the Al_{13}^{-} cluster corresponds to a closed shell magic number.[12] The study of boron clusters can be traced back to 1997 when Boustani[13] used the first-principles method to calculate the geometry and electrical properties of small-sized boron clusters B_n (n = 2–14). The study indicated that most steady-state structures of boron clusters are mainly composed of hexagonal and pentagonal cones when $n > 9$. For the stability of boron clusters, Aihara and Ishida[14] found that there are two kinds of aromatic boron clusters, one is δ-aromatic while the other is π-aromatic. Other than pure boron clusters, researchers also gave attention to X-doped (X = metal) boron clusters.[15–19] For example, simulated photoelectron spectra of $Al_nB_m^{-}$ ($n+m$ = 13) clusters have been reported,[16] and the structure and electronic properties were investigated by the density functional theory. Feng and Luo[20] studied the structure and stability of AlB_n (n = 1–12) clusters by the density functional theory. They found that the stable structures of aluminum-doped B clusters could be obtained by directly doping aluminum on boron clusters. Subsequently, Böyükata and Güvenç[21] presented the electronic and structural stability of AlB_n (n = 1–14) clusters and their various isomers using the density functional theory, and they showed that the AlB_9, AlB_{11} and AlB_{13} clusters have large chemical hardness. Meanwhile, Romanescu *et al.*[22] performed a joint experimental and theoretical study on the structures and chemical bonding of AlB_6^{-} and AlB_{11}^{-} clusters. They found that the structures and photoelectron spectra of the Al-doped clusters are similar to those of pure boron clusters. Additionally, Al–B master alloys are widely used in the production of electrical conductive grade aluminum to remove transition metal impurities.[23,24] Although there has been much research on Al-doped boron clusters, only a few studies were concerned with neutral or positively/negatively charged B-doped Al_{13} clusters. What are the differences among the $Al_{13}B_n^{\pm m}$ clusters? Can an "odd–even alteration" phenomenon be found for some properties like with X-doped (X = metal) boron clusters? To explore these questions, the geometric structures, stabilities and electronic properties of neutral and charged $Al_{13}B_n$ clusters were investigated in this study.

COMPUTATIONAL METHODS

To construct different types of initial structures, boron atoms were doped on the external positions of Al_{13} clusters. A systematic search was made for the global minimum energy for clusters of n = 1–4, whereas, the local minimum energy were considered for clusters of n = 5–6. The spin multiplicities were considered for the initial configurations of $Al_{13}B_n^{\pm m}$ clusters (n =

= 1–6 and $m = 0, 1$). To investigate the relative stability of different sized $Al_{13}B_n$ clusters, the average binding energy, fragmentation energy and the second-order difference in total energies were calculated. The average binding energy for $Al_{13}B_n$ clusters can be defined by the following formula:

$$E_b(n)^{\pm m} = \frac{\left[nE(\mathrm{B}) + E(\mathrm{Al}_{13})^{\pm m} - E(\mathrm{Al}_{13}\mathrm{B}_n)^{\pm m}\right]}{n+1} \tag{1}$$

where, $E(\mathrm{B})$, $E(\mathrm{Al}_{13})^{\pm m}$ and $E(\mathrm{Al}_{13}\mathrm{B}_n)^{\pm m}$ represent the energies of the most stable B, $Al_{13}^{\pm m}$ and $Al_{13}B_n^{\pm m}$ clusters, respectively.

The fragmentation energy can be defined by the following formula:

$$E_f(n)^{\pm m} = E(\mathrm{B}) + E(\mathrm{Al}_{13}B_{n-1})^{\pm m} - E(\mathrm{Al}_{13}\mathrm{B}_n)^{\pm m} \tag{2}$$

where $E(\mathrm{Al}_{13}\mathrm{B}_{n\text{-}1})^{\pm m}$ represents the energy of the most stable $Al_{13}B_{n\text{-}1}^{\pm m}$ cluster.

There is a sensitive quantity that can reflect the relative stability of clusters.[25] This parameter is the second-order difference of the total energies and it can be defined by the following formula:

$$\Delta_2E(n)^{\pm m} = E(\mathrm{Al}_{13}\mathrm{B}_{n+1}) + E(\mathrm{Al}_{13}B_{n-1})^{\pm m} - E(\mathrm{Al}_{13}\mathrm{B}_n)^{\pm m} \tag{3}$$

where $E(\mathrm{Al}_{13}\mathrm{B}_{n+1})^{\pm m}$ represents the energy of the most stable $Al_{13}B_{n+1}^{\pm m}$ clusters.

To investigate further the electronic properties, the HOMO–LUMO (highest occupied molecular orbital–lowest unoccupied molecular orbital) gaps energies and the chemical hardness for the most stable $Al_{13}B_n$ clusters were considered. Chemical hardness is defined as the resistance of the chemical potential to a change in the number of electrons[26,27] and is given by:

$$\eta = \frac{I - A}{2} \tag{4}$$

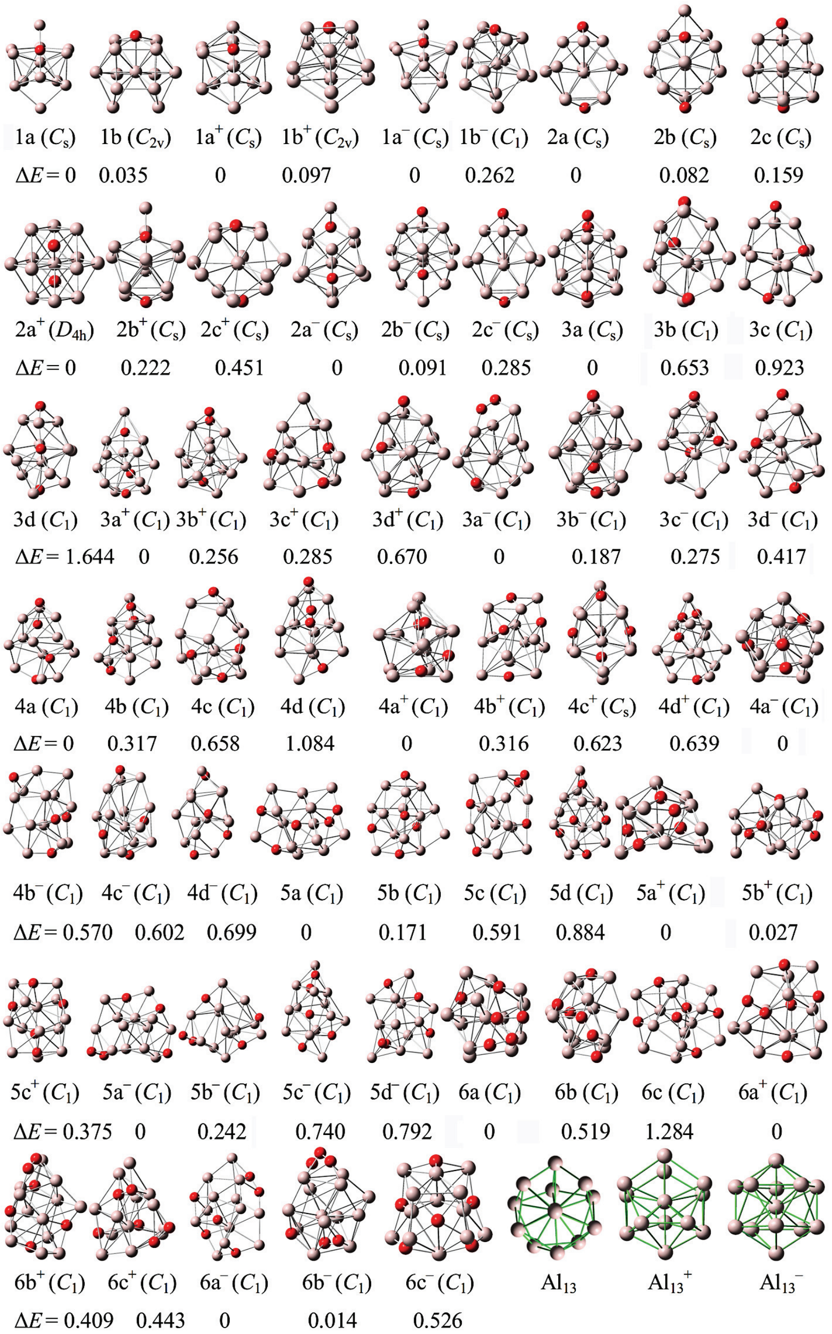
where I and A are the ionization potential and electron affinity, respectively.

Additionally, the size dependence of the average atomic charges for Al in clusters were analyzed by natural bond orbital (NBO) analysis.[28,29] Especially, in order to study the structural stability of the clusters, the deformation energy of the Al_{13} clusters were calculated. All the initial geometrical structures were fully optimized at the B3LYP/ 6-311+G(d) level, which was considered to be suitable for the families of Al–B clusters.[20,22] The optimized structures were characterized to be true local energy minima on the potential energy surfaces without imaginary frequencies. All the computations were performed through the Gaussian 09 package.[30]

RESULTS AND DISCUSSION

Stable geometric structures

The most stable and metastable structures of $Al_{13}B_n^{\pm m}$ and the most stable structures of $Al_{13}^{\pm m}$ ($n = 1$–6 and $m = 0, 1$) clusters are presented in Fig. 1. The symmetry and relative energy is denoted for each configuration. As can be seen in Fig. 1, the symmetry of the $Al_{13}B_n$ clusters gradually lowers when $n \geq 3$. This phenomenon could be explained by observing the deformation energy for Al_{13} clusters in Fig. 2, *i.e.*, the deformation energy of the Al_{13} moiety increases as the size n increases from 3.



1a (C_s) 1b (C_{2v}) 1a$^+$ (C_s) 1b$^+$ (C_{2v}) 1a$^-$ (C_s) 1b$^-$ (C_1) 2a (C_s) 2b (C_s) 2c (C_s)

$\Delta E = 0$ 0.035 0 0.097 0 0.262 0 0.082 0.159

2a$^+$ (D_{4h}) 2b$^+$ (C_s) 2c$^+$ (C_s) 2a$^-$ (C_s) 2b$^-$ (C_s) 2c$^-$ (C_s) 3a (C_s) 3b (C_1) 3c (C_1)

$\Delta E = 0$ 0.222 0.451 0 0.091 0.285 0 0.653 0.923

3d (C_1) 3a$^+$ (C_1) 3b$^+$ (C_1) 3c$^+$ (C_1) 3d$^+$ (C_1) 3a$^-$ (C_1) 3b$^-$ (C_1) 3c$^-$ (C_1) 3d$^-$ (C_1)

$\Delta E = 1.644$ 0 0.256 0.285 0.670 0 0.187 0.275 0.417

4a (C_1) 4b (C_1) 4c (C_1) 4d (C_1) 4a$^+$ (C_1) 4b$^+$ (C_1) 4c$^+$ (C_s) 4d$^+$ (C_1) 4a$^-$ (C_1)

$\Delta E = 0$ 0.317 0.658 1.084 0 0.316 0.623 0.639 0

4b$^-$ (C_1) 4c$^-$ (C_1) 4d$^-$ (C_1) 5a (C_1) 5b (C_1) 5c (C_1) 5d (C_1) 5a$^+$ (C_1) 5b$^+$ (C_1)

$\Delta E = 0.570$ 0.602 0.699 0 0.171 0.591 0.884 0 0.027

5c$^+$ (C_1) 5a$^-$ (C_1) 5b$^-$ (C_1) 5c$^-$ (C_1) 5d$^-$ (C_1) 6a (C_1) 6b (C_1) 6c (C_1) 6a$^+$ (C_1)

$\Delta E = 0.375$ 0 0.242 0.740 0.792 0 0.519 1.284 0

6b$^+$ (C_1) 6c$^+$ (C_1) 6a$^-$ (C_1) 6b$^-$ (C_1) 6c$^-$ (C_1) Al_{13} Al_{13}^+ Al_{13}^-

$\Delta E = 0.409$ 0.443 0 0.014 0.526

Fig 1. Low-lying structures of $Al_{13}B_n^{\pm m}$ and $Al_{13}^{\pm m}$ (n = 1–6 and m = 0, 1; aluminum atoms in brown and boron atoms in red. The digit in **1a**$^+$ denotes the number of boron and superscript in **1a**$^+$ denotes a positive charge, others are similar, ΔE / eV).

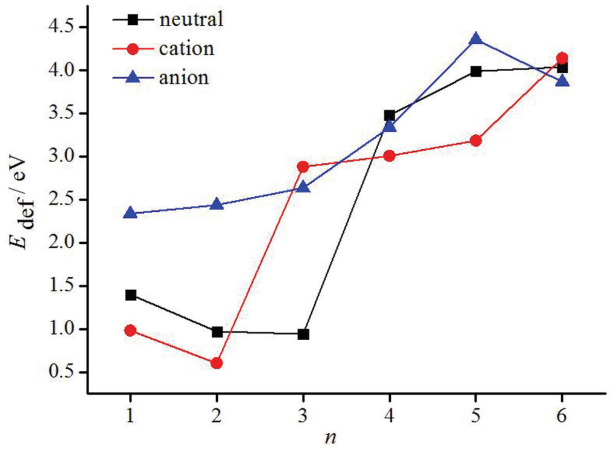


Fig 2. Cluster size (n) dependence of the deformation energy (E_{def}) of Al_{13} in $Al_{13}B_n^{\pm m}$ clusters.

As shown in Fig. 1, most of the lowest-energy conformations contain the B_2 moiety when $n \geq 3$. The $Al_{13}B_3^-$ (**3a**$^-$) cluster, for example, is a representative with a B_2 moiety in the lowest-energy structures. There is an external B_2 moiety in the $Al_{13}B_3^-$ cluster. This phenomenon may be because Al_{13}^- is a remarkably stable closed-shell cluster that has been referred to as a "superhalogen",[10,11] and after doping three B atoms in the Al_{13}^- cluster, the system continues to maintain the original stable configuration of the Al_{13}^- cluster, one of the B atoms fills in the Al_{13}^- cluster and the other two B atoms exist as a B_2 unit. To prove that the B_2 unit really exists, the shortest B–B bond lengths ($R_{B–B,min}$) and the average B–B bond lengths ($R_{B–B,ave}$) of the $Al_{13}B_n^{\pm m}$ clusters for the most stable structures in Table I were further investigated. Most clusters with $n \geq 3$ have a B_2 moiety with the shortest B–B bond length of 1.514 to 1.612 Å.

TABLE I. The shortest B–B bond lengths ($R_{B\text{-}B,\ min}$) and the average B–B bond lengths ($R_{B\text{-}B,\ ave}$) of the $Al_{13}B_n^{\pm m}$ (n = 1–6 and m = 0, 1) clusters for the lowest-energy structures[a].

System	Neutral		Cation		Anion	
	$R_{B\text{-}B,\ min}$	$R_{B\text{-}B,\ ave}$	$R_{B\text{-}B,\ min}$	$R_{B\text{-}B,\ ave}$	$R_{B\text{-}B,\ min}$	$R_{B\text{-}B,\ ave}$
$Al_{13}B$	–	–	–	–	–	–
$Al_{13}B_2$	–	–	–	–	–	–
$Al_{13}B_3$	1.514	1.514	–	–	1.519	1.519
$Al_{13}B_4$	–	–	–	–	1.525	1.525
$Al_{13}B_5$	1.612	1.612	1.593	1.593	1.528	1.528
$Al_{13}B_6$	1.559	1.650	1.682	1.682	1.540	1.540

[a]Bond lengths in Å

Additionally, the structures with different charges would also be changed in different ways. This indicates that the spatial configurations of the clusters are influenced by the electronic arrangement.[31,32]

The energy difference between the lowest-energy and low-lying structures (ΔE) and the Al–B bond length ($R_{\text{Al–B}}$) of $\text{Al}_{13}\text{B}_n^{\pm m}$ (n = 1–6 and m = 0, 1) clusters are listed in Table II.

TABLE II. Energy difference between lowest-energy and low-lying structure (ΔE) and bond length range ($R_{\text{Al-B}}$) of $\text{Al}_{13}\text{B}_n^{\pm m}$ (n = 1–6 and m = 0, 1) clusters.

Tested config.	Neutral		Cation		Anion	
	ΔE / eV	$R_{\text{Al-B}}$ / Å	ΔE / eV	$R_{\text{Al-B}}$ / Å	ΔE / eV	$R_{\text{Al-B}}$ / Å
1a	0.000	2.129–2.270	0.000	2.127–2.207	0.000	2.135–2.219
1b	0.035	2.103–2.548	0.097	2.114–2.355	0.262	2.105–2.402
2a	0.000	2.060–2.144	0.000	2.126–2.260	0.000	2.052–2.397
2b	0.082	2.060–2.273	0.222	2.102–2.269	0.091	2.095–2.267
2c	0.159	2.056–2.144	0.451	2.053–2.392	0.285	2.048–2.158
3a	0.000	2.053–2.441	0.000	2.025–2.381	0.000	2.034–2.304
3b	0.653	2.054–2.467	0.256	2.019–2.251	0.187	2.006–2.281
3c	0.923	1.993–2.442	0.285	2.043–2.336	0.275	2.038–2.362
3d	1.644	1.993–2.441	0.670	2.010–2.318	0.417	2.033–2.366
4a	0.000	2.031– 2.481	0.000	2.036–2.279	0.000	2.050–2.268
4b	0.317	2.062–2.306	0.316	2.066–2.313	0.570	2.009–2.350
4c	0.658	1.971–2.287	0.623	2.019–2.298	0.602	1.988–2.330
4d	1.084	2.008–2.385	0.639	2.041–2.489	0.699	2.024–2.229
5a	0.000	2.014–2.246	0.000	2.017–2.359	0.000	2.032–2.419
5b	0.171	2.012–2.246	0.027	2.077–2.479	0.242	1.999–2.419
5c	0.591	2.006–2.442	0.375	2.049–2.514	0.740	2.045–2.374
5d	0.884	2.015–2.329	0.423	2.040–2.247	0.792	2.003–2.373
6a	0.000	2.065–2.363	0.000	2.000–2.335	0.000	2.037–2.301
6b	0.519	2.033–2.383	0.409	2.024–2.386	0.014	1.992–2.493
6c	1.284	2.016–2.395	0.443	2.028–2.690	0.526	2.051–2.207

Overall, the shortest Al–B bond length is 1.971 Å, and the longest Al–B bond length is around 2.690 Å for $\text{Al}_{13}\text{B}_n^{\pm m}$ clusters. The minimum Al–B bond lengths of the most stable neutral and cationic clusters decreased as the size n increased. with the exception of $\text{Al}_{13}\text{B}_4^+$ (**4a**$^+$) and Al_{13}B_6 (**6a**) clusters, respectively. The differences in the Al–B bond lengths between the most stable neutral and charged clusters are in the range of 0.000 Å to 0.066 Å, indicating that the charge has a weak influence on bond lengths in these clusters. As seen from Table II, most energy differences between the isomers (ΔE) are within 1.000 eV for most clusters, and the maximum ΔE value of Al_{13}B_3 (**3d**) is 1.644 eV.

Relative stability

The relative stability of the differently sized Al_{13}B_n clusters can be evaluated by the average binding energy, fragmentation energy and second-order difference of the total energies. All the graphs of the above-calculated energies *versus* size *n* are plotted in Figs. 3–5, respectively. As can be seen from Fig. 3, when the neutral clusters obtain or loose one electron, their average binding energies change. Overall, the neutral clusters are more stable than the anionic clusters, but less stable than the cationic clusters as judged by the average binding energies. The average binding energy generally increases with increasing cluster size. Thus, the $Al_{13}B_n^{\pm m}$ clusters can continue to gain energy during the growth process, but the increment becomes smaller and smaller as *n* increases.

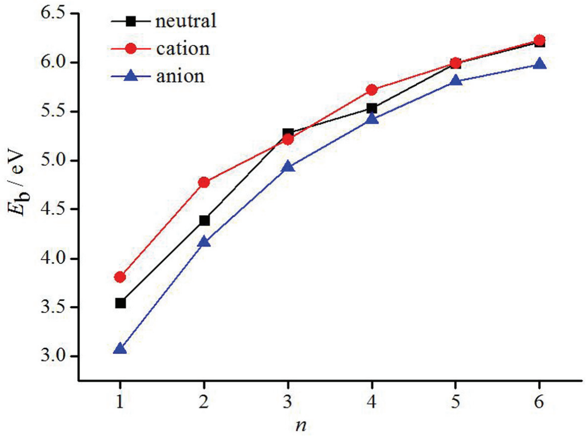


Fig 3. The dependence of the average binding energy (E_b) on the clusters size (*n*) for $Al_{13}B_n^{\pm m}$ clusters.

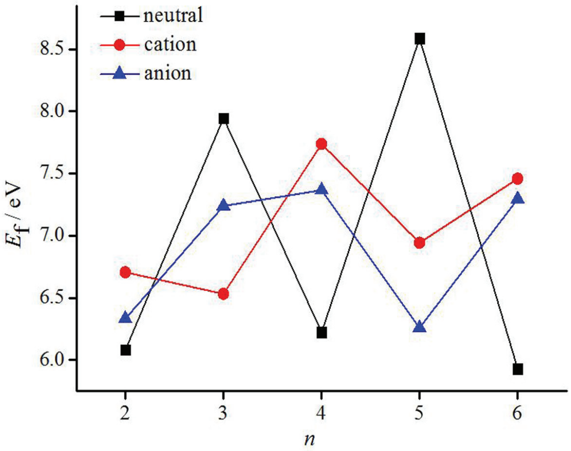


Fig 4. Dependence of the fragmentation energy (E_f) on the cluster size (*n*) for $Al_{13}B_n^{\pm m}$ clusters.

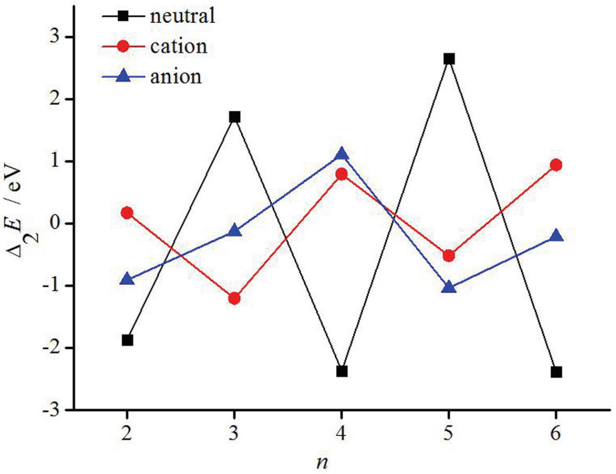


Fig 5. The dependence of the second-order difference energy (Δ_2E) on cluster size (n) for $Al_{13}B_n^{\pm m}$ clusters.

It could be seen from Fig. 4 that the local maximum fragmentation energies appear at $n = 3$ and 5 for neutral clusters, but the lowest fragmentation energies appear at the same sizes for cationic clusters. This indicates that $Al_{13}B_3$ and $Al_{13}B_5$ clusters are more stable than their neighbors are. However, $Al_{13}B_3^+$ and $Al_{13}B_5^+$ are less stable than their neighbors, which could also be seen from Fig. 3. For the anionic clusters, their local-minimum fragmentation energies appear at the sizes 2 and 5.

To demonstrate further the relative stabilities of $Al_{13}B_n$ clusters, the second-order difference of total energies were calculated. As can be seen from Fig. 5, the maxima are found at $n = 3$ and 5 for neutral clusters, but the local minimum of the cationic $Al_{13}B_n$ clusters are found at the same sizes. It is noteworthy that variations of the second-order difference of total energies with n values for the cationic and anionic clusters are similar. As shown in Figs. 4 and 5, the $Al_{13}B_2^+$, $Al_{13}B_3$, $Al_{13}B_5$ and $Al_{13}B_6^+$ clusters are more stable than their corresponding differently charged species of the same size.

Electronic property

The HOMO–LUMO gaps of $Al_{13}B_n^{\pm m}$ ($n = 1–6$ and $m = 0, 1$) clusters are presented in Fig. 6, from which it could be seen that the gap energies for all $Al_{13}B_n^{\pm m}$ clusters have a remarkable "odd–even alteration" as the size n increases. It was observed that the peaks in the gaps for the neutral clusters appear when n were odd, whereas, for the cationic and anionic clusters, these peaks appeared at even n values. The peaks mean that these clusters possess electronic stability, *i.e.*, these sized clusters are chemically more inert than their neighbors are. In general, the gaps of the anionic $Al_{13}B_n$ clusters are usually smaller than those of the cationic ones, indicating that the anionic $Al_{13}B_n$ clusters are more active in the process of electron excitation than are the cationic $Al_{13}B_n$ clusters.

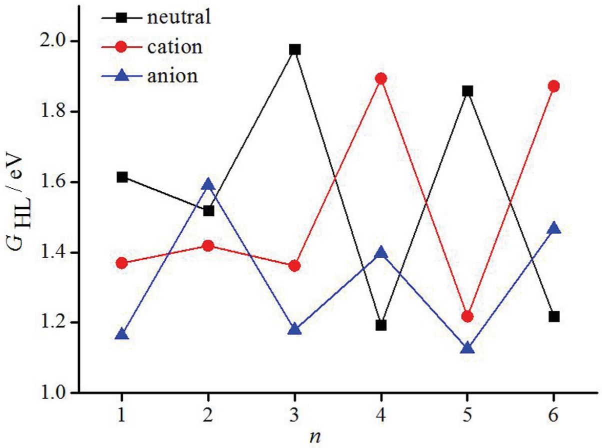


Fig. 6. Dependence of the HOMO–LUMO gap energy (G_{HL}) on cluster size (n) for $Al_{13}B_n^{\pm m}$ clusters.

In this study, the chemical hardness (η) was calculated for neutral $Al_{13}B_n$ clusters and the results are displayed in Fig. 7. The maximum hardness principle can be understood from Eq. (4). A larger η means a larger ionization potential and a smaller electron affinity, which implies that the system has a lower tendency to accept particles (electrons) and/or a lower tendency to give away particles, *i.e.*, the system is more stable.[33] Accordingly, the $Al_{13}B_3$ and $Al_{13}B_5$ clusters are more stable than their neighbors in Fig. 7 are. Moreover, this result is consistent with the results from Figs 4–6.

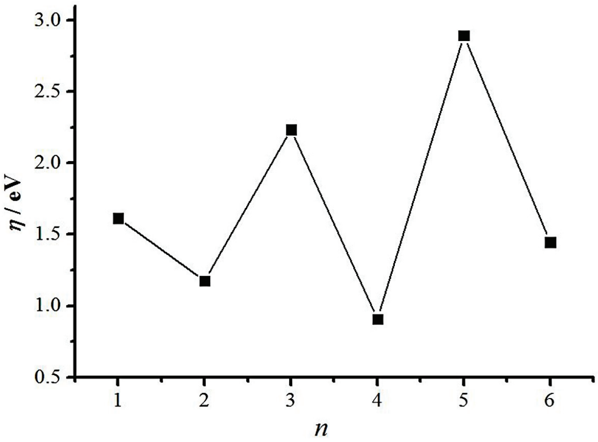


Fig. 7. Dependence of the chemical hardness (η) on cluster size (n) for neutral $Al_{13}B_n$ clusters.

The NBO method provides an effective electronic configuration for each atom in a cluster owing to the localized orbital constructed from the occupancy-weighted symmetric orthogonalized natural atomic orbital.[31] The average atomic charges of the Al atom *versus* the size *n* of the clusters are plotted in Fig. 8. Overall, the charge increases with increasing number of doped B atoms and the rate of increase is higher when $n \geq 3$. This indicates that more electrons transfer from Al to B when $n \geq 3$. The more electrons that transfer, the greater is the change of Al_{13} structure. This result is confirmed in Figs. 1 and 2. From Fig. 8, it is noteworthy that the variations of the Al charge *vs*. *n* are similar for the cationic and neutral clusters when $n \leq 3$, but contrary to the neutral clusters when $n \geq 4$. In addition, in combination with the fragmentation energy (Fig. 4) and second-order difference of the total energy (Fig. 5), it can be deduced that the ability of a B atom to obtain an electron from an Al atom is related to the stability of $Al_{13}B_n^{\pm m}$. The more the electrons transfer from Al to B, the more stable is the cluster; this phenomenon can also be found in AlB_n clusters.[20]

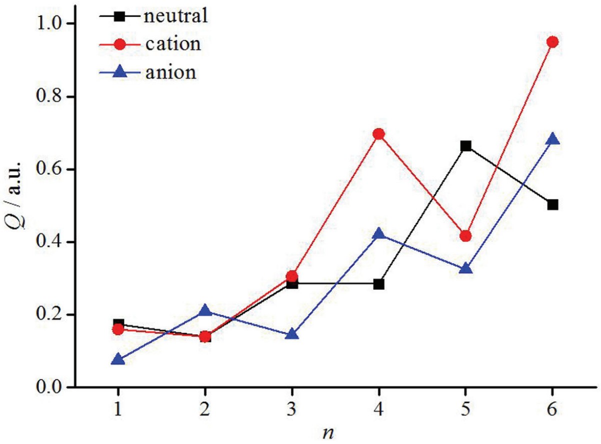


Fig. 8. Dependence of the average atomic charge of Al (*Q*) on the cluster size (*n*) in $Al_{13}B_n^{\pm m}$ clusters.

CONCLUSIONS

In this study, the stable configurations, relative stability and electronic properties of $Al_{13}B_n^{\pm m}$ (n = 1–6 and m = 0, 1) clusters were investigated at the B3LYP/6-311+G(d) level. The main results are as follows. The symmetry of the $Al_{13}B_n^{\pm m}$ (n = 1–6 and m = 0, 1) clusters was gradually reduced when $n \geq 3$; the $Al_{13}B_2^+$ cluster possesses the highest symmetry (D_{4h}). The average binding energies of the $Al_{13}B_n^{\pm m}$ clusters increased as size *n* increased, but the increment became smaller and smaller as the size *n* increased. Both the fragmentation energy and second-order energy of the $Al_{13}B_n^{\pm m}$ clusters indicated that the

$Al_{13}B_2^+$, $Al_{13}B_3$, $Al_{13}B_5$ and $Al_{13}B_6^+$ clusters had relatively higher stability than their corresponding differently charged species of the same size. As the $Al_{13}B_n^{\pm m}$ clusters grew from $n = 3$, most of the stable lowest-energy conformations contained a B_2 moiety, and the average B–B bond length increased with increasing n. The HOMO–LUMO energy gaps indicated that the anionic $Al_{13}B_n$ clusters were more active in the electron excitation process than the cationic $Al_{13}B_n$ clusters. The chemical hardness further proved that the $Al_{13}B_3$ and $Al_{13}B_5$ clusters were more stable than their neighbors were. Overall, the average charge of Al increased with increasing number of doped B atoms, indicating that more electrons were transferred from Al to B atoms with increasing size n.

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ИЗВОД

DFT ПРОУЧАВАЊЕ СТРУКТУРЕ И СТАБИЛНОСТИ КЛАСТЕРА $Al_{13}B_n^{\pm m}$

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Кластери $Al_{13}B_n^{\pm m}$ су проучавани DFT-UB3LYP/6-311+G(d) методом. Испитано је варирање структурних и електронских својстава са променом n и m. За кластере $Al_{13}B_n^{\pm m}$, геометрије њихових стабилних структура имају високу симетрију када је $n \leq 2$, као код $Al_{13}B$ (C_{2v}), $Al_{13}B^+$ (C_{2v}) и $Al_{13}B_2^+$ (D_{4h}). Разлике у дужинама веза Al–B међу најстабилнијим $Al_{13}B_n^{\pm m}$ кластерима не прелазе 0,066 Å, а разлике у енергијама међу изомерима (ΔE) су мање од 1,000 eV за већину кластера. На редослед стабилности кластера могу утицати наелектрисања. Структуре најниже енергије за $Al_{13}B_n^{\pm m}$ кластере садрже групу B_2 када је $n \geq 3$. У целини, просечна енергија везивања код неутралних кластера је већа него код одговарајућих анјонских кластера, али је мања него код катјонских кластера. Неутрални кластери имају највећу стабилност за $n = 3$ и 5, док су кластери $Al_{13}B_3^+$ и $Al_{13}B_5^+$ мање стабилни од својих суседа. И енергије раскидања и разлике другог реда у енергијама указују да су неки кластери стабилнији од њима одговарајућих другачије наелектрисаних молекулскх врста исте величине.

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