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Fragmentation and Coulomb explosion of multicharged small boron clusters

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We extensively study the fragmentation and Coulomb explosion of multiply charged small boron clusters B_n ($n = 2$–13), where n is the cluster size. Our calculations are based on *ab initio* quantum-chemistry methods. Highly charged unstable clusters dissociate spontaneously into several neutral or charged fragments, and large amounts of energy are produced, depending on the charge of the parent cluster. We argue that this mechanism makes boron clusters a clean, safe, and cheap energetic material.

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I. INTRODUCTION

There is an ever-increasing demand to find energetic materials which can be used as clean, safe, long-lasting, and cheap energy sources. In this sense nanosize energetic materials have been a great challenge in the last decade. The subject has stimulated scientists to reveal the most appropriate nanomaterials like atomic or molecular clusters, graphene-like two-dimensional sheets, and carbon-based cage structures. Boron is considered as an energetic material, like its neighbor carbon, due to its low weight, high coordination number, and high melting point. It has one of the highest volumetric and gravimetric energy densities. As a result, boron and boron-based structures are used in explosives and propellants in rocket boosters.[1–3] The addition of nano-sized boron particles to the propellants of ducted rockets increases the combustion stability.[4] Boron hydrides can store good amounts of hydrogen and release them upon chemical treatment when needed.[5]

The first experimental investigation of small boron clusters was reported in 1987 by Anderson *et al.*[6] They produced cationic boron clusters with a laser-ablation technique and studied their various fragmentation channels. La Placa *et al.*[7] produced cationic boron clusters up to size 52 from hexagonal boron nitride with a laser-ablation technique. Various *ab initio* studies have explored the electronic and atomic properties of small boron clusters both in neutral and charged states.[8–17] Electronic properties of neutral and anionic boron clusters of three and four,[18] five,[19] six,[20] seven,[21] eight and nine,[22] twelve,[23] and twenty[24] atoms were studied via photoelectron spectroscopy and *ab initio* methods. These studies show that small-size boron clusters prefer either planar- or quasiplanar-type atomic arrangements.

Fragmentation of clusters and their Coulomb explosion (CE) have been the subject of intense theoretical and experimental research in recent years. The CE of clusters is an efficient source of highly charged ions through an enhanced ionization process. It initiates when the repulsive Coulomb energy of positively charged ions in a cluster exceeds its binding energy. It was observed in the mass spectra of doubly charged metallic, ionic, and van der Waals clusters.[25] Depending on their size, doubly charged clusters either remained stable or disintegrated into singly charged cationic fragments. Iniguez *et al.*[26] studied some dissociation channels of cationic small sodium clusters by employing two independent models for the exchange correlation potential. A neutral sodium atom was predicted as one of the fragments in the most favorable binary dissociation of cationic clusters. Calvo tried to understand the role of the charge distribution in CE of multiply charged large metallic sodium clusters through molecular-dynamics simulations.[27] Brechignac *et al.*[28] experimentally studied fragmentation dynamics of small doubly charged potassium clusters and found that in predominant Coulombic binary fission of these systems the fragments carry equal amounts of charge. In theoretical calculations and experimental measurements, the dominant fragmentation channel is observed to have K_3^+ as a magic fragment. Singly, doubly, and triply charged lithium clusters were studied via *ab initio* techniques by Rao *et al.*[29] They noticed that singly charged lithium clusters are stable against dissociation, but doubly and triply charged systems disintegrate by exploding. As singly charged clusters dissociate, the charge stays on the larger fragment. Nevertheless, fragments of doubly and triply charged clusters carry equal charges.

In addition to metallic clusters, the stability of semiconductor clusters has also been studied from the viewpoint of fragmentation dynamics. In one of the earliest studies, Islam *et al.*[30] reported detailed *ab initio* computations investigating fragmentation attitudes of ionized carbon clusters with different structures. They predicted magic numbers with a well defined periodicity and computed the fragmentation energy (FE) of several channels. They found that as singly charged clusters dissociate, the charge is taken by a carbon monomer for small sizes. However, the charge is carried by the bigger fragment as the cluster size increases. Similar results were obtained for anionic carbon clusters. When the dissociation of doubly ionized cations into two singly ionized fragments was considered, they found CE for parents nearest to the magic numbers. Tendero *et al.*[31] also theoretically studied the fragmentation dynamics of neutral and cationic small carbon clusters. The authors predicted CE in the channel $C_n^{+2} \longrightarrow C_{n-1}^+ + C^+$ when $n \leqslant 4$. Due to their importance in technology, silicon clusters have been explored widely both theoretically[32] and experimentally.[33]

Striking chemical and physical properties of boron clusters can be extracted from their stability analyses. Anderson *et al.*[6] investigated the stability of $2-8$-atom cationic boron clusters with a collision-induced-dissociation technique. In channels having the lowest FEs, B_1^+ appeared as the major fragment at studied collision energies. Subsequently, Hanley *et al.*[34] explored the fragmentation attitudes of cationic clusters with up to 13 atoms by the same experimental method and compared their results with those obtained through the *ab initio* methods. They observed only binary fragmentations at low collision energies. Nevertheless, three or four fragments were detected at high collision energies as the parent size was increased. The charge remained on the free boron atom for small parents, but it was on B_{n-1} in the case of larger parents. Subsequently, the dissociation dynamics of singly and doubly ionized cationic boron clusters with up to 6 atoms were studied theoretically by Niu *et al.*[35] In their analysis, the boron atom carried the charge in the binary fragmentation of singly charged parents up to size 5, but it was neutral in the most favorable channel of B_6^+. They did not find any CE for doubly charged clusters.

In the present work we search for the possibility of CE in neutral and multicharged small boron clusters. For this purpose we study various dissociation channels and compute their FE values. The paper is organized as follows. Details of our numerical computations are explained in the next section. In Sec. III we discuss our results and compare them with the available literature. Our conclusions are presented in Sec. IV.

II. COMPUTATIONAL METHOD

We solved the Kohn-Sham equations by employing the first-principle calculations within the density-functional theory (DFT) framework. The exchange correlation potential was approximated by the generalized-gradient approximation (GGA) using the three-parameter hybrid exchange functional of Becke[36] and the nonlocal correlation functional of Lee, Yang, and Parr (LYP).[37] Geometry optimization and vibrational frequency computations were performed with the software package GAUSSIAN 03.[38] Our calculations were done through three stages. First, using a smaller basis set (3-21G), we obtained wave functions of each cluster and reliable geometries for them. Then, due to the possibility of an open-shell structure, we optimized these wave functions through a larger basis set (6-311 + G*) by allowing electrons to diffuse into shells of larger energies. Finally, we reoptimized the geometry and performed vibrational frequency computations in order to find equilibrium structure of the clusters. We did not impose any constraints on the symmetry during the computations.

We considered planar or quasiplanar boron clusters B_n^Q where n and Q represent, respectively, the number of atoms and the charge residing on them. The parameters vary as $2 \leqslant n \leqslant 13$ and $Q \geqslant -2$. The upper value of Q depends on the size n. Beyond a critical charge, a cluster becomes unstable relative to its constituent free atoms. We found that B_2^{+2}, B_3^{+2}, B_4^{+3}, B_5^{+3}, B_6^{+4}, B_7^{+4}, B_8^{+5}, B_9^{+5}, B_{10}^{+5}, B_{11}^{+6}, B_{12}^{+6}, and B_{13}^{+6} are all unstable.[8]

In order to find the equilibrium configuration of a charged cluster, we adopted the following recipe. Atomic positions of a relaxed neutral cluster were chosen as the initial coordinates of atoms in its own singly charged state. Then, we optimized this configuration and obtained the ground-state structure of the singly charged cluster. Similarly, the optimized geometry of a doubly charged cluster was obtained by adopting and re-relaxing the atomic positions of its singly charged state. The same procedure was followed for multicharged clusters. The ground-state spin multiplicity was determined for every charge state of each cluster. We further computed vibrational frequencies to verify the equilibrium geometry. Since "negative" frequencies refer to transition states, we perturbed the geometry and found the true ground-state configuration.

We also investigated the fission, or activation, barrier for one of the dissociation channels investigated here at the same level of theory. We used the basis set 6-311+G* and adopted the GGA by using the functional B3LYP.

III. RESULTS

In the present study we concentrate on the fragmentation of highly charged small boron clusters B_n^Q. Recently, we have investigated optimized geometries of these structures in the range $-2 \leqslant Q \leqslant 5$ and confirmed that they have either planar or quasiplanar geometries.[8] There, we also studied the vibrational frequencies, the binding energy per atom, the second energy difference, and a few dissociation paths. In this paper we proceed in determining further possible fragmentation channels for multicharged boron clusters as a function of their size and charge.

The fragmentation of clusters is induced typically by a femtosecond laser irradiation. Alternatively, they are collided with an energetic electron beam or highly charged ions or atoms. Clusters can also fragment at high temperatures. The energy released or required in a dissociation process, i.e., the FE, may be computed by

$$\Delta E_n^Q = \left(\sum_{j,k} E_k^j \right) - E_n^Q, \quad j \leqslant Q, \quad 1 \leqslant k < n, \tag{1}$$

where E_n^Q is the total energy of a n-atom cluster with charge Q, or the parent cluster. The sum over j and k considers the total energy of all fragments, or the daughters. The charge and mass conservation laws require $\sum j = Q$ and $\sum k = n$. If ΔE_n^Q is negative, the Q-fold charged parent cannot remain stable and dissociates spontaneously, i.e., a CE takes place. However, a positive ΔE_n^Q implies that the parent remains stable in that channel and needs a ΔE_n^Q amount of energy in order to dissociate. The most probable channels are those with the lowest FE values.

Ejection of a singly charged cationic atom is observed often in experiments. Hence, we start with the channel

$$B_n^Q \longrightarrow B_1^+ + B_{n-1}^{Q-1}. \tag{2}$$

We calculated FE values for this channel as a function of the parent size n and plotted them in Fig. 1. The highest curve shows the FEs of singly ionized clusters.

We have recently[8] studied the binary fragmentation of B_n^+. There we have found that while the appearance of B_1^+ together with B_{n-1} is energetically favorable for $n < 6$, the production of B_{n-1}^+ and B_1 is preferred for $n \geqslant 6$. As is observed in Fig. 1, all FE values for singly ionized clusters are positive,

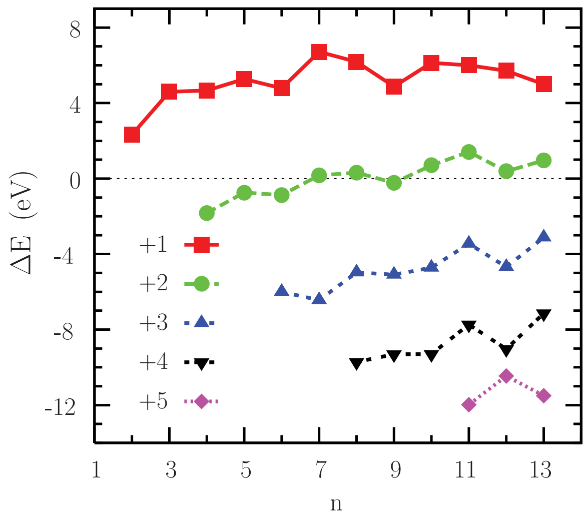

FIG. 1. (Color online) FE values for the reaction in Eq. (2). The legend denotes the charge state of the parents.

meaning they are stable and thus need external energy in order to fragment. Incidentally, the most and the least preferable channels are, respectively, of B_2^+ and B_7^+. In the case of +2-charged cations, the fragments B_1 and B_{n-1} carry unit charges. The ΔE is negative for parents B_4, B_5, B_6, and B_9, implying they are not stable for this dissociation, and a CE is likely to occur. The most and the least preferable channels are, respectively, of B_4^{+2} and B_{11}^{+2}. One must expect a CE for three-, four-, and five-fold-ionized clusters. More energy is released with increasing Q as expected. The most favorable channels are of B_7^{+3}, B_8^{+4}, and B_{11}^{+5}. In contrast, the least favorable paths are of B_{13}^{+3}, B_{13}^{+4}, and B_{12}^{+5}. We remark that B_7^+ is the most stable parent with $\Delta E = 6.72$ eV.

We now study the dissociation of a Q-fold charged parent into a doubly ionized atom and another fragment:

$$B_n^Q \longrightarrow B_1^{+2} + B_{n-1}^{Q-2}. \tag{3}$$

FE values for this channel are positive up to $Q = 3$, and parents with smaller charges need more energy to disintegrate as observed in Fig. 2. One of the fragments is a singly charged anion when $Q = 1$. Apparently, the production of B_1^{+2} and a singly charged anion together in a reaction is not favorable and needs a high energy input. Four- and five-fold-ionized parents have negative FE values, pointing to CEs. Fourfold-ionized parents yield charge-symmetric fragments. Smaller parents produce more energy as they explode. The highest amounts of energy are produced in the spontaneous fission of five-times-charged clusters. Parents B_2^+, B_4^{+2}, B_6^{+3}, B_8^{+4}, and B_{11}^{+5} have the most favorable channels in this reaction. Comparing Figs. 1 and 2, we conclude that the parents prefer fragmenting into B_1^+ rather than B_1^{+2}.

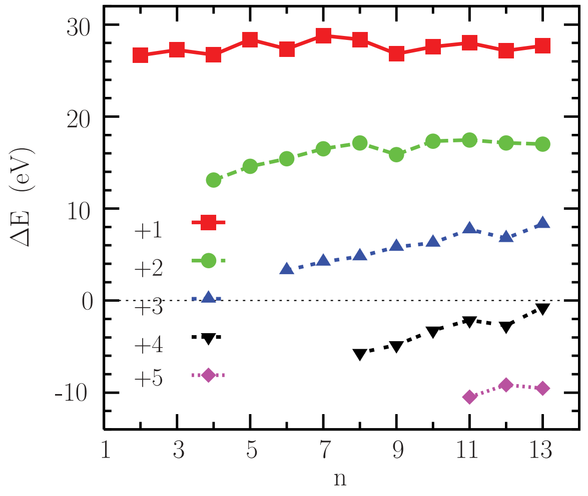

FIG. 2. (Color online) FE values for $B_n^Q \longrightarrow B_1^{+2} + B_{n-1}^{Q-2}$.

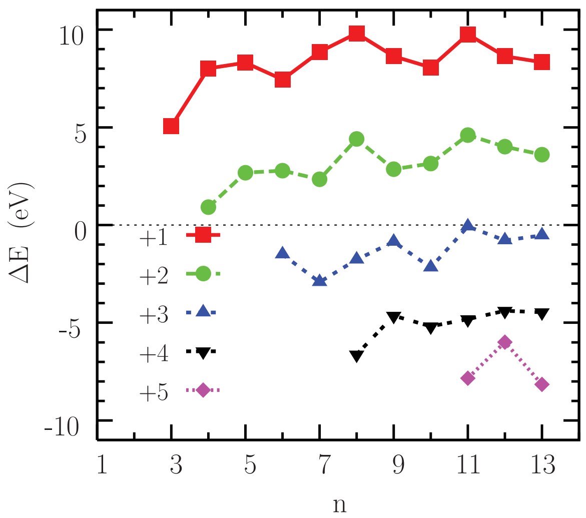

FIG. 3. (Color online) FE values for the reaction in Eq. (4).

It is curious if the emission of singly charged B_2 is preferable. We thus study the channel

$$B_n^Q \longrightarrow B_2^+ + B_{n-2}^{Q-1}. \tag{4}$$

The variation of the FE for this process is shown in Fig. 3. Notice that singly and doubly ionized parents need energy to fragment. Indeed, B_8 and B_{11} are the most stable parents when $Q = 1$ and 2. We expect CEs for parents with $Q \geqslant 3$. Clusters B_3^+, B_4^{+2}, B_7^{+3}, B_8^{+4}, and B_{13}^{+5} have the minimum FEs at their respective Q values.

Comparing ΔE values of the reactions analyzed so far, we conclude that in the binary fragmentation of multicharged boron clusters, B_1^+ is the predominant, or the most favorable, fragment, and next comes B_2^+. Parents prefer to emit B_2^+ instead of B_1^{+2}. This observation means that having a small charge is the decisive criterion for a fragment to be emitted easily.

The charge-symmetric double fragmentation of B_n^{+2} is

$$B_n^{+2} \longrightarrow B_x^+ + B_{n-x}^+, \tag{5}$$

where n and x assume integral values, respectively, in the ranges $10 \leqslant n \leqslant 13$ and $1 \leqslant x \leqslant 6$. As we see in Fig. 4, all parents considered are stable in this reaction. However, since the amounts of energy required for the dissociation of parents are small and can easily be achieved in experiments, this reaction is quite possible. Since both fragments have the same charge, we can find some basic relations between the sizes of parents and their fragments. We first notice that it is quite easy to find a singly ionized cationic atom as a fragment in this reaction. B_{11}^{+2} is found as the most stable parent almost for

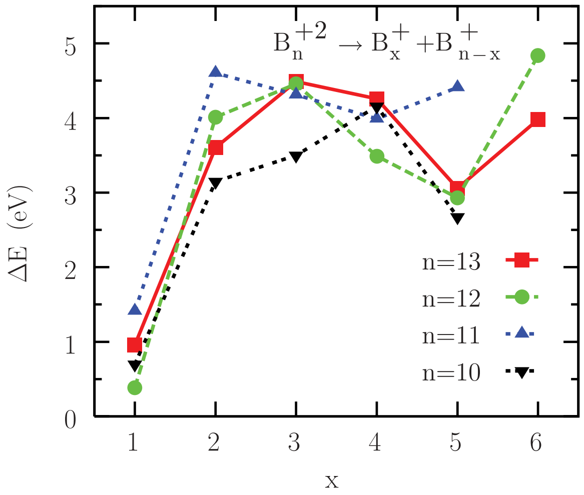

FIG. 4. (Color online) FE as a function of x in the charge-symmetric double fragmentation of B_n^{+2} for $10 \leqslant n \leqslant 13$.

all x values. Being smaller than other parents, doubly ionized B_{10} needs the smallest amount of energy in general. The ΔE of B_{10}^{+2} increases continuously, takes its maximum value at $x = 4$, and then sharply drops to its second-lowest value at $x = 5$. This behavior implies that it is energetically favorable for the cluster to fragment into two equal-charge and equal-size pieces. For B_{12}^{+2}, however, it is much easier to dissociate into B_5^+ and B_7^+. Fragmenting into identical pieces is not so easy; indeed, it requires the largest energy of all channels in this reaction. FE curves for parents B_{12}^{+2} and B_{13}^{+2} follow a similar variation with x. The production of B_5^+ in the dissociation of all parents except B_{11}^{+2} is favorable.

A possible charge-asymmetric double dissociation for threefold charged boron clusters is

$$B_n^{+3} \longrightarrow B_x^+ + B_{n-x}^{+2}. \tag{6}$$

FE values for this reaction as a function of x are depicted in Fig. 5. The fragmentation of B_{10}^{+3} and B_{12}^{+3} results in CEs for $x \leqslant 5$. Moreover, B_{11}^{+3} and B_{13}^{+3} show CEs, respectively, for $x \leqslant 3$ and $x \leqslant 2$. The fission of B_{10}^{+3} releases the greatest amount of energy. We notice that in favorable channels of all parents, a small fragment carries a unit charge, and the larger one takes the rest. Energy production is greater when the size difference between fragments is greater, similar to the reaction in Eq. (5).

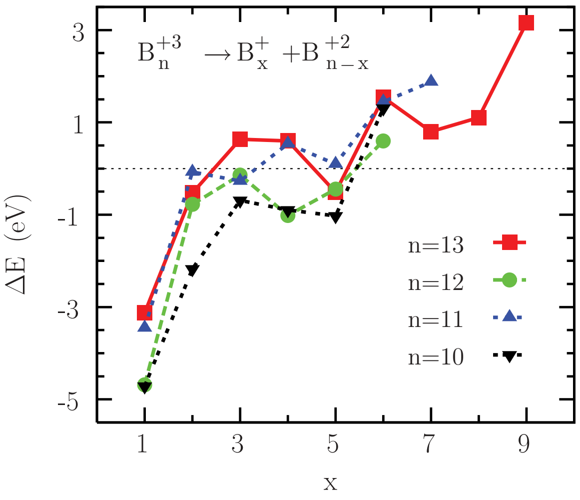

FIG. 5. (Color online) FE as a function of x in the charge-asymmetric double fragmentation in Eq. (6).

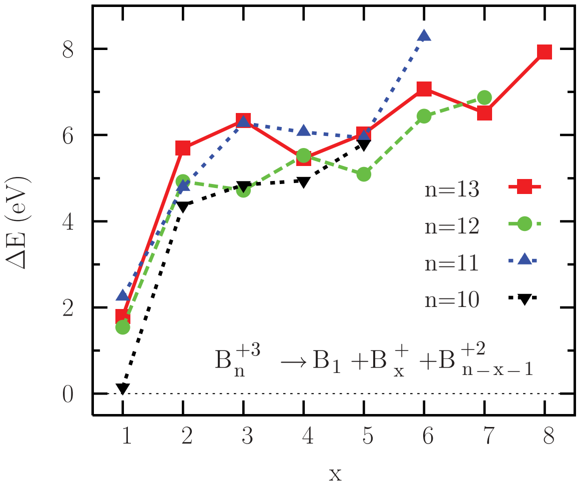

FIG. 6. (Color online) FE values for the charge-asymmetric fragmentation of B_n^{+3} via the reaction in Eq. (7).

We now consider the charge-asymmetric triple disintegration of B_n^{+3} in the reaction

$$B_n^{+3} \longrightarrow B_1 + B_x^+ + B_{n-x-1}^{+2}. \tag{7}$$

Figure 6 displays the FE values for this reaction. Obviously, a CE is not possible here. Parents need more energy to disintegrate for any x value compared to the reaction in Eq. (6). Thus, double fragmentation is more likely to occur compared to this one. B_{11}^{+3} and B_{13}^{+3} are the most stable parents. The easiest realizable channel produces B_1, B_1^+, and one larger fragment.

The charge-symmetric triple dissociation reaction of threefold-ionized boron clusters is

$$B_n^{+3} \longrightarrow B_1^+ + B_x^+ + B_{n-x-1}^+. \tag{8}$$

In contrast to previous triple fragmentation, here we expect CEs for all parents at certain x values. This means the equal, or symmetric, distribution of charge among fragments makes the parents unstable. As is seen in Fig. 7, the most energetic explosion is $B_{10}^{+3} \longrightarrow 2B_1^+ + B_8^+$. The energy gain decreases as the size of fragments B_x^+ and B_{n-x-1}^+ gets closer. In essence, the amounts of energy produced here are comparable with the process in Eq. (6).

The binary fragmentation of clusters B_n^{+4} may produce unequally charged fragments as

$$B_n^{+4} \longrightarrow B_x^+ + B_{n-x}^{+3}. \tag{9}$$

We notice in Fig. 8 that in this reaction all parents may explode spontaneously by releasing appreciable amounts of energy, especially for small x values. Energy produced in CEs decreases as the fragments become comparable in size. In other words, parents prefer fragmenting into singly charged atom rather than singly charged cluster. B_{13}^{+4} appears as the most stable parent as expected.

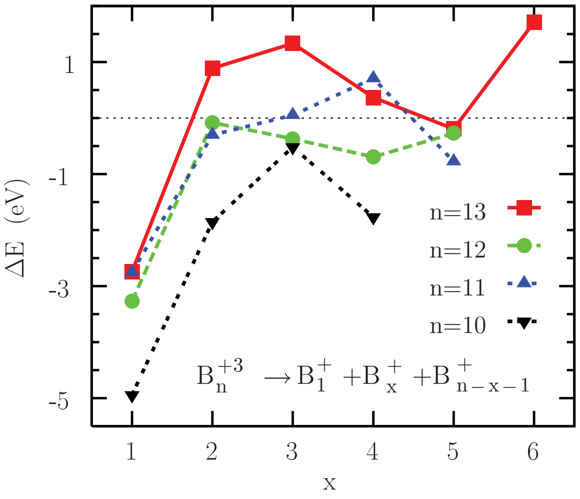

FIG. 7. (Color online) FE values for the charge-symmetric triple fragmentation of the threefold-ionized parents.

Another double dissociation path for fourfold-ionized boron clusters is the charge-symmetric one,

$$B_n^{+4} \longrightarrow B_x^{+2} + B_{n-x}^{+2}. \qquad (10)$$

For this reaction, there exist a smaller number of channels compared to previous reaction since we consider only stable structures as fragments. We already stated in Sec. II that doubly ionized B_2 and B_3 are not stable. Figure 9 shows that explosions of B_{10}^{+4} and B_{13}^{+4} produce, respectively, the largest and smallest amounts of energy. Thus, the energy gain is inversely proportional to the size of the parent. This is an expected result because larger clusters can sustain more stability as the charge increases. The energy outcome increases with increasing x for a parent. In this fission, more energy is released for $x \geqslant 4$ compared to the charge-asymmetric dissociation in Eq. (9).

One of the most favorable triple-dissociation paths for the fourfold-ionized boron cluster B_n^{+4} is

$$B_n^{+4} \longrightarrow B_1^+ + B_x^+ + B_{n-x-1}^{+2}. \qquad (11)$$

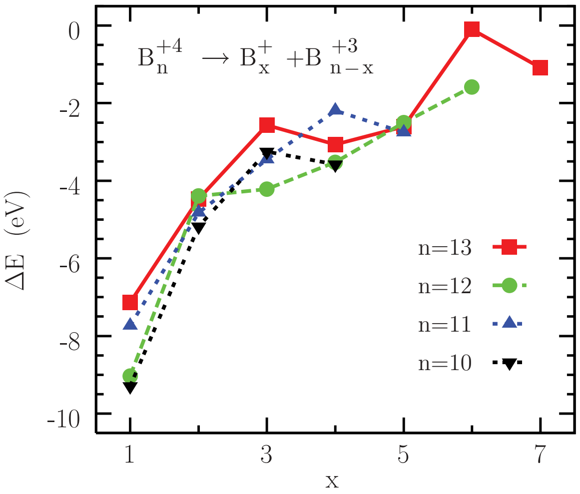

FIG. 8. (Color online) FE results for the charge-asymmetric dissociation of B_n^{+4}.

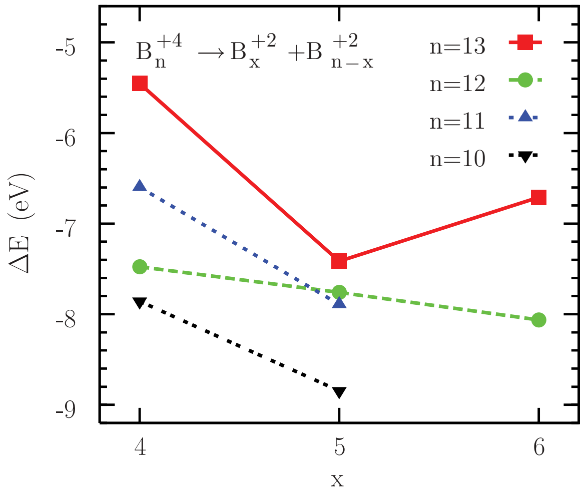

FIG. 9. (Color online) FE values for the charge-symmetric dissociation of B_n^{+4}.

In this reaction, a CE takes place for any n and x values. As is obvious in Fig. 10, the triple fission of four-times-charged parents yields more energy compared to their double fragmentations. Hence, triple disintegration is more advantageous for practical applications. Similar to threefold-ionized clusters, the explosion of B_{10}^{+4} generates the largest energy. This result is expected because B_{10} is not able to sustain more ionization. Other parents give off comparable energies, especially at $x = 4$ and 7. The fission of all parents into two singly ionized boron atoms and B_{n-2}^{+2} produces the largest energy, confirming a general observation that fragmenting into one or several smaller and one much bigger daughters is energetically favorable.

In the charge-symmetric dissociation of B_n^{+4} into four fragments, FE values are found even much smaller than those of Eq. (11), i.e., the energy gain is larger.

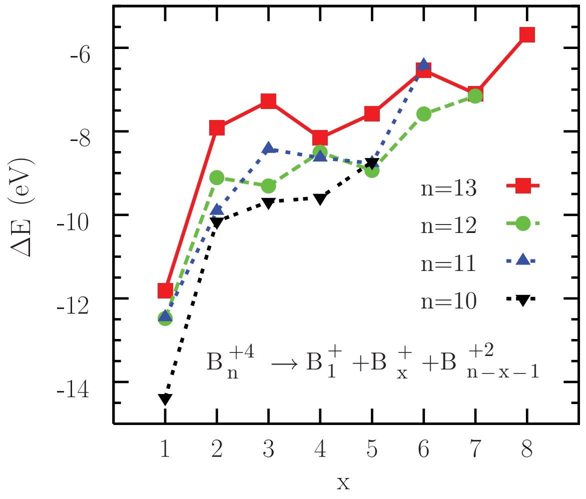

FIG. 10. (Color online) FE results for the triple fragmentation, as defined in Eq. (11), of the fourfold-ionized parents.

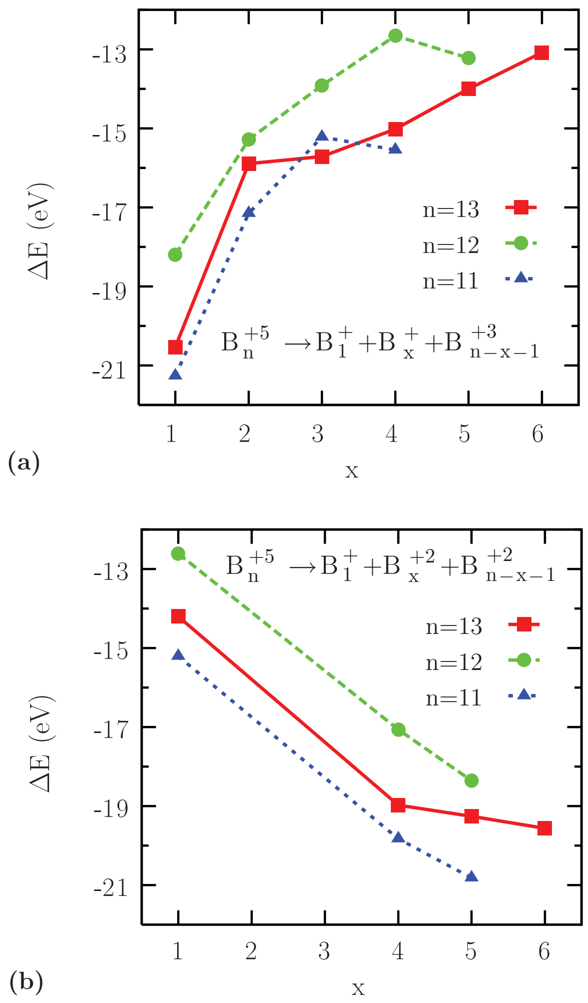

FIG. 11. (Color online) FE values for the triple fragmentation of fivefold-ionized parents in reactions (a) Eq. (12a) and (b) Eq. (12b).

In the case of fivefold-ionized boron clusters, we consider two distinct dissociation reactions:

$$B_n^{+5} \longrightarrow B_1^{+} + B_x^{+} + B_{n-x-1}^{+3}, \tag{12a}$$

$$B_n^{+5} \longrightarrow B_1^{+} + B_x^{+2} + B_{n-x-1}^{+2}. \tag{12b}$$

Clusters with $n < 11$ are unstable when $Q = 5$; thus, we only studied the dissociation of B_{11}, B_{12}, and B_{13}. FE values for the reaction in Eq. (12a) are presented in Fig. 11(a). The explosion of fivefold-ionized clusters yields the largest amount of energy compared to all previous reactions because of the fact that more excess charge in a cluster means a larger Coulomb energy. The FE increases with increasing x. Fragmentation of B_{11}^{+5} and B_{12}^{+5} yields, respectively, the largest and smallest energies. In contrast, Fig. 11(b) tells us that ΔE for the reaction in Eq. (12b) decreases as x increases. Figure 9 also displays a similar behavior. The largest and minimum amounts of energy are obtained, respectively, in the explosions of B_{11}^{+5} and B_{12}^{+5} as in the reaction in Eq. (12a).

Interplay between the cohesive energy and the Coulomb repulsion usually results in the formation of a fission, or activation, barrier which prevents a cluster from decaying immediately even if it is energetically favorable. Hence, a minimum amount of energy, as much as the height of the activation barrier (AB), has to be transferred to the cluster in order to make the fission possible. This issue has been studied in detail for various charged-cluster systems.[39]

The AB is defined as the energy difference of the equilibrium- and transition-state structures. Hence, once the optimized transition state is found, one can calculate the AB of a reaction as

$$\text{AB} = \text{E[TS]} - \text{E[EG]}, \tag{13}$$

where E[TS] is the total energy of the true transition-state structure linking the reactant and products, and E[EG] is the total energy of the reactant in its own equilibrium geometry.

A transition state is a saddle point lying above the equilibrium structure on the potential-energy surface (PES). The true, or optimized, transition state has one imaginary frequency. The main issue in the calculation of AB is to find the true transition state connecting the reactant and products in a reaction pathway. On the PES, there exist many hills and valleys that makes searching for the corresponding transition state very complicated. We made use of the synchronous transit-guided quasi-Newton (STQN) method[40] and QST2 option in the GAUSSIAN 03 package to find the optimized transition state. Unlike geometry optimization, the STQN method with the QST2 option requires structures of the reactant and products as its input. The algorithm first makes an initial suitable guess for the transition-state structure linking the reactant and products in the reaction of interest and then renders the optimized transition state if it really exists on the PES.

We computed the AB against the dissociation in the channel $B_9^{+4} \longrightarrow B_1^{+} + B_8^{+3}$ in order to understand the reaction mechanism. We have recently[8] obtained equilibrium geometries of the reactant and products as quasiplanar. Equation (1) yields the energy released in this reaction as −9.31 eV. The same value is obtained as the enthalpy of the reaction by separate computations of the energies for the most stable structures of the products and reactants without a zero-point-energy (ZPE) correction (considering thermal enthalpies), and with the ZPE correction, it is found as −9.36 eV. Thus, the reaction is exothermic.

There exists a great deal of pathways connecting the reactant and products that can be taken into account in our reaction. We consider two possible routes: the parent ejects a cationic boron atom either from its periphery or from its center.

The removal of a side atom at the periphery of reactant B_9^{+4} leads to the expected final product configuration of quasiplanar B_8^{+3}. The ejected cationic boron atom moves away on the same plane of the reactant. Due to the high symmetry with respect to the central atom, we should expect to reach the true transition state if any one of the eight peripheral atoms is dislodged. Thus, we focused on the removal of an arbitrary side atom. The optimized transition state is further confirmed by a separate computation. Using Eq. (13), we found the AB as 0.25 eV. This small value makes sense since the structure dissociates by a CE with an additional electron loss.

Now consider the removal of the central atom perpendicularly away from the plane. We found that this is not a preferred pathway on the PES because this route does not end up with a quasiplanar geometry for B_8^{+3}. Rather, it tends to be optimized as a ring-shaped structure. However, it is outside of the scope of this paper and does not deserve attention since it is not the ground-state geometry.

IV. CONCLUSIONS

In this paper we have theoretically studied various dissociation channels for multiply charged boron clusters. The reactions considered are the most possible double and triple fragmentations. We calculated the fragmentation energies in these paths via Eq. (1) by using the total energies of clusters at their equilibrium configurations, which were computed through the first principles as a function of cluster size n and charge state Q.

We observed that in the binary fragmentation of multicharged boron clusters, B_1^+ is the major fragment. Parents prefer to emit B_2^+ instead of B_1^{+2}, meaning that having a small charge is the decisive criterion for a fragment to be produced. In the charge-symmetric fragmentation of three- and four-fold-ionized parents, a CE is favorable. This implies that the dissociation of parents produces more energy if their charge is distributed evenly among the fragments. In Coulombic fission, the energy gain is inversely proportional to the size of the parent for a specific charge because larger clusters can sustain more stability as they are highly ionized. The energy released in the CE increases with increasing Q.

In the charge-symmetric double fragmentation of clusters B_n^{+2} with sizes $n \geqslant 10$, we did not observe any CE. Nevertheless, since their FE values can easily be accessible in experiments, it can be considered as a possible channel. The CE is not possible in the charge-asymmetric triple disintegration of threefold charged clusters. Symmetric and asymmetric double dissociations and triple fragmentation for four-times-ionized parents make the CE possible. Although the smallest parent provides the largest energy in its CE, the biggest parent gives off the smallest energy when it explodes.

Clusters preferably fragment into B_1^+ and B_{n-1}^{Q-1} for any Q value. A cationic boron dimer is likely to be produced in the dissociation of parents except B_9^{+4} and $Q = 5$ instead of a multicharged boron atom. More energy is produced if B_9^{+4} and fivefold charged clusters decay into a doubly ionized boron atom. Other fourfold charged clusters render higher amounts of energy in their CEs by producing a cationic boron dimer. We determined the size of the parents whose explosions generate the maximum energy for a given Q. In general, the stability of parents emitting a doubly ionized boron atom increases monotonically with size for $Q \geqslant 2$. If a fragment B_{n-1}^{Q-1} has a charge greater than one, a CE is expected. On the other hand, when both fragments have an equal charge, a CE can only be observed for clusters with sizes 4, 5, 6, and 9. Similarly, a CE is possible when a fragment B_{n-2}^{Q-1} carries more charge than a cationic dimer.

Finally, the height of the barrier against dissociation is computed for a sample channel. We concluded that in most of the reactions, this barrier is reasonably small so that CEs can take place and produce good amounts of energy.

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