Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Theoretical study on the line defects in β_{12}-borophene: the enhanced direct-current and alternating-current conductances

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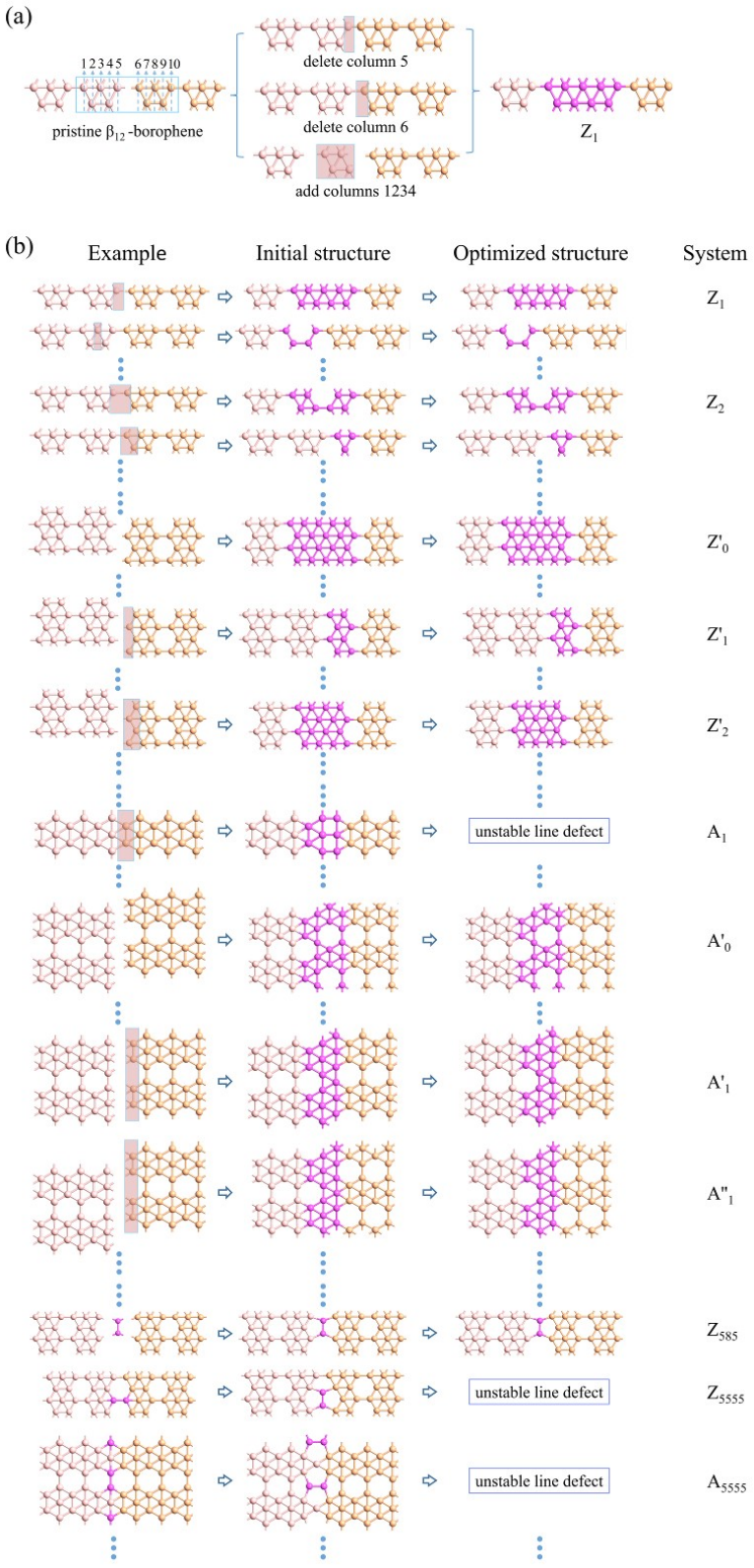

Fig. S1 (a) An example of how to design the initial structure of a line defect. (b) Some typical design processes for the line defects. The pink and yellow balls represent the B atoms of the perfect β_{12}-borophene, while the purple balls represent the B atoms of the line defect.

The design method of the initial structures of the line defects is important. According to the structure of the perfect β_{12}-borophene, here three design methods were used to construct the initial structures of the line defects:

I. By directly deleting or adding different columns of B atoms in β_{12}-borophene, we can obtain various initial structures.

Owing to the symmetry and periodicity of β_{12}-borophene, an initial structure can be obtained by different design processes. For example, as shown in Fig. S1(a), by deleting the column 5 or 6, or adding the four columns of B atoms, we can obtain three initial structures, but they are the same.

Fig. S1(b) shows some typical design processes for various line defects. For a given category, the notation Z_n or A_n represents the corresponding lowest-energy structure. For instance, by deleting or adding one column of B atoms, we can obtain many initial structures for this kind of line defect. After structural optimization at the DFT level, some initial structures were found to be unstable. Among the rest of the stable line defects, the lowest-energy structure is designated as Z_1. Here, the letter Z indicates that the line defect is along the zigzag direction, while the subscript '1' indicates this lowest-energy structure is obtained by deleting or adding 'one' column of B atoms.

II. By introducing various possible line dislocations in the initial structures from the design method I, we can also obtain new initial structures.

In this method, the notations Z'_n and A'_n represent the related lowest-energy structures and the superscript 'apostrophe' indicates that there exists line dislocation in the structure. Z'_0 (A'_0) represents the lowest-energy structure of the line defect along the zigzag (armchair) direction, in which only the line dislocation exists. By introducing various possible line dislocations, and deleting or adding one column of B atoms at the same time, the obtained lowest-energy structure is Z'_1. The second lowest-energy structure is Z''_1 (this structure is not given in the figure).

III. By deleting, adding or rotating several B atoms, some typical line defects can be constructed.

For example, the line defect Z_{585} can be obtained by this method; this line defect is

similar to those well-known structures observed in other 2D materials such as graphene and transition metal dichalcogenides. In this method, the subscript usually represents the corresponding structure (*e.g.*, for Z_{585} the subscript '585' indicates that in a periodic unit the line defect contains two five-membered B rings and one eight-membered B ring).

Based on the three design methods, we obtained and optimized a variety of structures of line defects. We found that all the optimized structures keep flat. It is worthy to note that the initial structures of the line defects from the three design methods can include the experimental results. In addition, to the best of our knowledge, there is no systematic or special nomenclature for the line defects in 2D materials. Nevertheless, we believe the notations and explanations mentioned above can be effectively used to distinguish these different line defects in β_{12}-borophene.

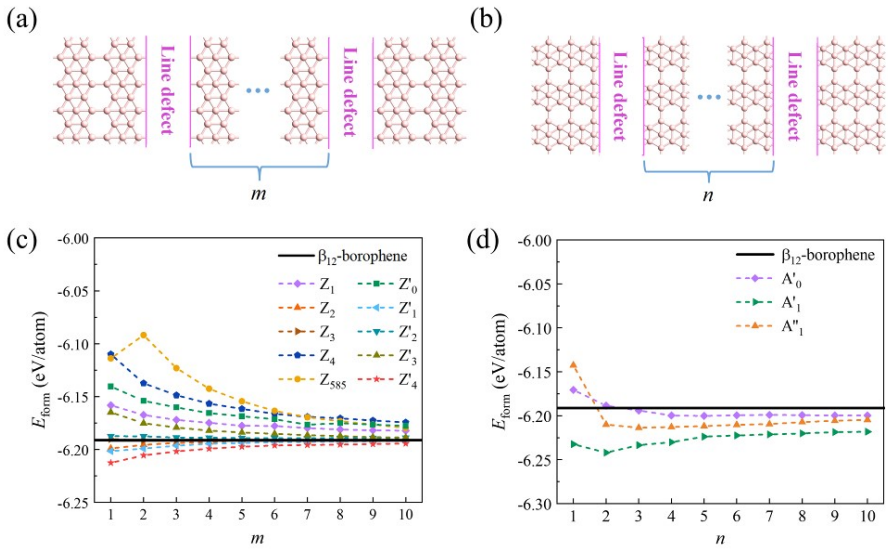

Fig. S2 The Schematic diagram of the two adjacent line defects along the (a) zigzag direction and (b) armchair direction of β_{12}-borophene, and *m* or *n* is the number of the corresponding periodic units. (c) and (d) The formation energies as the functions of *m* and *n*. The formation energy of β_{12}-borophene is also given for comparison.

The interaction between two adjacent line defects is a complicated problem. For example, if the distance of two line defects is small enough, one may incorporate with

the other, leading to the formation of a new line defect. Here, we only consider a simple case, *i.e.*, the distance of two adjacent line defects is large enough and the related interactions can be neglected. Fig. S2 shows the schematic diagram and the calculated results. It can be seen that the formation energies of these line defects are converged when m (n) is no less than 6 (9); this also means that the changes of the formation energies do not exceed 10^{-3} eV/atom. As a result, the interaction of two adjacent line defects can be effectively avoided by choosing suitable supercells.

Table S1 The formation energies of β_{12}-borophene and the line defects under PAW method.

	E_{form} (eV/atom)		E_{form} (eV/atom)
β_{12}-borophene	-5.802	Z'_1	-5.804
Z_1	-5.794	Z'_2	-5.802
Z_2	-5.805	Z'_3	-5.791
Z_3	-5.801	Z'_4	-5.810
Z_4	-5.779	A'_0	-5.806
Z_{585}	-5.738	A'_1	-5.821
Z'_0	-5.788	A''_1	-5.823

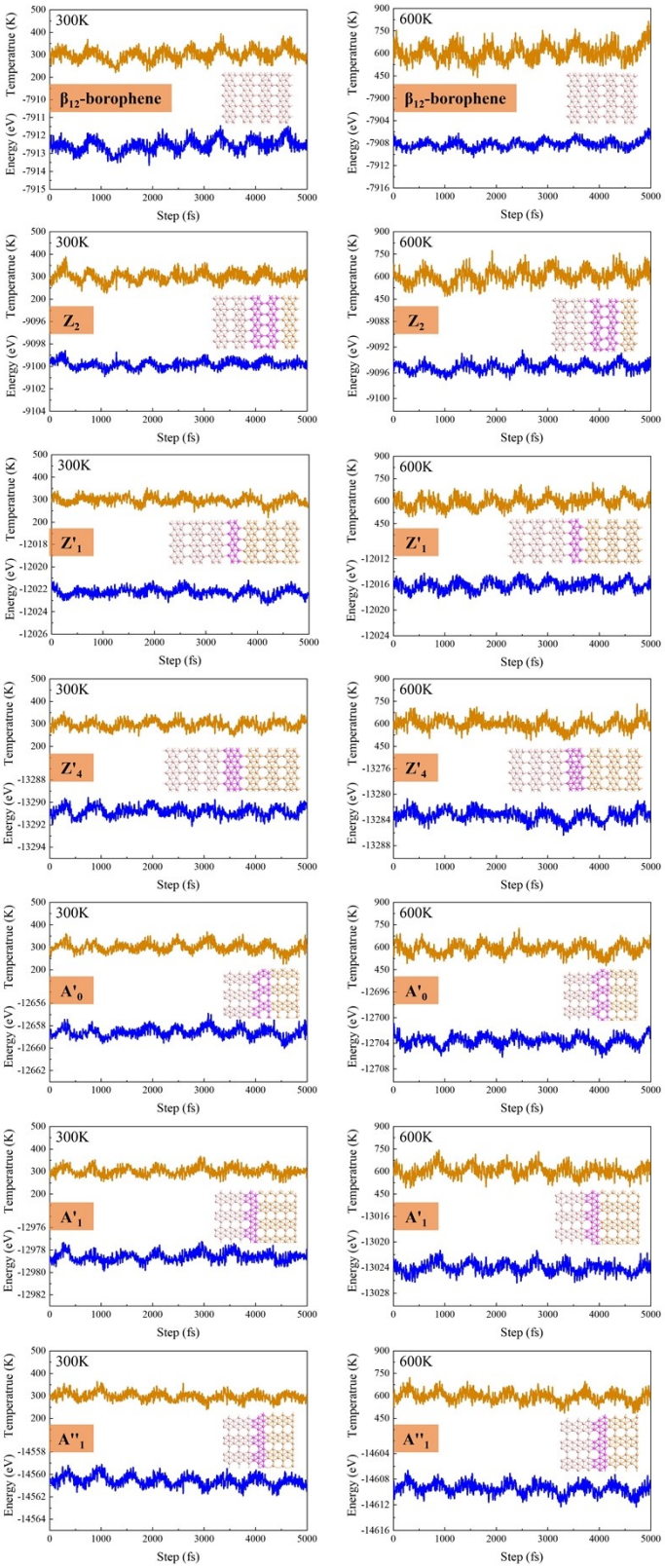

Fig. S3 The fluctuations of temperature and free energy with time for β_{12}-borophene and the six line defects at 300 and 600 K. The insets show the corresponding structures after 5000 time steps.