

The electronic and transport properties of borophane with defects: A first principles study

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ABSTRACT

Recent works well confirm the stability of hydrogenated borophene, known as borophane. Here, first principles studies have performed on the electronic and transport properties of borophane with defects. The calculations indicate that the introduction of defects results in different behavior of charges redistribution along x and y directions. The intrinsic electronic structure of borophane with Dirac cone is destroyed in various degrees by each type of defect. The inducing defect states lead to the occurrence of flat bands, which are not benefit for the electronic transport properties. According to the transmission spectra and I-V characteristics, these defects decrease the transmission intensity and the current value both along two directions. However, the transport anisotropy can be efficiently tuned by defect, which may contribute to the design of functional device.

1. Introduction

Since the discovery of graphene [1], two dimensional (2D) materials have been intensively studied due to their novel mechanical, electronic, and catalytic properties [2–6]. As carbon's neighbour, boron is always expected to be explored as 2D nanostructures, though they have long proven difficult to prepare. The quasiplanar B36 cluster obtained in early experiment shows the viability of single layer boron sheets [7,8]. And eventually, the latest experiments succeed in synthesizing of 2D boron films [9,10]. Three main types are known as borophene, β_{12} and χ_3 boron sheet, synthesized by Mannix et al. and Feng et al., respectively. Especially borophene, which possesses out-of-plane buckling structure and shows metallic characteristics, has been extensive investigated in theory beyond experiment [11–14]. First principles calculations have been carried out to predict that borophene has highly anisotropic mechanical properties [15,16], unexpectedly low lattice thermal conductivity [17] and tunable superconducting transition temperature [18].

Despite the merit of borophene seems promising, the easy chemical degradation in ambient conditions still drawback its practical applications [9]. A feasible method to enhance the stability of borophene is surface chemical functionalization, which has been applied in other 2D materials to modify their properties [19,20]. The hydrogenated form of borophene, known as borophane, confirmed the stability in recent work [21], has also attracted a great attention. It is demonstrated that

borophane possesses a Dirac cone in its band structure with ultrahigh Fermi velocity, rendering it ideal for nanoelectronic applications [22]. Similar to borophene, the mechanical properties borophane is also highly anisotropic [23]. Further studies also verify that borophane is auxetic with a surprising negative Poisson's ratio and ferroelastic with a remarkable orientation switch of the anisotropic Dirac transport channels [24].

We note the above aspects mainly concentrate on the perfect borophane. However, considering the practical fabrication process, the experimentally available borophane may not perfect but with vacancies, which may greatly impact its electronic and transport properties. Referred to the past work, it found little mentioned about the effects of such defects on the properties of borophane, therefore, clear clarification that is necessary. In the present work, we firstly create defects by removal of hydrogen and boron atoms. Such defects may be experimentally realized by using high energy ion beams. Then, we reveal the nature of borophane with defects based on the analysis of the formation energy, the charges distribution as well as the electronic band structure. And finally, we construct a two-probe system to clarify electronic transport properties borophane with defects.

2. Computational details

The geometry optimizations and electronic structure calculations are

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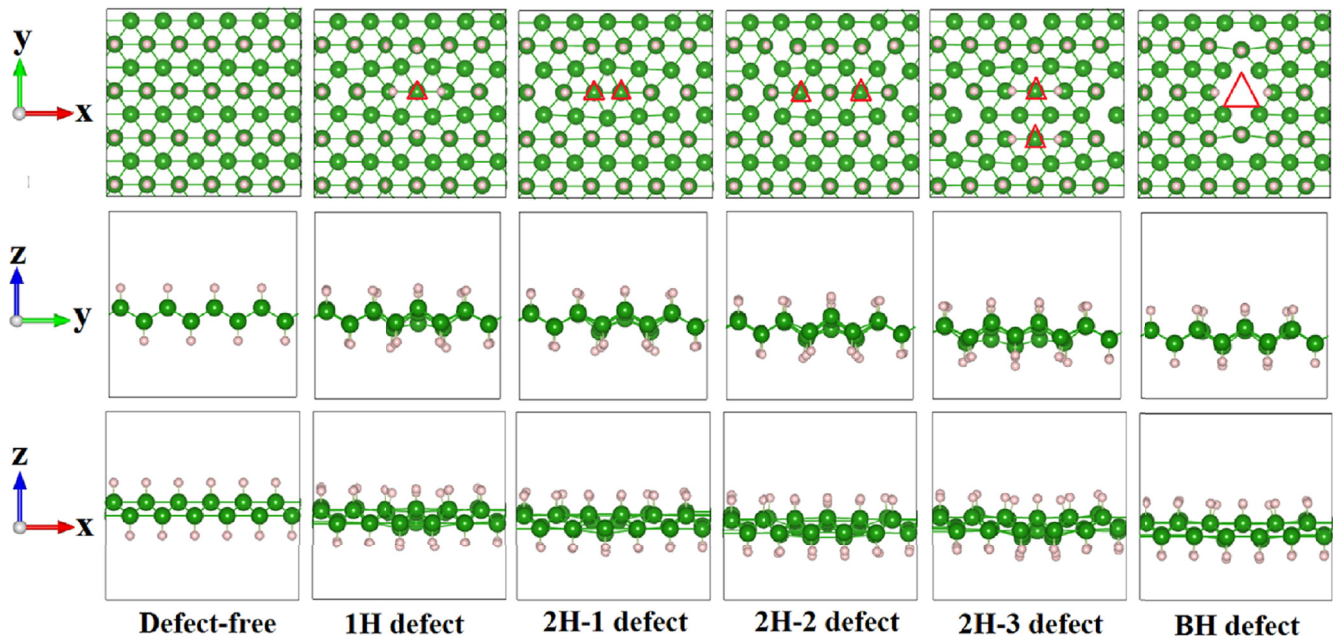


Fig. 1. The geometry structures of borophane with defects.

carried out in the Vienna ab initio simulation package (VASP) [25] with the projector-augmented wave (PAW) method and generalized gradient approximation (GGA) functional of Perdew, Burke and Ernzerhof (PBE) [26]. The cutoff energy is chosen as 500 eV for the plane-wave basis set and a Monkhorst-Pack mesh of $6 \times 6 \times 1$ is employed for the Brillouin zone integration. To avoid artificial interactions between adjacent images, larger than 15 \AA vacuum layer is used.

The electronic transport properties are investigated by using the nonequilibrium Green's function (NEGF) method executed in the TRANSIESTA program [27]. The transport current is obtained according to the Landauer–Büttiker formula:

$$I = \frac{2e}{h} \int T(E, V) [f_L(E) - f_R(E)] dE$$

where $T(E, V)$ is the transmission coefficient and $f(E)$ is the Fermi distribution functions at electrode. Single- ζ plus polarization basis set is used with a mesh cutoff 150 Ry. $1 \times 100 \times 100$ k-point samplings are adopted for the transmission spectra calculations.

3. Results and discussion

At the beginning of our calculations, five types of defect are designed as shown in Fig. 1. 1H defect is constructed by individually removing single hydrogen from defect-free borophane with dimensions $11.617 \text{ \AA} \times 11.236 \text{ \AA}$. Two hydrogen atoms in different relative positions are removed name as 2H-1, 2H-2 and 2H-3 defect, respectively. BH defect is obtained by getting rid of a B-H group. The supercell of defect-free borophane contains 96 atoms, including 48 B atoms and 48 H atoms. As the introduction of defect in perfect borophane, 95, 94, 94, 94 and 94 atoms are included in 1H, 2H-1, 2H-2, 2H-3 and BH supercell, respectively. Note that both spin-unpolarized and spin-polarized computations have been performed to determine the ground state of borophane with defects. No energy discrepancy is found in each configuration except 1H defect with spin-polarized calculated total energy 0.01 eV lower than spin-unpolarized calculated total energy. Thus, 1H defect has a magnetic ground state with magnetic moment $0.89 \mu_B$ and other configurations have nonmagnetic ground states. As carefully check each optimized configuration, the hydrogen atoms around the defect obvious lean to the defect position due to repulsive effect from other hydrogen atoms. The

boron atom which loses hydrogen atom slides down $\sim 0.74 \text{ \AA}$, 0.33 \AA , 0.48 \AA and 0.79 \AA in 1H, 2H-1, 2H-2 and 2H-3 defect, respectively. The B–B bond length surrounding the defects are changed in various degrees compared with that in perfect borophane.

After confirm the ground states of borophane with defects, the formation energy of each configuration is evaluated by formula, $E_f = E_{\text{defect}} + \sum_i n_i \mu_i - E_{\text{borophane}}$, where E_{defect} and $E_{\text{borophane}}$ represent the total energy of borophane with and without defect, n_i indicates the number of atoms of type i that have been removed from the perfect borophane, and μ_i are the corresponding chemical potentials of these species. Here, μ_H and μ_B are given as the single atom energy in H_2 and borophane, respectively. The calculated results are shown in Fig. 2. As can be seen that the formation energy of 1H defect is $\sim 0.52 \text{ eV}$, which is much smaller than that of single hydrogen vacancy formed in graphane ($\sim 2.3 \text{ eV}$) [28]. As for two hydrogen removal case, their formation energies are extremely sensitive to the relative positions of two removal hydrogen atoms. Given there is no coupling effect between two removal hydrogen atoms, the formation energy twice as much as 1H defect is marked with red dash line. It is worth to note that the formation energies

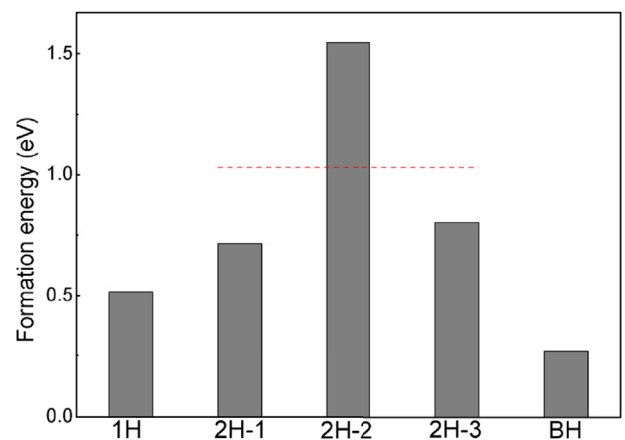


Fig. 2. The formation energy of each configuration. Red dash line represents the formation energy twice as much as 1H defect. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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