Study on the Influence of Hydrogen Surface Passivation on the Light Absorption Properties of Borophenes

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Abstract

The unique two-dimensional hexagonal honeycomb structure of Borophenes gives it the energy band structure of the Dirac cone and the novel quantum effect. Its superior electrical, mechanical and thermal properties have been highly expected by the scientific community. However, the lack of electrons causes to the honeycomb Borophenes to not exist stably in the free state. Therefore, the paper adopts hydrogen surface passivation method to modulate the stability of borophenes to control the light absorption characteristics. The electronic structure and light absorption characteristics of the borophenes have been studied using the first priciples method. The results shown that the best absorption rate of 20% hydrogen passivation was in the energy range of 7eV~13eV, and the maximum was 32500. The best absorption rate of 60% hydrogen passivation was in the energy range of 4eV~13eV, and the maximum was 19500. The best absorption rate of 100% hydrogen passivation was in the energy range of 11.8eV~13.8eV, and the maximum was 27500. The more stable structure can be obtained by hydrogen passivation of the borophenes, and its light absorption characteristics were significantly improved. The calculation results provide theoretical guidance for the further research and development of borophenes.

Keywords

Borophenes, First-priciples, Hydrogen passivation, Energy band structure, Llight absorption characteristics.

1. Introduction

Graphene is a two-dimensional carbon nanomaterial with a hexagonal honeycomb lattice composed of carbon atoms and sp^2 hybrid orbitals. Because of its excellent optical, electrical, and mechanical properties, it has important application prospects in materials science, micro-nano processing, energy, biomedicine, and drug delivery, and is known as "the revolutionary material in the future." Borophenes has been placed high hopes by the scientific community due to its superior electrical, mechanical and thermal properties, and it may become another "magic nanomaterial" after graphene. Borophenes are similar in structure to graphene. The hexagonal network is composed of boron atoms. The center of the hexagon periodically has an

extra boron atom. The unique two-dimensional hexagonal honeycomb structure gives it the energy band of the Dirac cone. Structure and novel quantum effects. But theoretical calculations show that due to the lack of electrons, the honeycomb-shaped Borophenes cannot exist stably in the free state. Due to the unique electronic structure of boron, through the interface charge transfer between the substrate and Borophenes.

Borophenes is one of the most effective ways to obtain stable honeycomb Borophenes. It was first born not in the laboratory, but in the computer: more than 20 years ago, scientists proved the existence of Borophenes through computer simulations and predicted their properties. Graphene is formed by sp^2 hybridization of sp^2 electrons of each carbon atom to form three σ bonds, and the remaining p_z electron is perpendicular to the surface of the sheet to form a large π bond. Therefore, this hexagonal honeycomb structure The model has four valence tracks. The arrangement of the valence electrons of boron is $2s^2 2p^1$, and there are 3 valence electrons in the outer layer, one electron less than the carbon atom. If Borophenes is designed as a graphene-like structure, it means that the valence orbitals of Borophenes cannot be filled. The Borophenes system of this configuration usually tends to form multi-center bonds, which will greatly affect the properties and stability of the system Sex. The graphene-like configuration of Borophenes is very unstable, and the phonon spectrum results strongly prove this point. That is, there are more imaginary frequencies in the phonon spectrum of the hexagonal honeycomb boron monolayer, indicating that its configuration is unstable, so it is theoretically unreasonable to design Borophenes directly according to the structure of graphene.

Tang designed two new types of Borophenes, called α-sheet boron monolayer and β-sheet boron monolayer, both of which are a mixture of three-membered and six-membered rings. In addition, Tang found that changing the ratio of the three-membered boron ring to the six-membered boron ring will result in many different configurations of Borophenes, but when the ratio of the two is 12:1, the overall energy is the lowest, and the corresponding configuration the most stable, all boron atoms in this boron monolayer structure will be on the same plane, without any wrinkles on the surface of the material. Since then, new Borophenes single-layer structures have been designed, many of which are based on the nested combination of three-membered boron rings and six-membered boron rings, but the combination methods are different. For example, Zope designed a boron single-layer structure called snub-sheet, which has a slightly higher energy than α-sheet boron single-layer structure; Penev predicted several boron planes with nearly equal energy Structure (g1/8-sheet and g2/15-sheet); Boustani proposed the β12-sheet boron single-layer structure. It is worth mentioning that the particle swarm optimization algorithm to globally search for the lowest energy configuration of the boron monolayer, and found a total of more than 9,000 Borophenes structures, of which two configurations have lower energy than α-sheet Borophenes.

2. Calculation method

This paper uses the first-principles pseudo-potential plane wave method based on density functional theory to simulate and calculate the optical properties of Borophenes, and the hydrogen passivation simulation of Borophenes with 20%, 60% and 100% hydrogen passivation. All the calculations were executed using CASTEP (Cambridge serial total energy package) software package[16]. The interaction between Lonic and electeonic interaction were calculated by Ultra Soft Pseudo Potential and Norm-conserving, respectively. The exchange-correlation potential was calculated by the PBE(Perdew Burker Emzerhof) of GGA(Generalized Gradient Approximation) method, the brillouin zone integration using Monkhorst-Pack method, the K-points was set as 4×6×3, the convergence accuracy was set $1×10^{-6}$, all the calculation was in the reciprocal space.

3. Results and discussion

3.1. The absorption properties

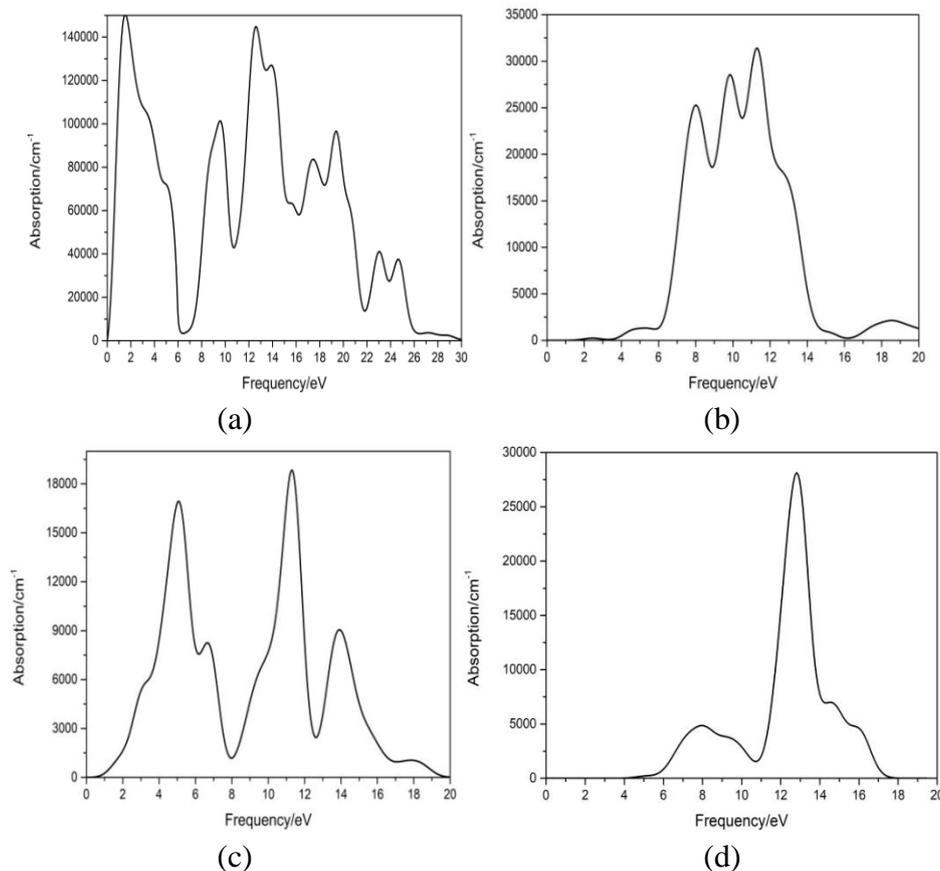$$(a) \qquad\qquad\qquad (b)$$

$$(c) \qquad\qquad\qquad (d)$$

Fig 1 the absorption of borophenes ((a) the absorption of borophenes, (b) the absorption of borophenes with 20% hydrogen passivation, (c) the absorption of borophenes with 60% hydrogen passivation, (d) the absorption of borophenes with 100% hydrogen passivation)

Figure 1(a) was the absorption spectrum of borophenes. The preliminary observation shows that the absorption spectrum fluctuates relatively greatly. In the range of 0eV~1.6eV, the absorption spectrum almost rises linearly, and the absorption spectrum is most obvious at 1.6eV. The first peak (the largest peak) appears, the absorption spectrum was decreased at 2eV~6eV, the absorption spectrum almost shows an upward trend in the range of 7.2eV~10eV, and the second peak appears at 9.1eV and the third peak at 12.8eV. The peak value tends to be stable after 16eV. So the best range of borophenes absorption was between 11.25eV~14.85eV. Figure 1(b) and Figure 1(c) are the absorption spectra of borophenes with 20% hydrogen passivation and with 60% hydrogen hydrogen passivation, respectively. There are three peaks absorption of borophenes with 20% passivation, the first peak The (minimum peak) appeared at 7.8eV, the second peak appeared at 9.65eV, and the third peak (maximum peak) appeared at 11.5eV. The best absorption rate was between 7eV and 13eV. There are four peaks in the absorption of borophenes with 60% hydrogen passivation. The first peak (the second largest peak) was at 5eV, the second peak (the smallest peak) was at 6.6eV, and the third peak (the largest peak) was at 11.eV. , The fourth peak was at 14eV, and the best absorption rate was between 4eV~13eV. Compared with the borophenes with 20% hydrogen passivation, the peak appeared red-shifted. Figure 1(d) was the absorption spectrum of the borophenes with100% hydrogen passivation. It can be seen that the light absorption effect was the best in the photoelectron range of 11.8eV~13.8eV, and the whole absorption chart shown a process of

rising and then falling in the range of 11eV~14eV, and the peak appeared at 12.8eV photoelectron, the absorption rate in other photoelectron ranges tends to be flat.

3.2.   The bond analysis

Table 1 bonding analysis of borophenes

Bond	Population	Length(A)
B1--B3	0.85	1.30952
B1--B5	0.85	1.30952
B2--B4	1.76	1.37992
B3--B5	1.44	1.38096
B4--B5	0.24	1.39512
B2--B3	0.24	1.39512
B1--B2	-0.10	1.42778
B3--B4	-0.10	1.42778
B2--B5	-0.60	2.35805
B3--B4	-0.60	2.35805

Table 1 shown the bond formation on the surface of borophenes. From the table, it can be concluded that B1 and B3 were formed a chemical bond. The bond length is 1.30952. The probability that they can bond in the entire region was 0.85. The bond length of the chemical bond formed by B2 and B4 was 1.37992 , The probability of forming a bond between the two was 1.76, the bond length of the chemical bond formed by B4 and B5 was 1.39512, the probability of forming a bond was 0.24, the bond length of the chemical bond formed by B1 and B2 was 1.42778, and the probability of forming a chemical bond was -0.10, and B1-B2 was formed an anti-bonding state. The preliminary conclusion through analysis was that there was no direct relationship between the bonding ability of a chemical bond and the bond length, and the bonding was related to the charge transfer between atoms and the relative position.

3.3.   The charge analysis

Table 2 the charge distribution table of borophenes

Species	Ion	s	p	d	f	Total	Charge(e)
B	1	0.78	0.78	0.78	0.78	3.08	3.08
B	2	0.91	0.91	0.91	0.91	2.86	2.86
B	3	0.91	0.91	0.91	0.91	3.09	3.09
B	4	0.82	0.82	0.82	0.82	2.86	2.86
B	5	2.30	2.30	2.30	2.30	3.09	3.09

Table 2 was shown the electron distribution of borophenes. From the table, we can see that the charge on the electron orbital of the s, p, d, and f states of the boron atom were 0.78, and the final electron was 3.08 , The total charge was also 3.08. For the second boron atom and the third boron atom, their charge distribution on the atomic orbitals of the s, p, d and f states were all 0.91, and the total electron of the second boron was 2.86 , The obtained electron was also 2.86, the total electron of No. 3 boron was 3.09, and the obtained electron was also 3.09. The charge distribution of No. 4 boron on the atomic orbitals of the s, p, d and f states were 0.82, and the total electron was 2.86 , The obtained electron was also 2.86, the charge distribution of the No. 5 boron atom in the s, p, d and f state atomic orbitals were 2.30, the total electron was 3.09, and the obtained electron was also 3.09.

4. Conclusion

The electronic structure and light absorption characteristics of the borophenes have been studied using the first priciples method. The results shown that the best absorption rate of 20% hydrogen passivation was in the energy range of 7eV~13eV, and the maximum was 32500. The best absorption rate of 60% hydrogen passivation was in the energy range of 4eV~13eV, and the maximum was 19500. The best absorption rate of 100% hydrogen passivation was in the energy range of 11.8eV~13.8eV, and the maximum was 27500. The more stable structure can be obtained by hydrogen passivation of the borophenes, and its light absorption characteristics were significantly improved. The calculation results provide theoretical guidance for the further research and development of borophenes.

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