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The Effect of the Light Absorption Properties of Borophenes with S-doping

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Abstract

The light absorption properties of borophene with s-doping were studied by the first-principles methods. The research shown that T the energy band structure of borophenes was formed the direct band gap with a band gap value of 1.87eV. The electrons in the valence band can easily pass through the fermi level and jump to the bottom of the conduction, and exhibited the metallic properties, with surface s-doping. The energy band structure of borophenes bulk s-doping was formed the direct band gap with a band gap value of 1.375eV. the s-doping surface makes borophenes become a conductor, and the electronic transition enhancement. The refractive index of borophenes film, the refractive index of borophenes film is always higher than the extinction coefficient. The light absorption properties of borophenes were enhanced by S-doping.

Keywords

Borophenes, First-priciples, S-doping, Light absorption.

1. Introduction

Borophenes is a two-dimensional material with a single atomic layer, which is composed of boron atoms. Boronphenes has excellent mechanical, electrical, thermal and other properties. Compared with graphene, it is stronger, more flexible, lighter, and more prone to chemical reactions, these properties were applied in the fields of sensors, batteries, and catalytic chemistry, application value. Borophenes was first born nor in a laboratory, but in a computer. Scientists proved the existence of borophenes through computer simulations and predicted their properties. The graphene is formed by sp^2 hybridization of s, p_x, p_y 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 configuration has four valence orbitals. The arrangement of the valence electrons of boron is $2s^22p^1$, 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

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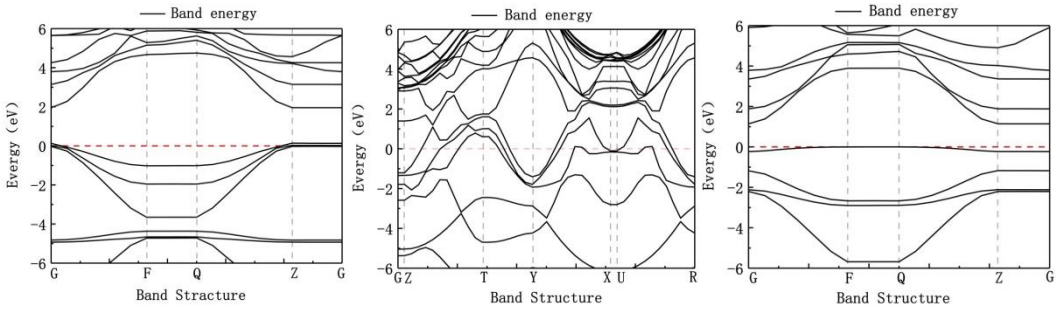
orbitals of borophenes cannot be filled. The borophenes system of this configuration usually tends to form multi-center bonds, which will greatly affect the properties and stability of the system. The graphene-like configuration of borophenes is very unstable, and the phonon spectrum results strongly 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, therefore, it is not reasonable to design borophenes directly according to the structure of graphene. Therefore, this paper proposes to realize the charge transfer between doping and borophenes through surface doping, and to inject electrons into borophenes to obtain stable honeycomb boron.

2. Calculation method

The light absorption properties of borophene with s-doping were studied by the frist principles method, 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 energy band structure of borophenes



(a) (b) (c)

Fig 1 the energy band structure diagram(a. the band structure of borophenes films, b. the band structure of borophenes surface s-doping, c. the band structure of borophenes bulk s-doping)

The figure 1 were the energy band structure of borophenes, in the fig 1(a) the energy band structure of borophenes was formed the direct band gap with a band gap value of 1.87eV. In the fig 1(b) shown that there are three energy bands cross the fermi level from the valence band to the conduction band and then return to the valence band, but there is no overlap mechanism with the conduction band. The electrons in the valence band can easily pass through the fermi level and jump to the bottom of the conduction, and exhibited the metallic properties. The fig 1(c) shown that the energy band structure of borophenes bulk s-doping was formed the direct band gap with a band gap value of 1.375eV. the s-doping surface makes borophenes become a conductor, and the electronic transition enhancement.

3.2 The light absorption characteristics of borophenes

The figure 2 were the light absorption characteristics of borophenes. The fig 2(a) shown that the absorption spectrum of borophenes film was happen in the energy range of 0.79eV~10.85eV, the spectrum overall shown the upward trend. There are three obvious peaks in this energy range, and the largest peak is 122100 at the point of 10.85eV. The absorption spectrum of s-doping in the surface was shown in the fig 2(b). The absorption spectrum was rises sharply and reaches the first peak, in

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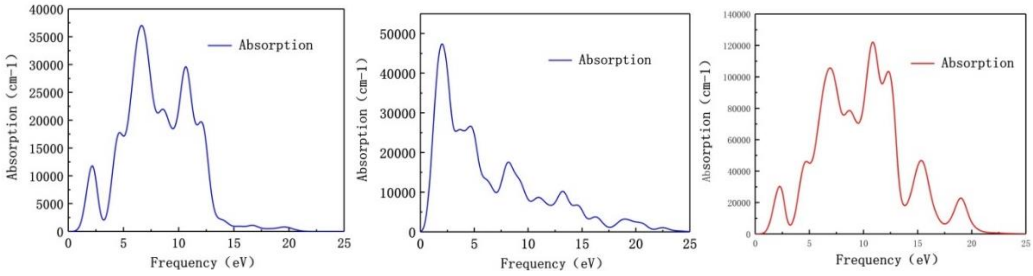
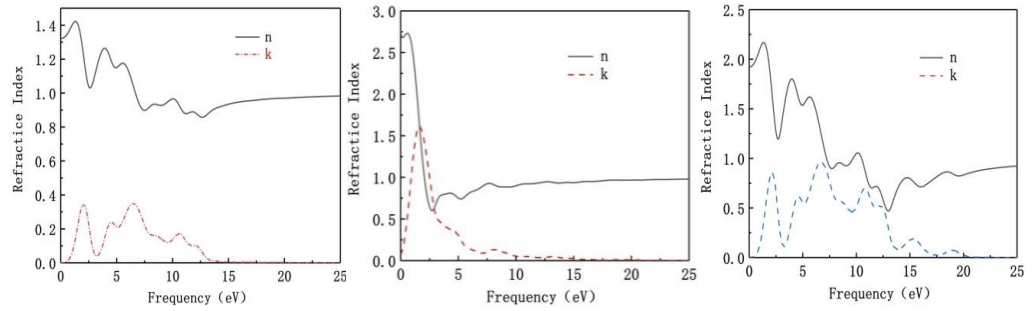
the energy range of 0eV~2.27eV. The second peak was appeared in the energy range of 3.3eV~4.77eV, and the maximum peak appear at the 7.95eV, the maximum value was 77500, after that, with the energy increase the spectrum showed the downward trend. The absorption spectrum of s-doping in the bulk was shown in the fig 2(c). the absorption spectrum was shown that the major absorption spectrum was appeared in the energy range of 0.01 eV~2.007eV, the absorption spectrum was increased from 11.24 to the maximum of 47360. In the energy range of 2.007eV~7.04eV, the absorption spectrum begin decreased which decreased from 47360 to 9514, after 7.04eV, the fluctuation of the absorption spectrum was reduced. It is concluded that the absorption sprctrum of the borophenes is reduced after s-doping.



(a) (b) (c)

Fig 2 the light absorption characteristics of borophenes (a. the band structure of borophenes films, b. the band structure of borophenes surface s-doping, c. the band structure of borophenes bulk s-doping)

3.3 The refractive index of borophenes



(a) (b) (c)

Fig 3 the refractive index of borophenes (a. the refractive index of borophenes films, b. the refractive index of borophenes surface s-doping, c. the refractive index of borophenes bulk s-doping)

The figure 3 were the refractive index of borophenes. The fig 3(a) shown that the refractive index of borophenes film, the refractive index of borophenes film is always higher than the extinction coefficient. At 1.35eV, the refractive index has a maximum value of 2.17. After 7.71eV, the refractive index was decreased, and the extinction coefficient value was increased which from 0.01 to 2.13. the first peak was appeared at the 6.69eV, the maximum was 0.962. the refractive index and extinction coefficient of the borophenes with the surface s-doping were intersect at the energy of 2.245eV and 2.68eV. The maximum peak was appeared at 0.98eV, and the value is 2.705. In the energy range of 0eV~2.245eV, the extinction coefficient was increased, the maximum peak was appeared in the 2.2245eV, and the value is 1.51. the fluctuation trend of the refractive index and the extinction coefficient were approximately the same.

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4. Conclusion

In this paper, the light absorption characteristics of borophenes with s-doping using the first principle method based on density functional theory. The results shown that the energy band structure of borophenes was formed the direct band gap with a band gap value of 1.87eV. The electrons in the valence band can easily pass through the fermi level and jump to the bottom of the conduction, and exhibited the metallic properties, with surface s-doping. The energy band structure of borophenes bulk s-doping was formed the direct band gap with a band gap value of 1.375eV. the s-doping surface makes borophenes become a conductor, and the electronic transition enhancement. The absorption spectrum of borophenes film was happen in the energy range of 0.79eV~10.85eV, the largest peak is 122100 at the point of 10.85eV. The maximum absorption spectrum of s-doping in the surface was and peak appear at the 7.95eV, the maximum absorption spectrum of s-doping in the bulk was the of 47360. The fluctuation of the absorption spectrum was reduced. It is concluded that the absorption sprctrum of the borophenes is reduced after s-doping. The refractive index of borophenes film, the refractive index of borophenes film is always higher than the extinction coefficient. The light absorption properties of borophenes were enhanced by S-doping.

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