ISSN: 2688-8645

First-Principles Study of Novel Two-dimensional Materials Cr_4BA (A=C, N)

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Abstract

For material research, it is important to have an in-depth understanding of the basic laws of crystal structure. For materials, their properties are inextricably linked to their structure, that is, the structure determines the properties, which in turn affects their application. Therefore, the study of the electronic properties of materials is more helpful for us to understand and apply the properties of materials. The electronic properties of novel two-dimensional materials Cr_4BA (A=C, N) predicted based on first-principles were studied, namely, the phonon spectrum, band structure, and density of states of the two-dimensional materials Cr_4BA (A=C, N) were analyzed. It is shown that the Cr_4BA (A=C, N) structure has metallic properties and dynamic stability.

Keywords

Two-dimensional Structure; First Principles; Energy Band Structure; Density of States.

1. Introduction

Environmental protection and sustainable development are key pillars of social development today [1]. Reducing carbon emissions and promoting the widespread use of clean energy are important measures to address pollution, climate change, and global clean energy demand and storage [2]. Rechargeable ion batteries, especially lithium-ion batteries [3,4], have become an important technology in the field of clean energy storage and have received much attention in current research. However, for batteries with high capacity requirements, existing materials cannot meet the needs. Therefore, there is an urgent need to develop high-performance anode materials with high storage capacity.

The discovery of graphene in 2004 opened up new avenues for researchers to study two-dimensional materials [5]. A large number of 2D materials have been reported, such as graphene derivatives (reduced graphene oxide and graphene oxide) [6], graphene-like materials (phosphorene, borophene, silicene, germanene) [7-9]. Numerous studies have shown that two-dimensional materials can provide higher battery charge and discharge rates and the theoretical specific capacity of batteries [10, 11]. Some typical two-dimensional materials are introduced below.

Graphene is a layered two-dimensional material that exhibits a honeycomb-like hexagonal morphology. It has the advantages of high mechanical strength, electrical conductivity, thermal conductivity, and chemical stability. However, there are still some problems in its practical application, such as the high preparation cost of graphene, and the need to improve the stability and purity of the finished product.Therefore, there is a need for further research and development of efficient, stable, and low-cost two-dimensional materials.

Phosphorene is a two-dimensional material composed of phosphorus atoms, similar to graphene. The most significant feature of phosphorene is its advantages, such as high mechanical strength, electrical conductivity, thermal conductivity, and optical properties. However, due to the relatively complex preparation process and technical difficulties,

ISSN: 2688-8645

phosphorene is currently still in the research stage, and its application prospects remain to be further explored [12, 13].

Two-dimensional MXenes represent a large family of two-dimensional materials with the chemical formula $M_{n+1}X_nT_x$, where M is a transition metal and T_x represents the functional groups introduced on its surface during the synthesis of MXenes. A class of boron carbides called X_2BC (where X = Mo, V, Nb, Ta, and W) has attracted attention due to its unique hybrid properties.

Inspired by these studies, a novel and unexplored two-dimensional Cr_4BA (A=C, N) material was investigated.

2. Computational Methods

In the past 20 years, first-principles calculation methods have been widely used in the research and development of new materials, and have become one of the most important methods in computational materials science today. Using the first-principles calculation method, the physical properties of two-dimensional materials Cr_4BC and Cr_4BN as anode materials for lithium-ion batteries are calculated and studied. In structural optimization, the plane wave cutoff energy is set to 500 eV, the energy convergence criterion is set to 1.0×10^{-7} eV, and the stress convergence criterion acting on each atom in the system is -0.01 eV/Å. The k-point for calculating the properties of the primitive cell structure and electronic structure is set to 14×8×1. In order to eliminate the van der Waals force interaction between layers, a vacuum layer of 25 Å was set in the c-axis direction.

For data processing, the crystal structure was analyzed using the modeling software VESTA, first-principles calculations were performed using the software VASP, and the energy band structure data and density of states data obtained from the calculations were processed using Origin software for plotting to obtain corresponding graphs.

3. Results and Discussion

3.1. Structural Analysis

The Cr_4BA (A=C, N) structure possesses an orthorhombic crystal structure with the Pmm2 space group. The optimized monolayer structure consists of three atomic layers arranged as Cr-A/B-Cr, similar to transition metal dichalcogenides MoS_2 and WS_2. The top and side views of the optimized structure are shown in Figures 1 and 2.

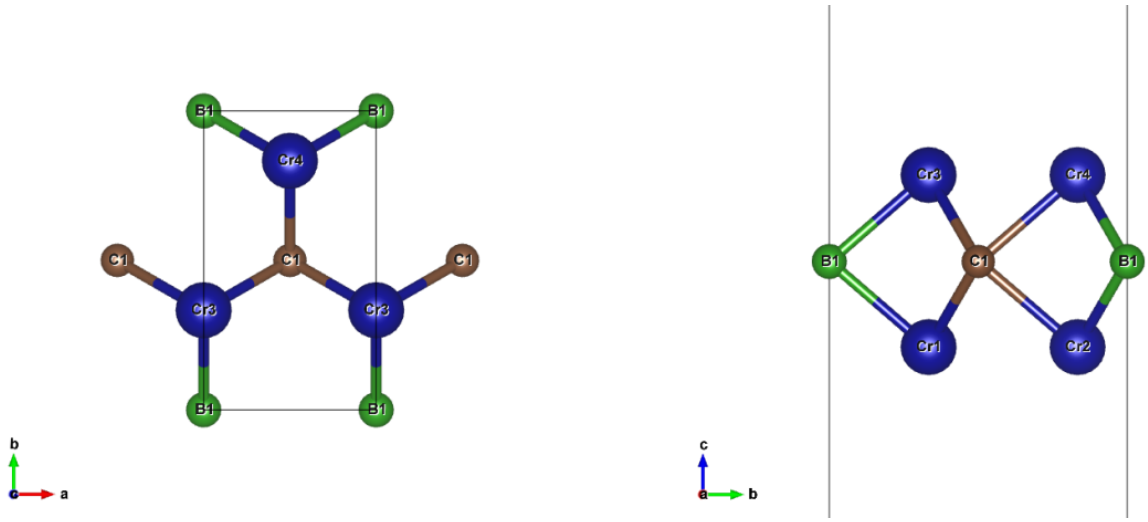

Fig 1. Top and side views of the optimized crystal structure of Cr_4BC.

ISSN: 2688-8645

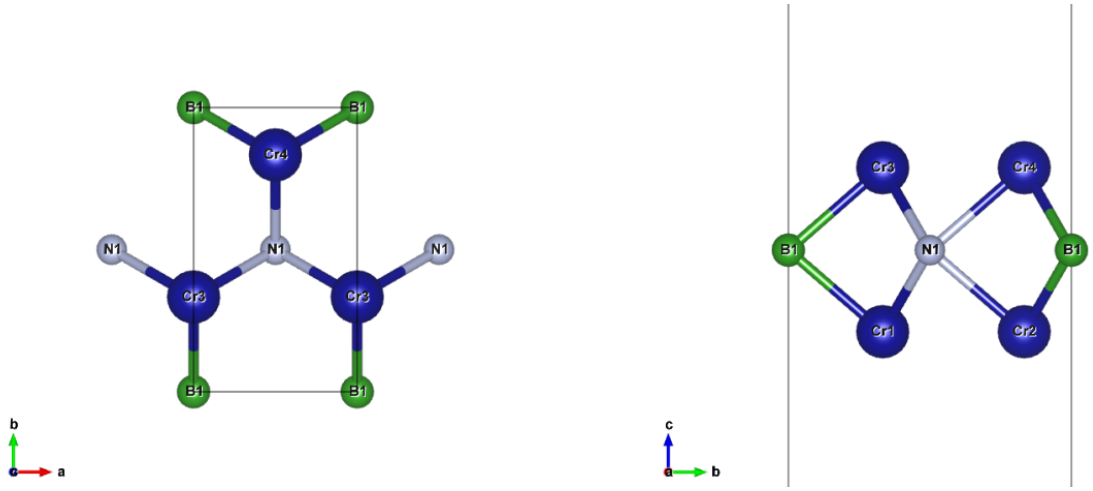

Fig 2. Top and side views of the optimized crystal structure of Cr_4BN

3.2. Band Structure and Density of States Analysis

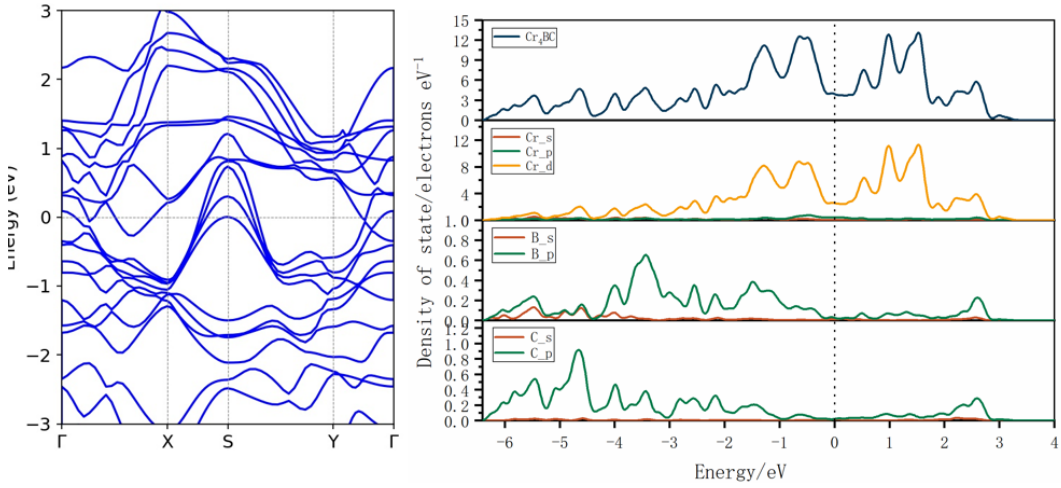

Fig 3. Cr_4BC band structure and density of states.

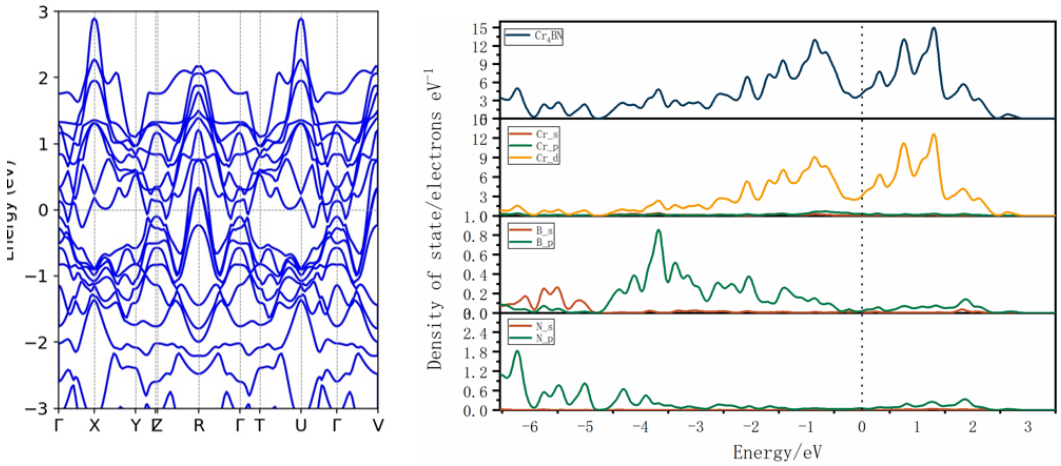

Fig 4. Cr_4BN band structure and density of states.

The band structures and density of states of Cr_4BC and Cr_4BN were calculated, and the results are shown in Figures 3 and 4. The density of states diagram and the band structure diagram correspond to each other, and the density of states diagram is a visualization of the band

ISSN: 2688-8645

structure. According to the electronic density of states (DOS), the distribution of electronic energy levels in the energy band can be understood. According to the band structure diagram, Cr_4BA (A=C, N) has no band gap, so its property is metallic. By analyzing the total density of states (DOS) and partial density of states (PDOS) of Cr_4BC and Cr_4BN, the valence bond properties and electronic properties of Cr_4BC and Cr_4BN are analyzed. The electronic density of states value at the Fermi level $E_F > 0$, indicating metallic properties, which is consistent with the results shown in the band structure diagram.

Meanwhile, the DOS at the Fermi level is mainly contributed by the Cr-3d orbitals. The results show that Cr_4BA (A=C, N) has good electrical conductivity and dynamic stability.

3.3. Phonon Spectrum Calculation and Analysis

The calculated phonon spectrum results are shown in Figure 5. No imaginary frequency was found in Cr_4BC and Cr_4BN, indicating that they have dynamic stability.

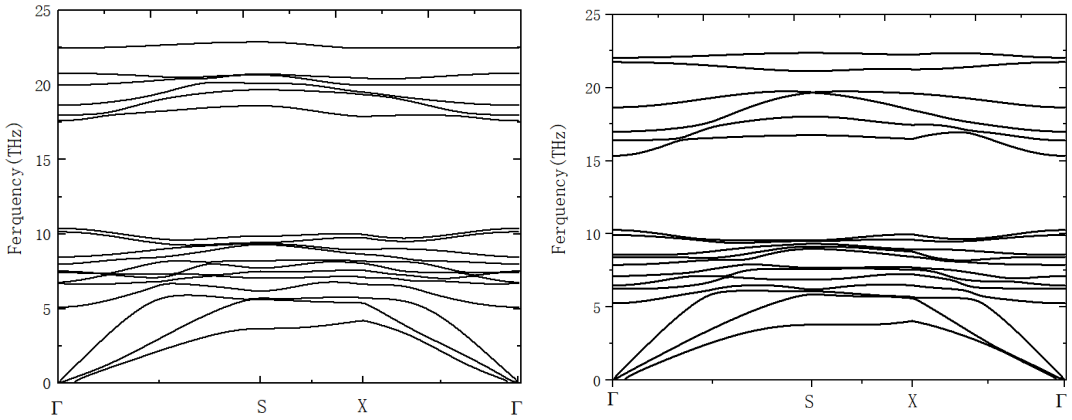

Fig 5. Phonon spectra of Cr_4BC and Cr_4BN

4. Conclusion

This article studies the electronic properties of the predicted novel two-dimensional materials Cr_4BA (A=C, N) based on first-principles, that is, analyzes the phonon spectrum, band structure, and density of states of the two-dimensional materials Cr_4BA (A=C, N). The results show that:

The Cr_4BA (A=C, N) structure has an orthorhombic crystal structure with the Pmm2 space group. The optimized monolayer structure consists of three layers of atoms arranged as Cr-A/B-Cr.

The band structure and density of states diagrams show that Cr_4BA (A=C, N) has metallic properties.

The phonon spectrum shows that Cr_4BA (A=C, N) has dynamic stability, providing a theoretical reference for subsequent research.

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