

Phosphorene: A Promising Two-Dimensional Material for Advanced Electronic Applications

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Abstract

Phosphorene, a two-dimensional material, has garnered significant attention for its promising applications in optoelectronics due to its unique electronic properties. In this study, we employed Density Functional Theory (DFT) calculations, using the Quantum Espresso package, to investigate the electronic structure of phosphorene with an orthorhombic structure. The calculations utilized ultrasoft pseudopotentials and the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional, with a k-point mesh of $20 \times 20 \times 1$ and a vacuum of 10 \AA along the z-axis to mitigate interlayer interactions. Our results revealed a direct band gap of $E_g = 0.9 \text{ eV}$ at the Gamma point, as confirmed by both the band structure and density of states (DOS) analyses. This direct band gap is particularly advantageous for optoelectronic applications such as light-emitting diodes (LEDs) and photodetectors, where efficient electron-hole recombination is crucial. The high density of states near the band edges suggests enhanced optical absorption and emission properties, making phosphorene a promising candidate for next-generation photodetectors and solar cells. Our findings provide a deeper understanding of the electronic properties of phosphorene, highlighting its potential for various optoelectronic applications.

Keywords: Phosphorene; DFT; Electronic properties

Introduction

The landmark discovery of graphene in 2004 by Novoselov and Geim [1] revolutionized materials science. They succeeded in isolating a single layer of carbon atoms arranged in a hexagonal lattice from graphite, a breakthrough that earned them the Nobel Prize in Physics in 2010 [2]. Graphene's remarkable attributes, such as outstanding electrical and thermal conductivity [3], high transparency [4], and superior mechanical strength [5], have led to extensive research and various applications in fields like electronics, photovoltaics, energy storage devices [6-9], and biomedical sciences [10].

The remarkable achievements of graphene have sparked a wave of interest in two-dimensional (2D) materials [11-16], leading to the discovery of numerous other 2D materials such as hexagonal boron nitride (h-BN) [17], MXenes [18], carbon nitride [19], transition metal oxides [20], elemental 2D materials like germanene, silicene, and stanene, and transition metal dichalcogenides (TMDs) [21, 22]. These materials exhibit diverse physical, chemical, and electronic properties, making them promising candidates for advancing post-silicon device technologies. Among them, molybdenum disulfide (MoS₂) is particularly noteworthy [23], as it offers a tunable bandgap ranging from 1.8 eV in monolayers to 1.2 eV in the bulk state. However, despite its impressive ON/OFF ratio in devices, MoS₂ has lower charge carrier mobility compared to graphene.

Phosphorene, a single layer derived from black phosphorus [24-26], stands out as an exciting addition to the 2D material family due to its impressive optical absorption, high carrier mobility, and distinctive anisotropic orthorhombic crystal structure. These attributes confer phosphorene with exceptional mechanical [27-34], electronic [35-37], optical [38-42], and transport properties, making it a compelling candidate for electronic and optoelectronic applications. Recent progress in the synthesis, functionalization, and deployment of phosphorene-based devices highlights its potential for high-speed electronics, optoelectronics, and emerging biomedical applications.

In this article, we present the results of density functional theory (DFT) calculations performed using the Quantum Espresso package, which reveal the presence of a direct band gap in phosphorene. This finding underscores phosphorene's potential as a highly promising 2D material for diverse technological applications. Our study contributes to the growing body of research on phosphorene, aiming to deepen the understanding of its unique properties and foster future advancements in the field of 2D materials.

Computational Methods

Density Functional Theory (DFT) is a crucial computational method in materials science, widely used for predicting and understanding the electronic structures of various materials. By solving the Kohn-Sham equations, DFT allows for the determination of ground state properties of many-electron systems, balancing accuracy and computational efficiency. This approach employs the exchange-correlation functional to effectively account for electron-electron interactions, making it highly effective for investigating a broad spectrum of materials.

The electronic structure of phosphorene was investigated using Quantum Espresso, a highly regarded open-source plane-wave DFT code [43]. This software is known for its efficient solution of the Kohn-Sham equations, utilizing plane-wave basis sets and pseudopotentials. Quantum Espresso's parallelization capabilities allow for the handling of complex systems with large supercells and dense k-point grids. Ultrasoft pseudopotentials of the Rappe, Rabe, Kaxiras, and Joannopoulos type were applied, with a cutoff energy of 544.23 eV. The exchange-correlation effects were incorporated using the Perdew-Burke-Ernzerhof (PBE) functional within the Generalized Gradient Approximation (GGA) [44]. For the self-consistent field (SCF) calculations, the energy convergence threshold was set to 10⁻⁵ eV.

For our model system, we utilized the orthorhombic structure of phosphorene, depicted in Figure 1. We sampled the Brillouin zone with a dense Monkhorst-Pack grid of 20 × 20 × 1 k-points to ensure precise integration over the reciprocal space. To prevent interactions between periodic images and accurately represent the two-dimensional characteristics of phosphorene, we included a vacuum layer of 10 Å along the z-axis. Periodic boundary conditions were enforced in the x and y directions, while a vacuum of 10 Å was applied along the z-axis. This approach effectively isolates the phosphorene layers, enabling us to investigate their inherent electronic properties without the influence of boundary effects.

The total energy of the system was calculated using the Kohn-Sham equations:

$$E_{\text{total}} = \sum_i f_i \langle \psi_i | \hat{H}_{KS} | \psi_i \rangle + E_{\text{xc}}[n] + E_{\text{ion}} \quad (1)$$

where f_i is the occupation number, ψ_i are the Kohn-Sham orbitals, \hat{H}_{KS} is the Kohn-Sham Hamiltonian, $E_{xc}[n]$ is the exchange-correlation energy functional, and E_{ion} is the ion-ion interaction energy. The electronic density $n(\mathbf{r})$ was obtained from the Kohn-Sham orbitals as:

$$n(\mathbf{r}) = \sum_i f_i |\psi_i(\mathbf{r})|^2 \quad (2)$$

The self-consistent field (SCF) cycle aimed to minimize the total energy, iterating until the change in total energy between cycles was below the threshold of 10^{-5} eV.

By employing these computational methods, we ensured accurate and reliable results for the electronic properties of phosphorene, paving the way for a deeper understanding of its potential applications in optoelectronic devices.

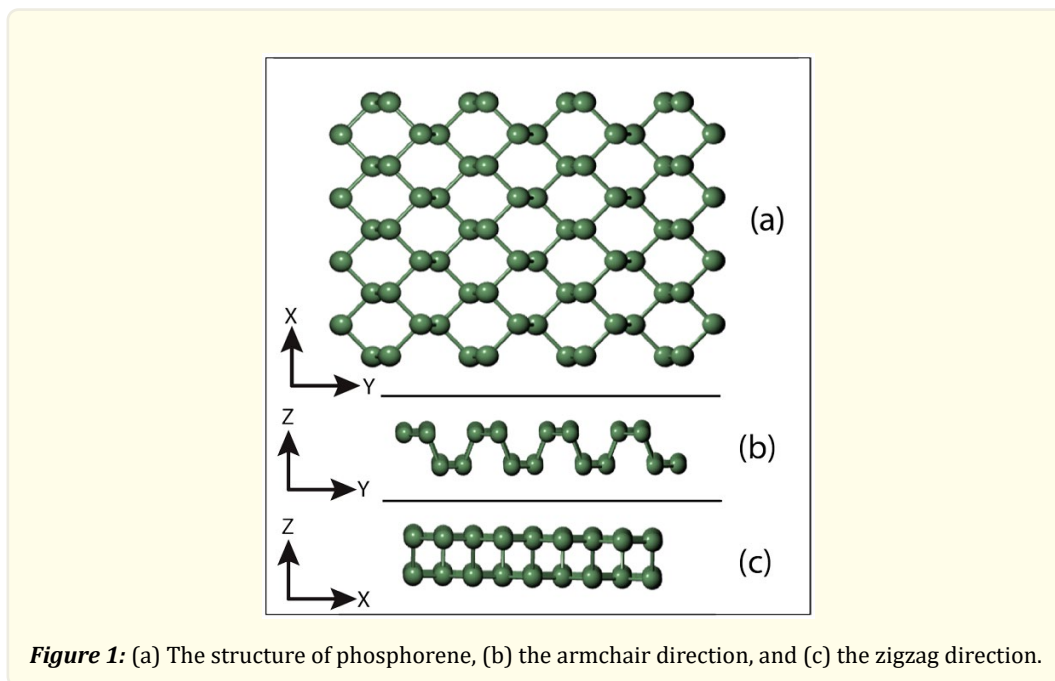


Figure 1: (a) The structure of phosphorene, (b) the armchair direction, and (c) the zigzag direction.

Results and Discussion

We utilized density functional theory (DFT) calculations with the Quantum Espresso package to explore the electronic properties of phosphorene. The calculated band structure and density of states (DOS) provide valuable insights into the electronic characteristics of this two-dimensional material. As depicted in Figure 2, the band structure of phosphorene shows a direct band gap at the Gamma point with a value of $E_g = 0.9$ eV. This direct band gap is essential for optoelectronic applications, such as light-emitting diodes (LEDs) and photodetectors, where efficient electron-hole recombination is vital. Our results are consistent with previous studies, such as those by Liu et al. [45] and Li et al. [46], which also reported a direct band gap in phosphorene, supporting its potential for optoelectronic uses. Additionally, Rudenko and Strelkov [47] corroborate the presence of a direct band gap and discuss its implications for electronic properties.

The DOS plot (Figure 2) aligns with the band structure results, indicating a distinct separation between the valence band maximum and the conduction band minimum, which confirms the direct band gap nature. The pronounced peaks in the DOS near the band edges indicate a high density of states, potentially enhancing optical absorption and emission properties. This increased optical activity is especially beneficial for applications in photodetectors and solar cells, where a high density of electronic states can lead to better device performance.

The direct band gap of 0.9 eV makes phosphorene a promising material for numerous optoelectronic applications [48-50]. Phosphorene's efficient photon absorption and electron-hole pair generation can be harnessed in photodetectors, where its direct band gap ensures high quantum efficiency, enabling detection of light over a wide spectral range. Additionally, the direct band gap favors efficient electron-hole recombination, which is advantageous for LED applications, potentially enabling phosphorene-based LEDs to emit light from the infrared to the visible spectrum, depending on specific band gap modifications.

Moreover, phosphorene's direct band gap can be adjusted to enhance solar absorption, positioning it as a promising candidate for solar cell applications. Incorporating phosphorene into solar cell designs can improve light harvesting capabilities, potentially leading to higher power conversion efficiencies. As a two-dimensional material, phosphorene's flexibility allows it to be used in flexible optoelectronic devices. Its combination of mechanical and electronic properties makes it suitable.

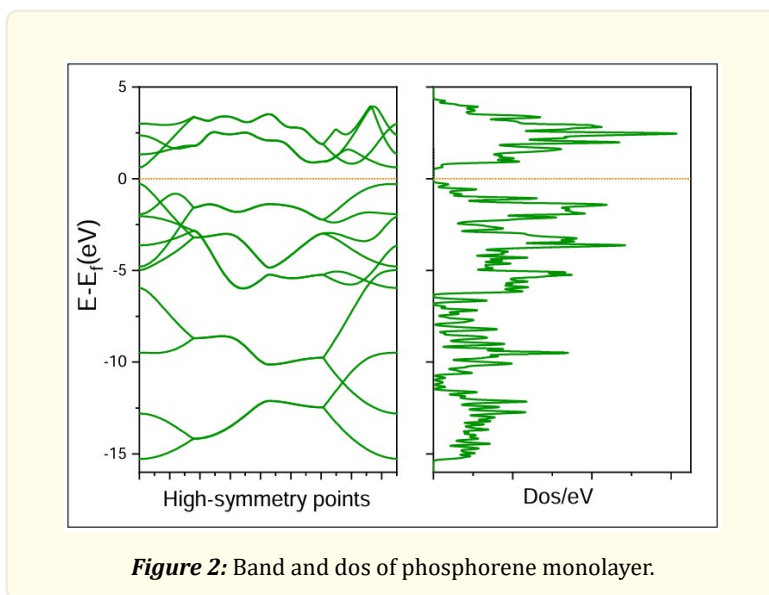


Figure 2: Band and dos of phosphorene monolayer.

Conclusion

In this study, we investigated the electronic properties of phosphorene using Density Functional Theory (DFT) calculations with the Quantum Espresso package. Our findings revealed a direct band gap of $E_g = 0.9$ eV at the Gamma point, highlighting phosphorene's potential for optoelectronic applications. The detailed analysis of the band structure and density of states (DOS) indicated significant electronic properties, such as high optical absorption and emission capabilities, which are essential for developing efficient light-emitting diodes (LEDs) and photodetectors. Moreover, the high density of states near the band edges suggests that phosphorene could substantially enhance solar cell performance. This work provides a comprehensive understanding of phosphorene's electronic behavior, paving the way for further research and development in the field of two-dimensional materials. Our insights underscore phosphorene's suitability for next-generation optoelectronic devices, highlighting its promising future in various high-performance applications.

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