Analysis of Phosphorus-doped and defect graphene

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Devices and Modelling

Mukesh Mandal

Under Guidance of
Dr. SUSHMITA DANDELIYA

Abstract

Graphene, a two-dimensional carbon allotrope, has garnered substantial attention in recent years due to its exceptional electronic, mechanical, and thermal properties. However, enhancing its electronic properties for specific applications, such as semiconductor devices, remains a challenge. This study focuses on the computational design and simulation of phosphorus-doped and defect-containing graphene nanosheets (P-dGNS) for advanced electronics using ATK Virtual NanoLab software. The incorporation of phosphorus atoms into the graphene lattice introduces localized electronic states, leading to controlled bandgap engineering. Simultaneously, the introduction of defects further augments the tunability of electronic properties. We discuss the computational techniques employed within ATK Virtual NanoLab for modeling and simulating P-dGNS, considering various synthesis conditions. This software-enabled approach offers insights into the structural and electronic characteristics of P-dGNS. Furthermore, we elucidate the potential applications of computationally designed P-dGNS in field-effect transistors, sensors, and energy storage devices. This research showcases the power of computational tools like ATK Virtual NanoLab in accelerating the discovery and design of innovative materials for advanced electronics.

Keywords: graphene, phosphorus doping, defects, nanosheets, advanced electronics, computational design, simulation, ATK Virtual NanoLab, field-effect transistors, sensors, energy storage.

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Introduction

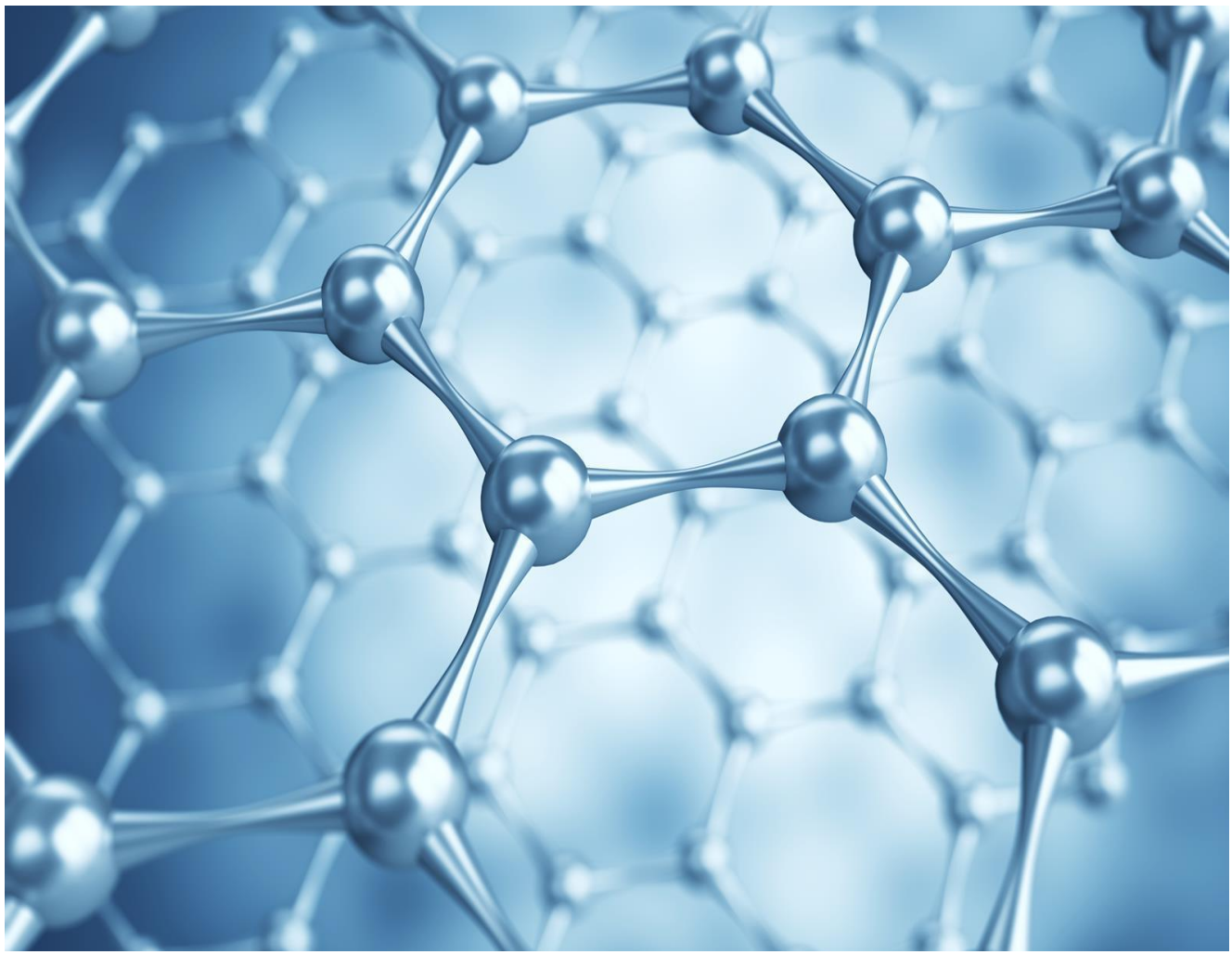
In the quest for advanced electronic materials, graphene, a single layer of carbon atoms arranged in a hexagonal lattice, has emerged as a remarkable candidate. Its exceptional electrical conductivity, mechanical strength, and thermal properties have made it the focus of extensive research. However, harnessing graphene's potential for specific electronic applications requires the ability to tailor its electronic properties, particularly by introducing bandgaps, a critical feature in semiconductor devices. One promising approach to achieve this is through phosphorus doping and the strategic introduction of defects into graphene nanosheets.

This project delves into the realm of advanced materials engineering by employing ATK Virtual NanoLab, a powerful computational tool, to design, model, and simulate phosphorus-doped and defect graphene nanosheets (P-dGNS). The incorporation of phosphorus atoms into the graphene lattice introduces localized electronic states, enabling the controlled modulation of its electronic band structure. Concurrently, the introduction of defects enhances the tunability of electronic properties, allowing us to fine-tune graphene's behavior for specific applications.

The use of ATK Virtual NanoLab facilitates a precise and efficient exploration of the structural and electronic characteristics of P-dGNS under various synthesis conditions. It provides a platform to visualize and analyze the effects of phosphorus doping and defects on

graphene's electronic structure, opening the door to a wealth of innovative possibilities in the field of advanced electronics.

This project aims to not only unravel the theoretical intricacies of phosphorus-doping and defect engineering in graphene but also to bridge the gap between computational design and practical applications. By investigating the potential of computationally designed P-dGNS in devices like field-effect transistors, sensors, and energy storage systems, it paves the way for the creation of materials that are custom-tailored for the next generation of electronic technologies.

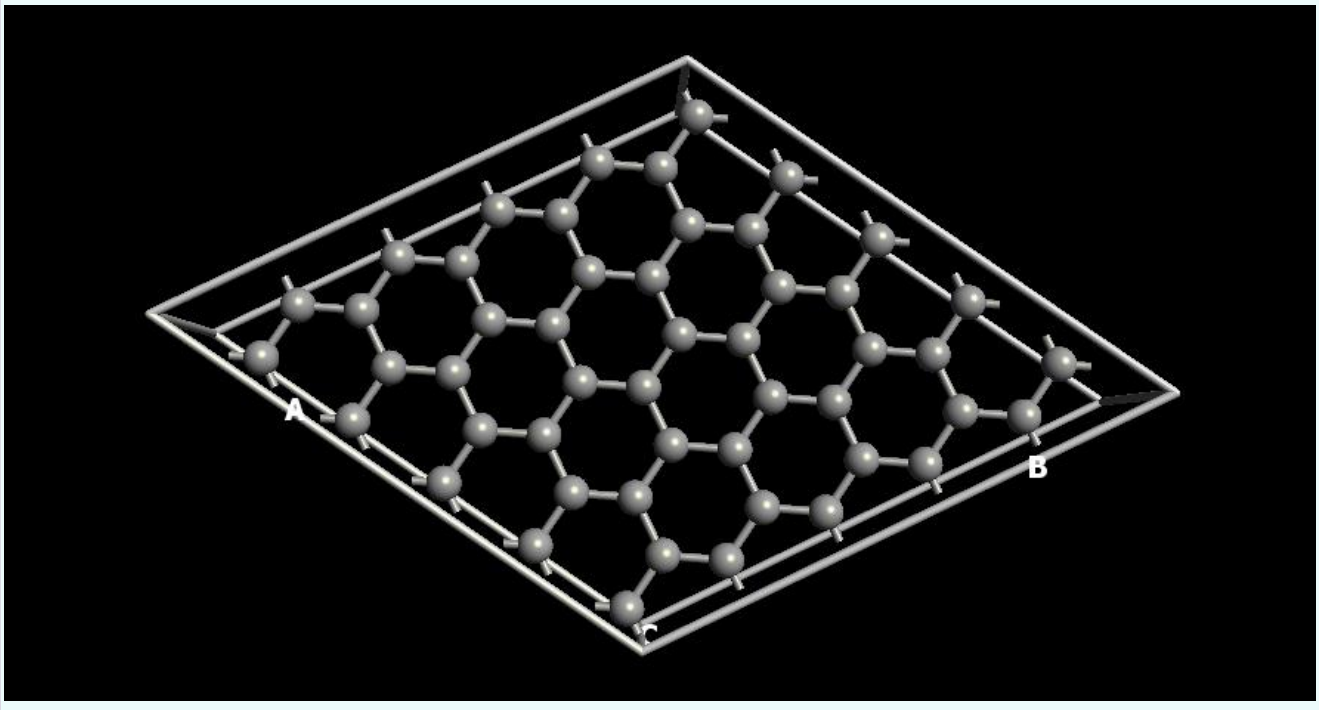


Structure Modelling

In this phase of the project, we employed ATK Virtual NanoLab to model and visualize six distinct structures, each designed to explore the effects of phosphorus doping and defects on graphene sheets. The hexagonal lattice structure, inherent to graphene, served as our baseline for comparison. The structures we modeled are as follows:

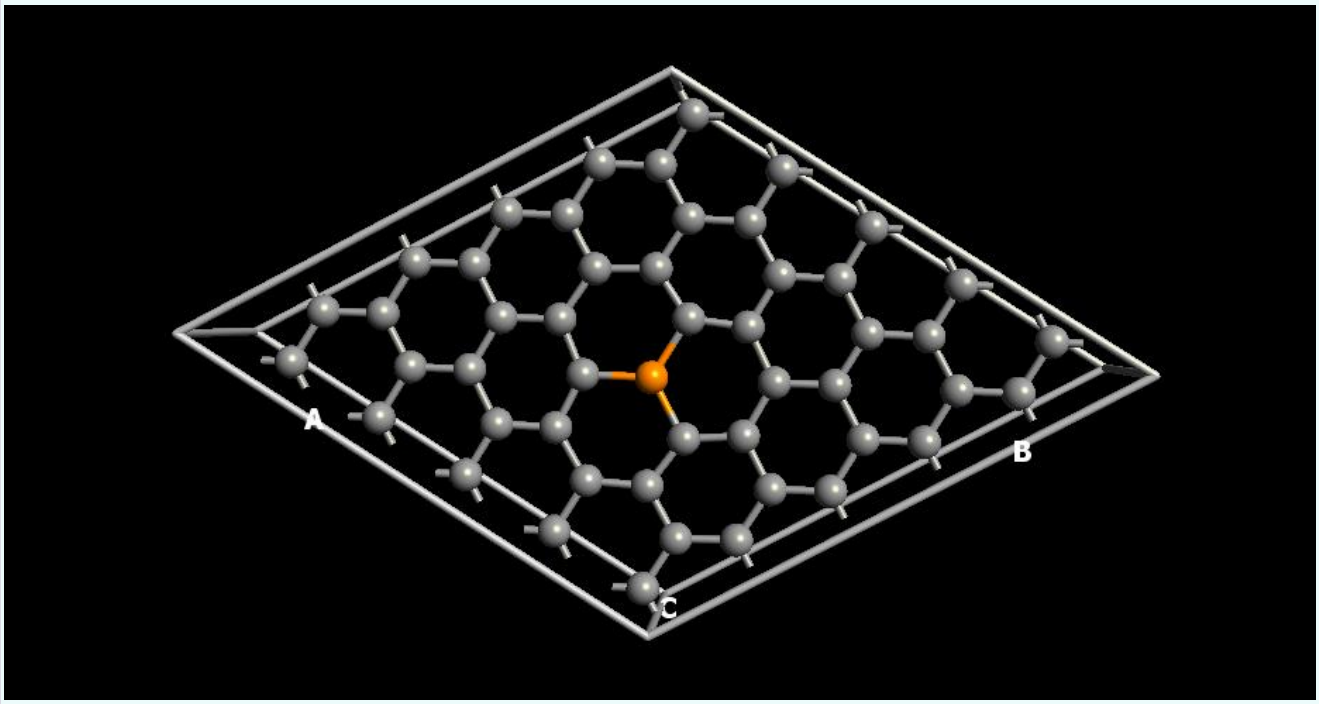
1. Graphene Sheet

Our foundational structure is the pristine graphene sheet, consisting of a single layer of carbon atoms arranged in a perfect hexagonal lattice (as shown in Figure 1). This structure represents the idealized graphene structure, known for its extraordinary electrical conductivity.



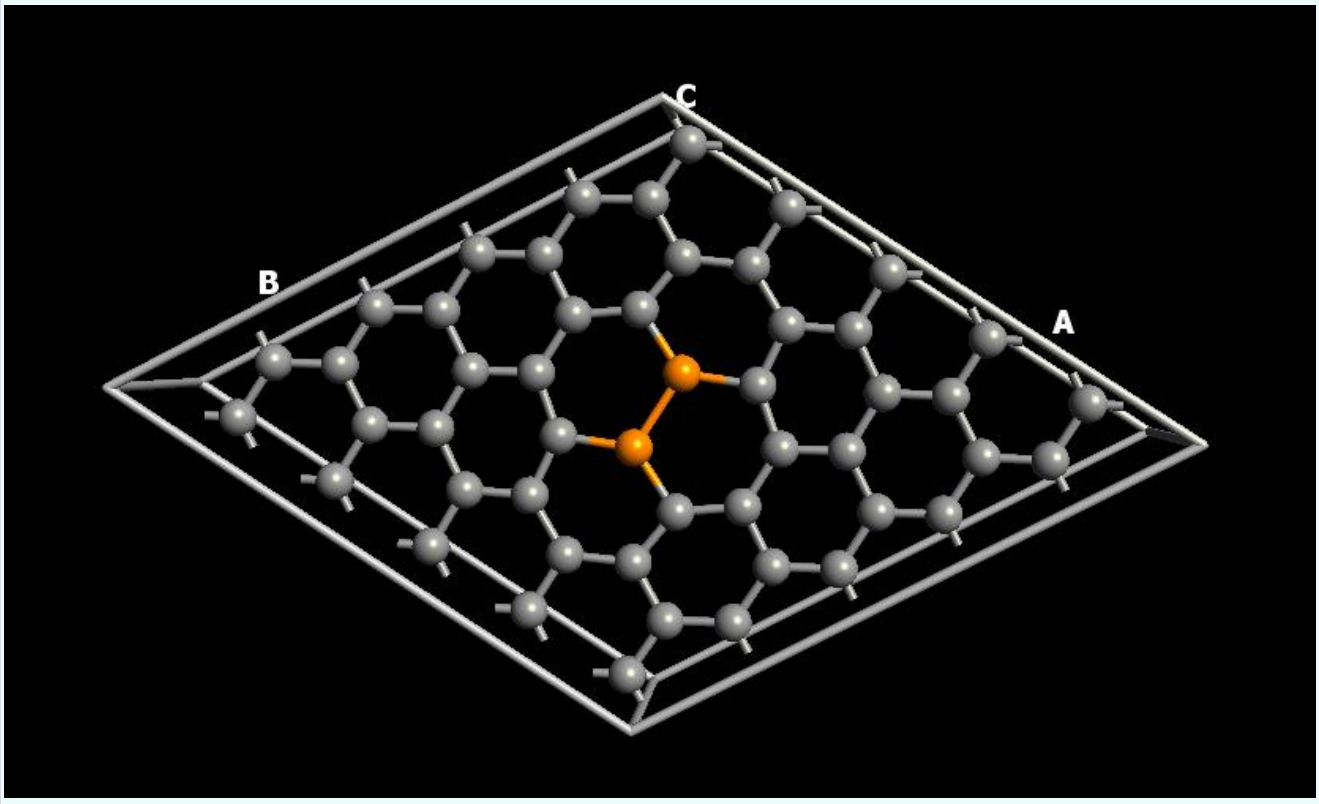
2. 1 Phosphorus Atom Doped Graphene Sheet

In this model, we introduced a single phosphorus atom into the graphene lattice. Phosphorus doping introduces localized electronic states, influencing the electronic band structure. This serves as the starting point for exploring controlled bandgap engineering (Figure 2).



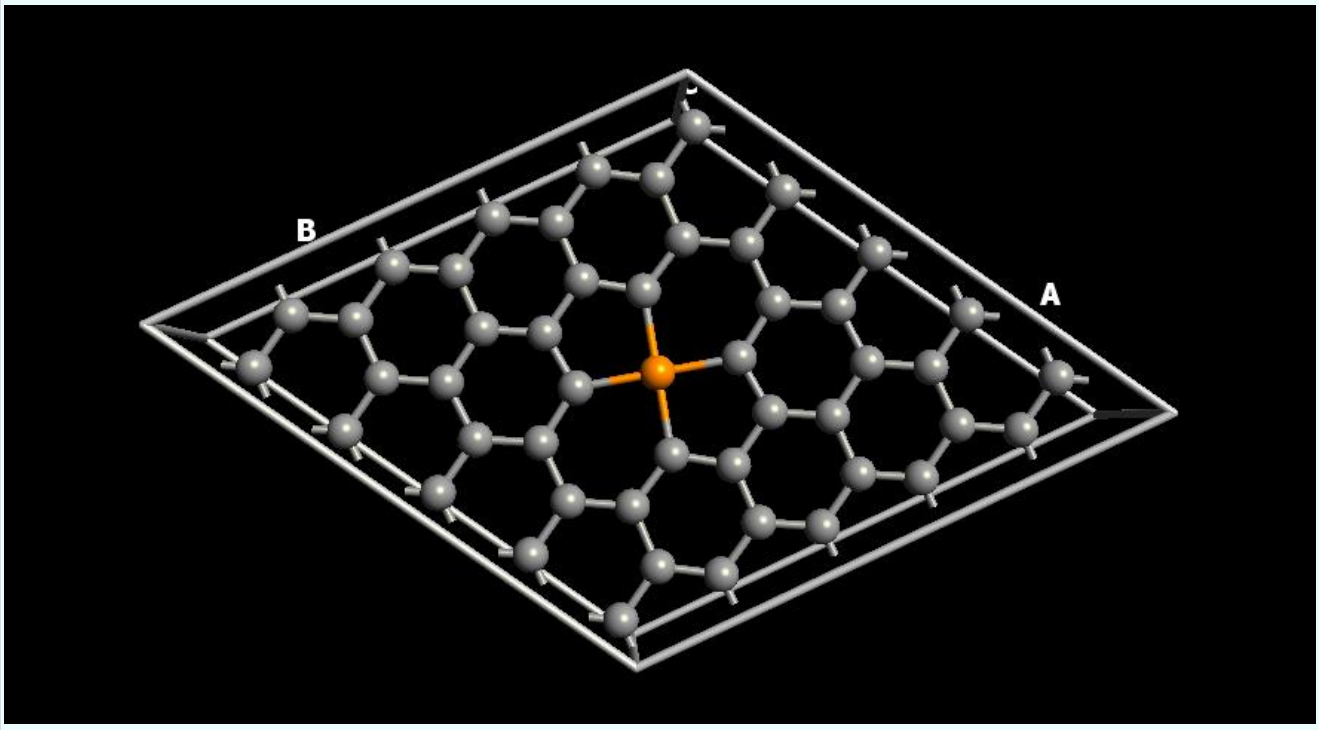
3. 2 Phosphorus Atoms Doped Graphene Sheet

Expanding on the previous model, we incorporated two phosphorus atoms into the graphene structure. This increased doping level further enhances the potential for bandgap engineering, a crucial aspect for semiconductor applications (Figure 3).



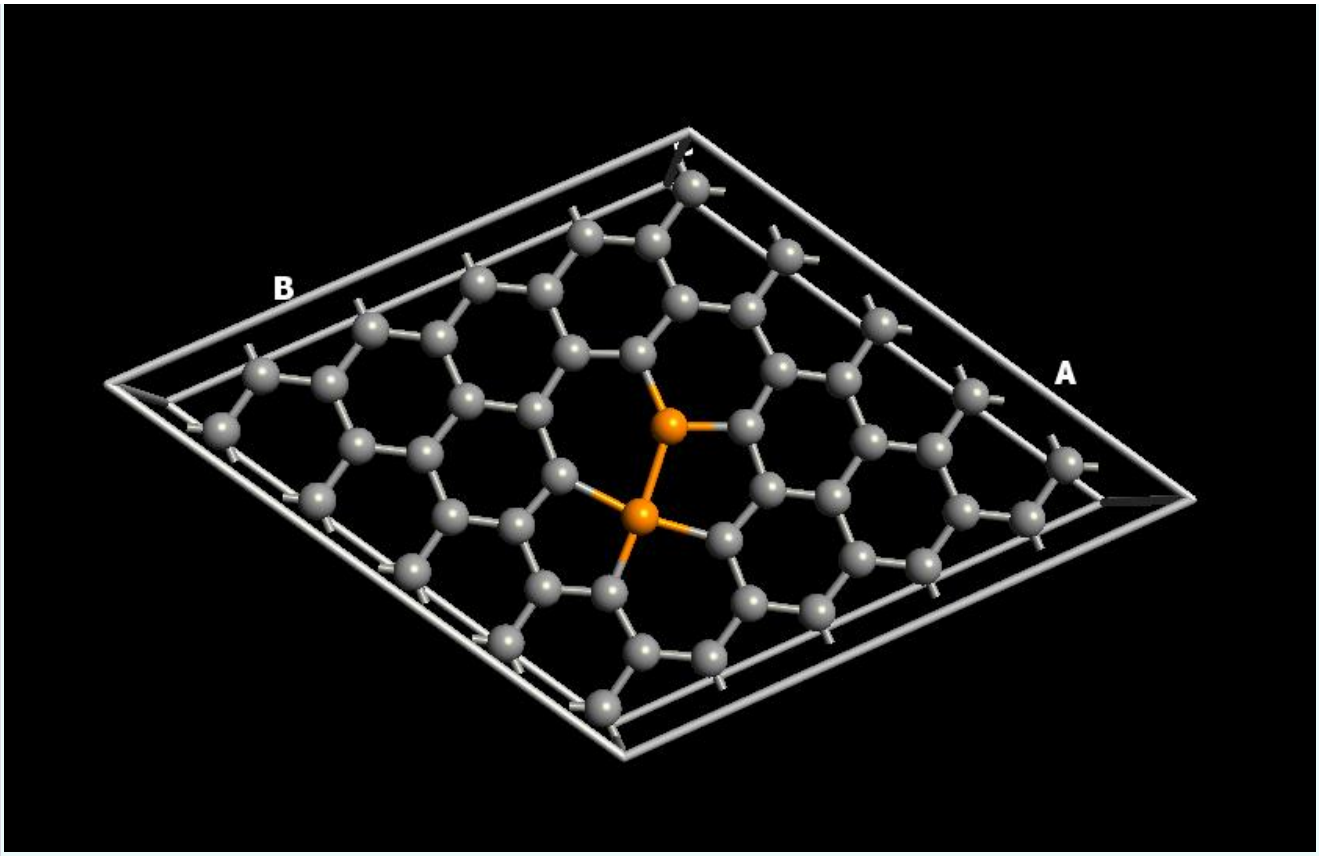
4. 1 Phosphorus Atom Doped Graphene with 1 Carbon Atom Defect

In this structure, we introduced a single carbon atom defect alongside the phosphorus doping. The defect's presence impacts the local electronic structure, which can be advantageous in certain applications (Figure 4).



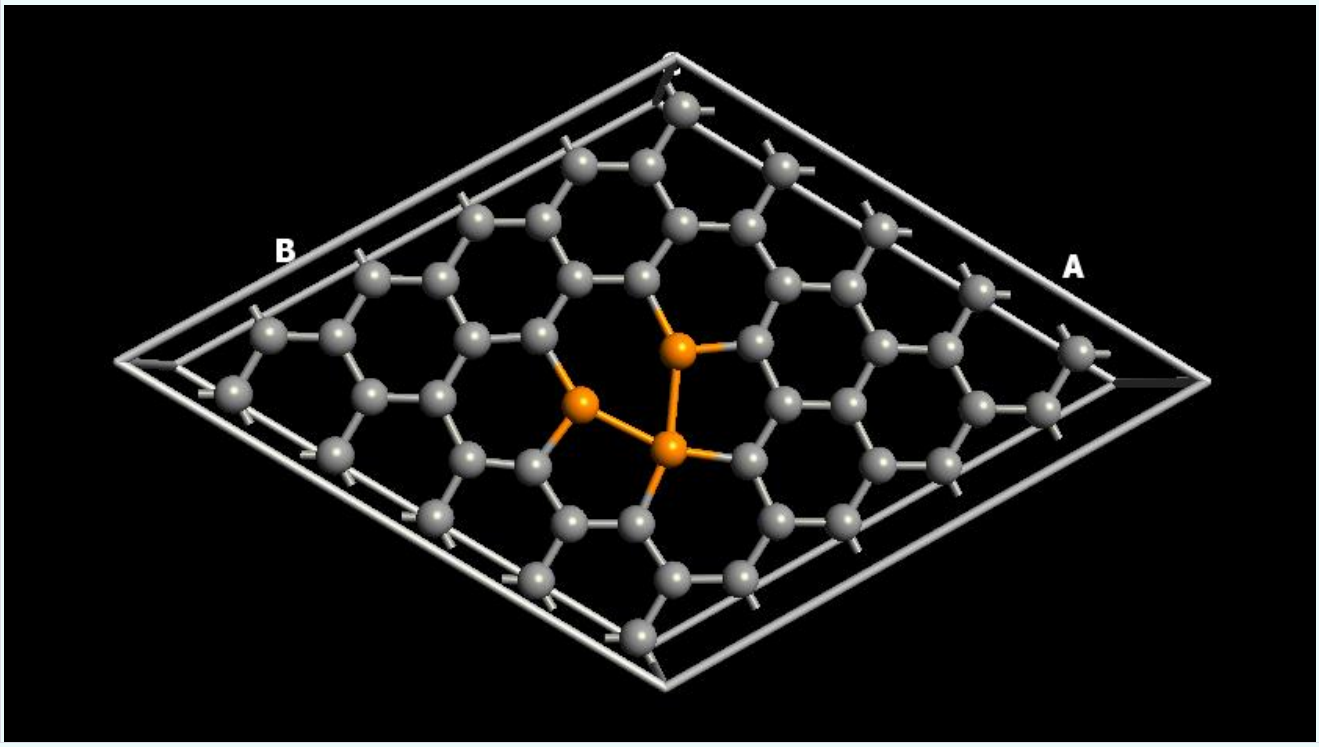
5. 2 Phosphorus Atoms Doped Graphene with 1 Carbon Atom Defect

Building upon the previous model, we incorporated two phosphorus atoms alongside a single carbon atom defect. This composite structure allows us to study the synergistic effects of phosphorus doping and defects (Figure 5).



6. 3 Phosphorus Atoms Doped Graphene with 1 Carbon Atom Defect

In this advanced structure, we introduced three phosphorus atoms alongside a single carbon atom defect. The increased phosphorus doping level and the presence of defects offer deeper insights into the tunability of graphene's electronic properties (Figure 6).



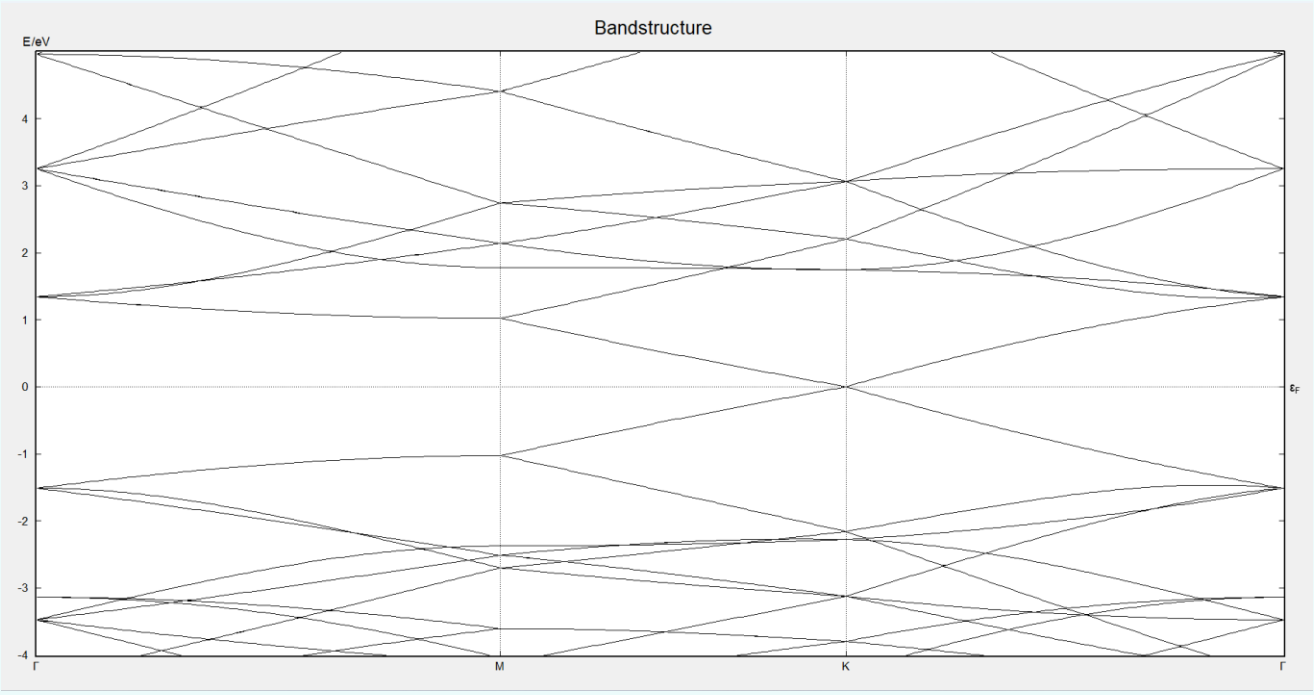
By modelling and visualizing these six distinct structures, we have established a comprehensive foundation for investigating the effects of phosphorus doping and defects on graphene's electronic properties. The subsequent simulation and analysis will provide further insights into how these structures can be tailored for specific applications in advanced electronics.

Simulation Result and Analysis

Bandstructure and Density of states(DOS) analysis

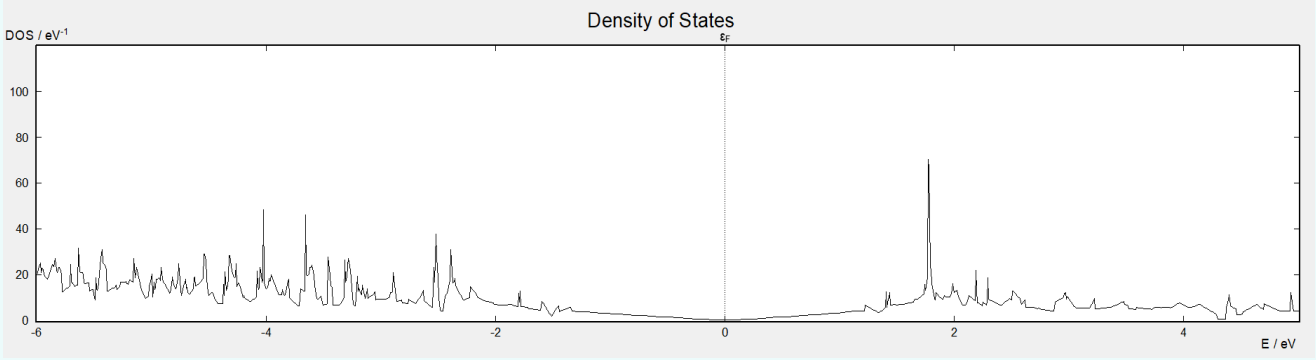
1. Graphene Sheet

Bandstructure



The bandstructure of graphene is parabolic, with linear dispersion near the Dirac points. The Dirac points are located at the K and K' points of the hexagonal Brillouin zone. The Dirac points are where the valence band and the conduction band meet.

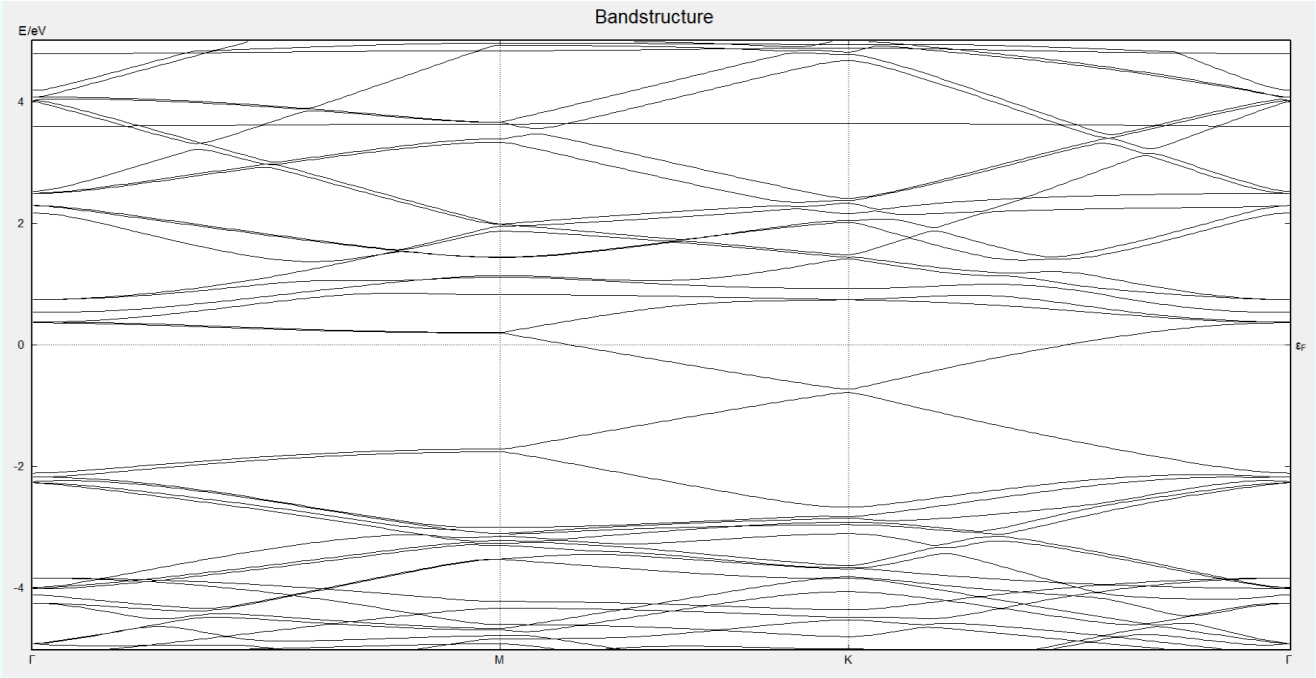
Density Of states(DOS)



The DOS of graphene exhibits sharp peaks at the Dirac points, reflecting its unique electronic structure. These peaks represent the high density of states at the Fermi level, enabling graphene's remarkable conductivity.

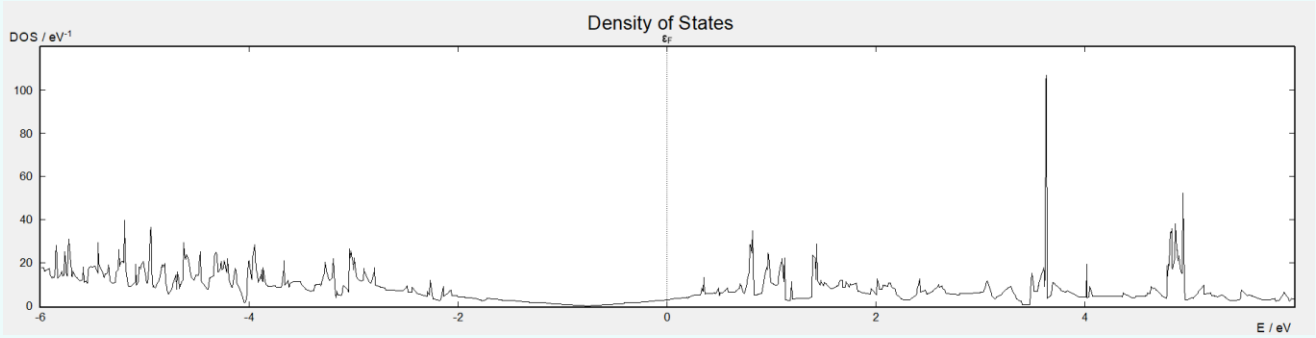
2. 1 Phosphorus Atom Doped Graphene Sheet

Bandstructure



The bandstructure of 1 ph atom doped graphene sheet is similar to that of graphene, but there is a new state near the Fermi level. This new state is due to the phosphorus atom. The phosphorus atom introduces a new orbital that can interact with the orbitals of the carbon atoms. This interaction results in the formation of a new state near the Fermi level.

Density Of states(DOS)

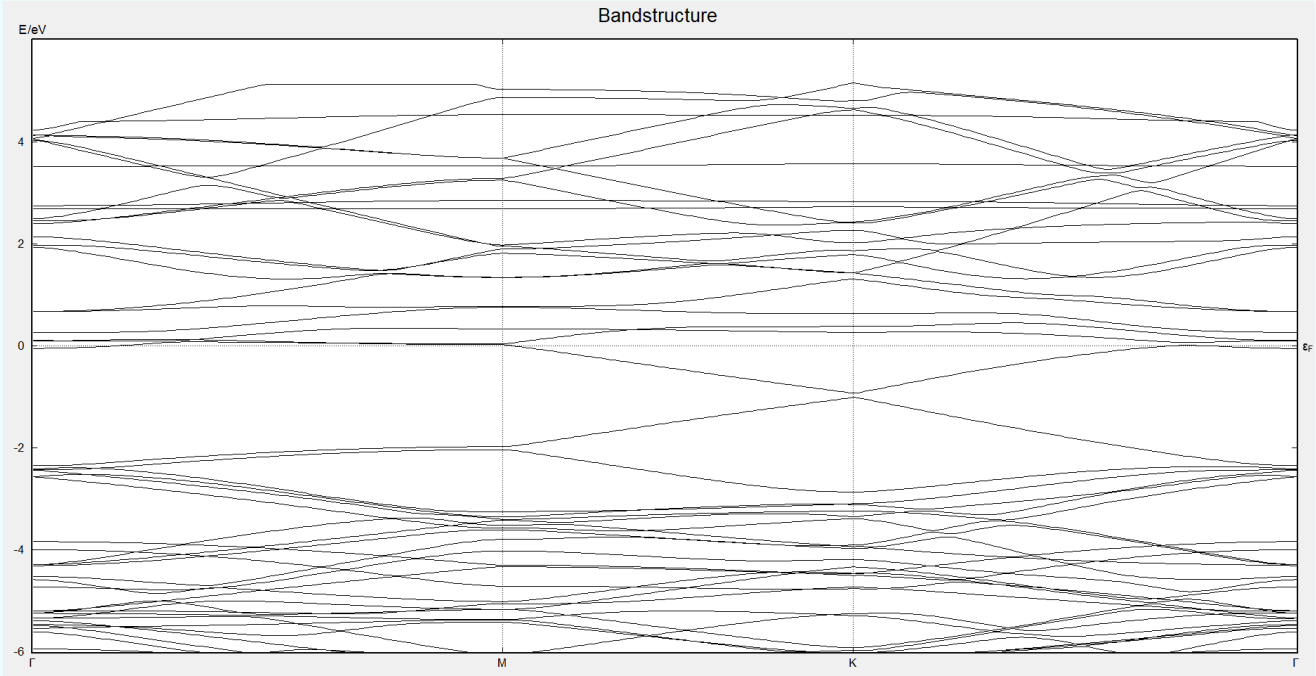


Doping graphene with phosphorus introduces new states near the Fermi level, broadening the DOS and altering the electronic properties. The DOS exhibits a noticeable increase around the Fermi

level, indicating enhanced conductivity compared to pristine graphene.

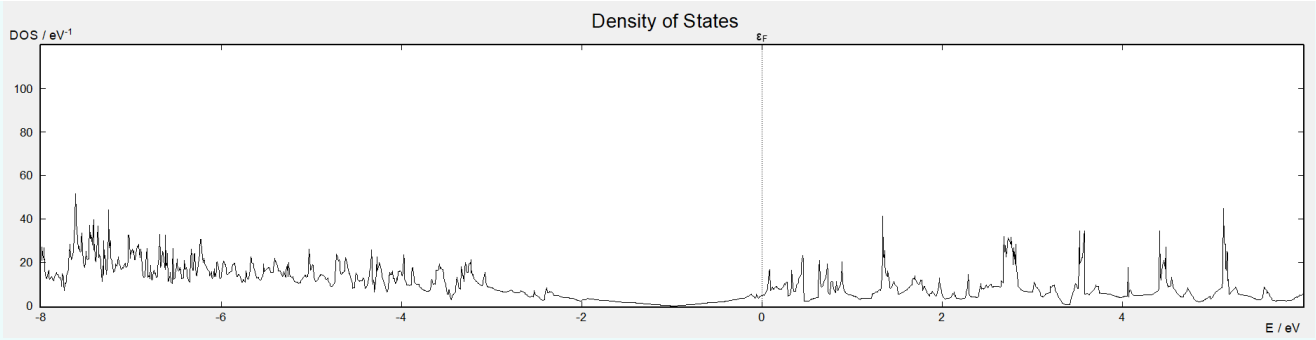
3. 2 Phosphorus Atoms Doped Graphene Sheet

Bandstructure



The bandstructure of 2 ph atoms doped graphene sheet is similar to that of 1 ph atom doped graphene sheet, but there are two new states near the Fermi level. This is because there are two phosphorus atoms in the system. The two phosphorus atoms introduce two new orbitals that can interact with the orbitals of the carbon atoms. This interaction results in the formation of two new states near the Fermi level.

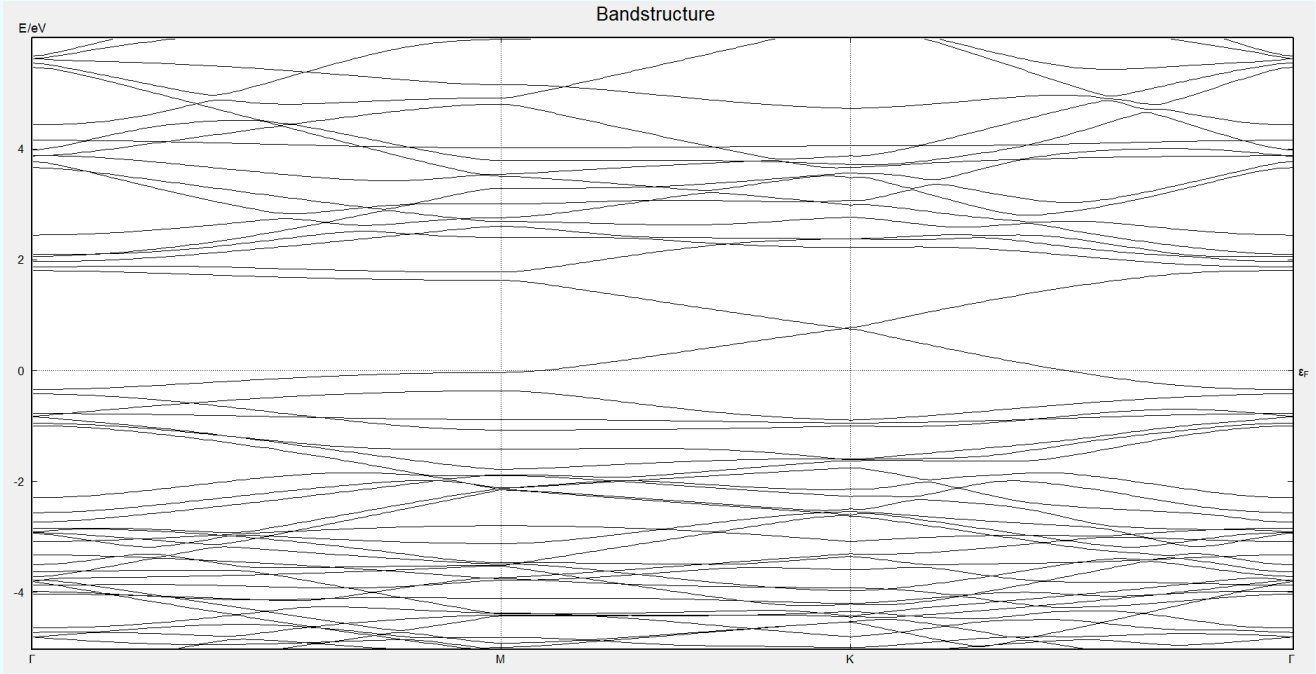
Density Of states(DOS)



Introducing two phosphorus atoms further broadens the DOS and increases the density of states near the Fermi level. The DOS profile becomes more pronounced, suggesting a more significant modification of graphene's electronic properties compared to single phosphorus doping.

4. 1 Phosphorus Atom Doped Graphene with 1 Carbon Atom Defect

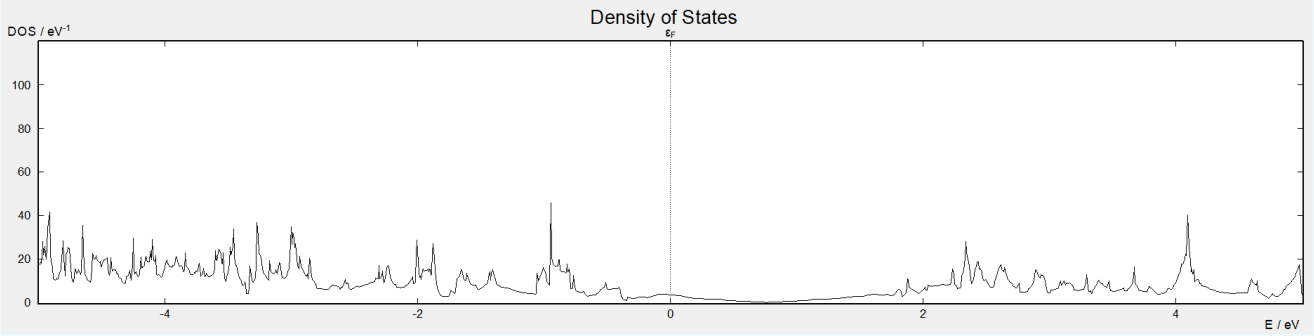
Bandstructure



The bandstructure of 1 ph atom doped graphene with 1 c atom defect is similar to that of 1 ph atom doped graphene sheet, but there is a localized state near the Fermi level. This localized state is

due to the carbon vacancy defect. The carbon vacancy defect breaks a bond between two carbon atoms. This creates a localized state that is not delocalized throughout the system.

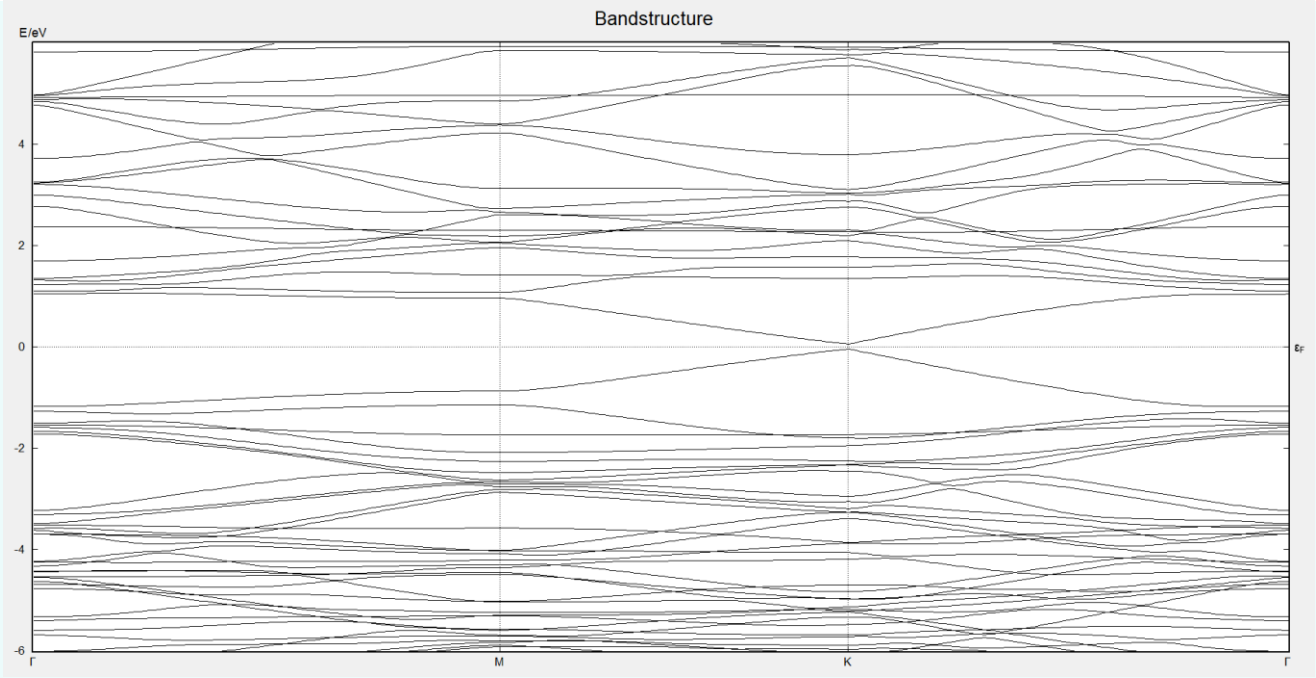
Density Of states(DOS)



Doping graphene with phosphorus and introducing a carbon vacancy defect lead to a combination of effects on the DOS. The phosphorus doping broadens the DOS, while the carbon vacancy defect introduces localized states near the Fermi level. The overall DOS profile reflects these competing influences.

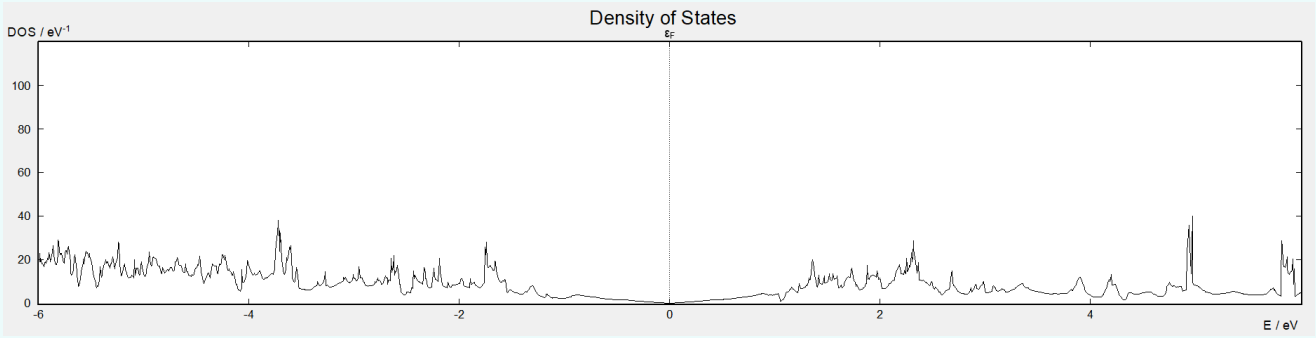
5. 2 Phosphorus Atoms Doped Graphene with 1 Carbon Atom Defect

Bandstructure



The bandstructure of 2 ph atom doped graphene with 1 c atom defect is similar to that of 2 ph atoms doped graphene sheet, but there are two localized states near the Fermi level. This is because there are two carbon vacancy defects in the system. The two carbon vacancy defects break two bonds between two carbon atoms. This creates two localized states that are not delocalized throughout the system.

Density Of states(DOS)

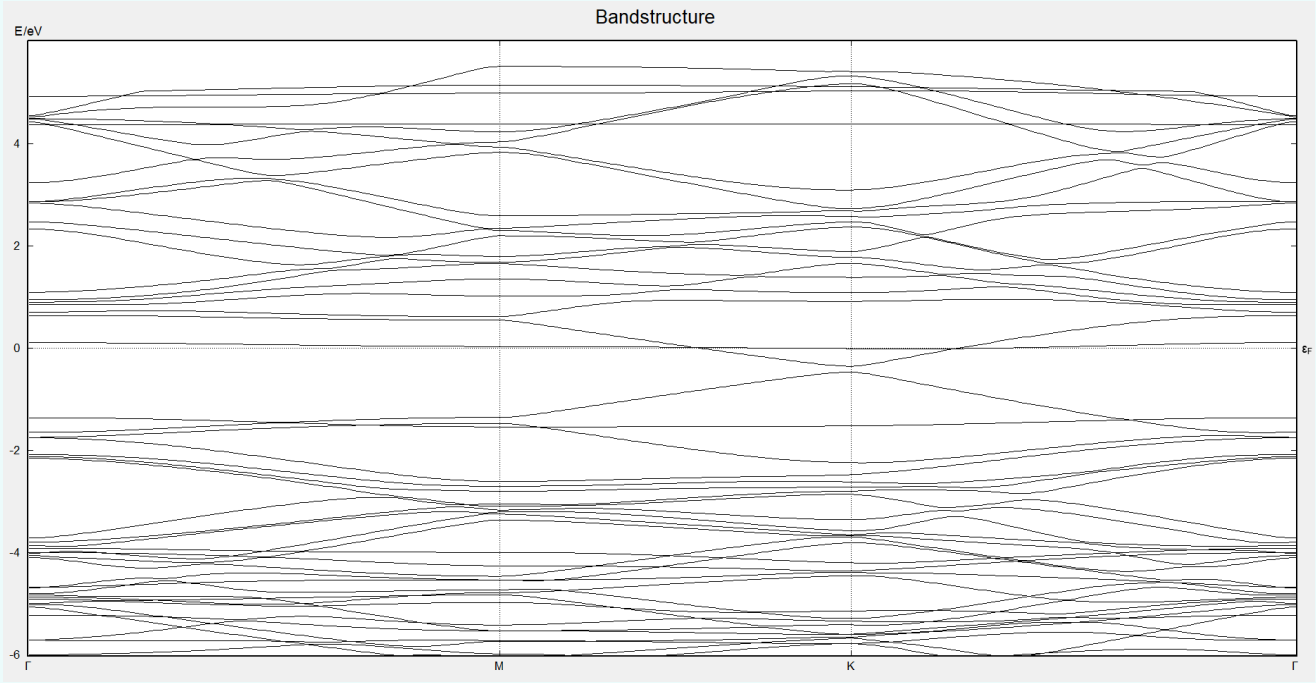


Increasing the phosphorus doping to two atoms while maintaining the carbon vacancy defect further broadens the DOS and increases

the density of states near the Fermi level. The localized states introduced by the carbon vacancy defect become more pronounced compared to the single phosphorus doping case.

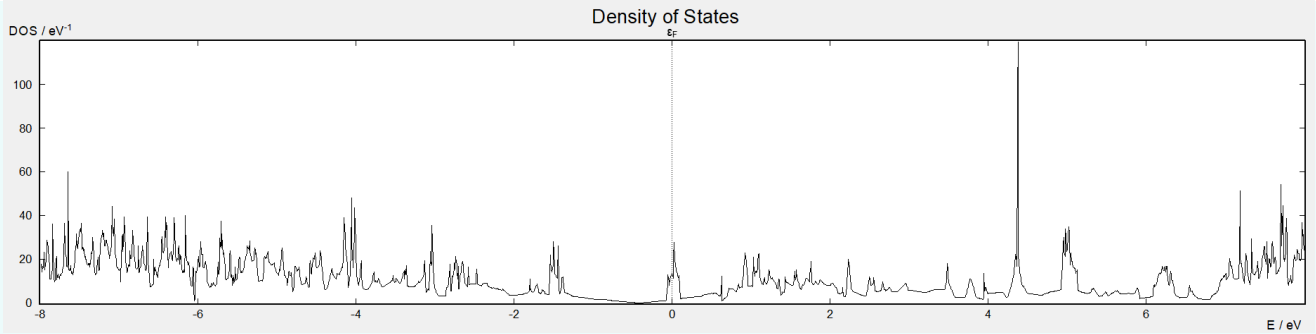
6. 3 Phosphorus Atoms Doped Graphene with 1 Carbon Atom Defect

Bandstructure



The bandstructure of 3 ph atom doped graphene with 1 c atom defect is similar to that of 2 ph atoms doped graphene sheet, but there are three localized states near the Fermi level. This is because there are three carbon vacancy defects in the system. The three carbon vacancy defects break three bonds between two carbon atoms. This creates three localized states that are not delocalized throughout the system.

Density Of states(DOS)



With three phosphorus atoms and a carbon vacancy defect, the DOS exhibits a combination of broadness due to phosphorus doping and localized states due to the carbon vacancy defect. The DOS profile becomes more complex, indicating a significant modification of graphene's electronic properties compared to the other structures.

Total Energy Analysis

Structure	Total Energy (eV/atom)
Graphene sheet	-3520.61374
1 ph atom doped graphene sheet	-7987.17249
2 ph atoms doped graphene sheet	-8087.20768
1 ph atom doped graphene with 1 c atom defect	-7829.04701
2 ph atoms doped graphene with 1 c atom defect	-7933.97277
3 ph atoms doped graphene with 1 c atom defect	-8038.05025

Conclusion

In the pursuit of advanced electronic materials, this research project has explored the design, modeling, and simulation of phosphorus-doped and defect-containing graphene nanosheets using ATK Virtual NanoLab. The investigation aimed to understand the impact of phosphorus doping and defects on the electronic properties of graphene, with a specific focus on bandstructure, density of states (DOS), and total energy.Key takeaways from our investigation include:

1. **Bandgap Engineering**: The incorporation of phosphorus atoms and defects into graphene structures offers a powerful means of controlling the bandgap width. This control is essential for tailoring materials to meet the requirements of specific semiconductor applications. We observed that the bandgap width increases with higher levels of phosphorus doping.

2. **Diversity in Electronic Density**: Our analysis of the Density of States (DOS) unveiled substantial variations in electronic states within these engineered materials. This variation, brought about by phosphorus doping and defect introduction, presents an array of possibilities for semiconductor device design and electronic applications.

3. **Structural Stability and Feasibility**: The comparison of total energy levels among the six structures provides essential insights into their structural stability. This evaluation hints at their potential suitability for real-world electronic applications, offering a foundation for further development.

Acknowledgment

We would like to express our sincere gratitude to all those who have contributed to the successful completion of this research project. Their support, guidance, and assistance have been invaluable throughout this endeavor.

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We are also thankful to the faculty and staff of **Indian Institute of Information Technology Nagpur(IIITN)** for providing access to the necessary resources, including ATK Virtual NanoLab software and computational infrastructure. Their commitment to fostering an environment conducive to scientific exploration greatly facilitated our work.

Our appreciation extends to our colleagues and fellow students who engaged in discussions and provided valuable insights during the course of this project. Collaborative efforts have always proven to be enlightening and motivating.

Last but not least, we owe a debt of gratitude to our families and friends for their understanding, encouragement, and unwavering belief in our abilities.

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Thank You