MAGNETIC PROPERTIES OF MOLECULAR NITROGEN ADSORBED PHOSPHORENE

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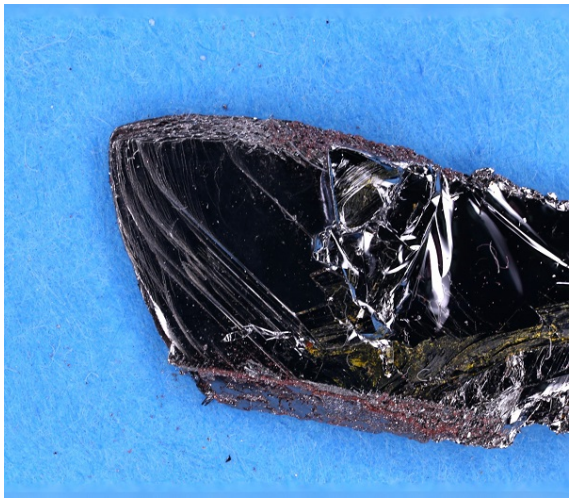
OUTLINES

- Introduction / Motivation
- Theoretical Background
- Computational Details
- Results and Discussion
- Conclusions and Concluding Remarks
- Acknowledgements

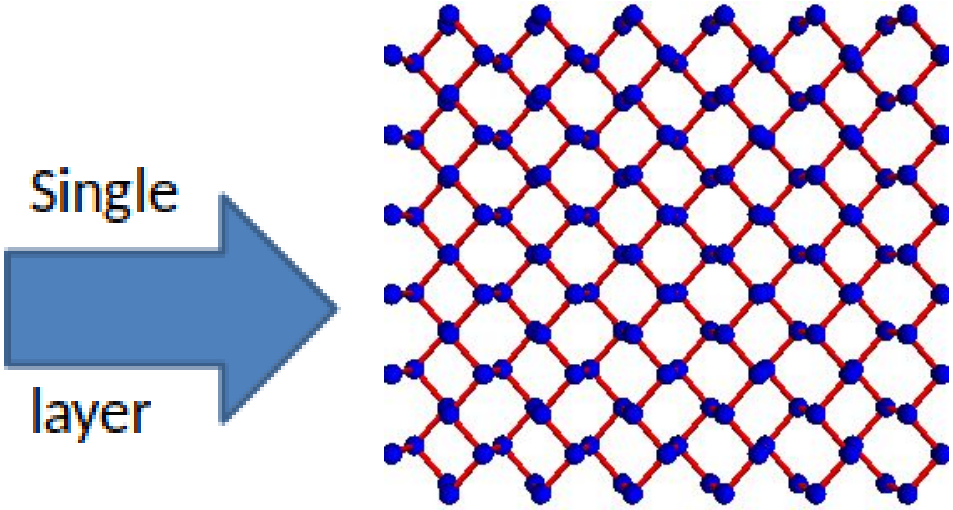
Introduction

Phosphorus and Phosphorene

- Phosphorus (P) exists in different allotropic forms:
  Red P, Black P, Yellow P, White P, Blue P.
- **Black phosphorus** is a layered crystalline allotrope.
- An individual layer of *black phosphorus* is named *phosphorene*.



(a) Black Phosphorus



(b) Phosphorene

- 2D material first isolated in 2014 by Han Liu and his team.

Fig. source: `www.plasmamaterials.com`

Introduction / Motivation

Structure of Phosphorene

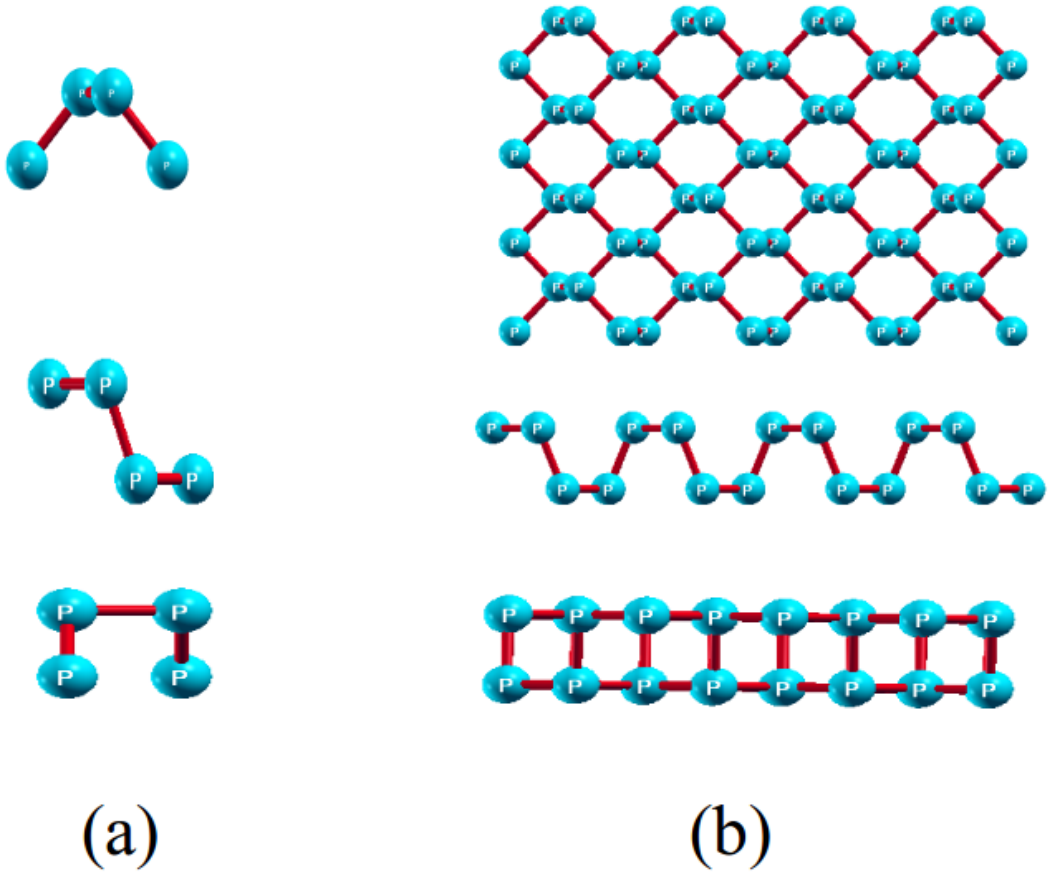


Fig.(a): Unit cell of Phosphorene (a = 4.57Å , b = 3.31Å)
Fig.(b): Propagation of unit cell to form a supercell

Introduction / Motivation

Notable Properties of Phosphorene

- **Direct and tunable band gap** depending upon number of layers (1.51 eV for a monolayer to 0.59 eV for a five layer sample)[1].
- **High hole mobility**; μ ~10,000 cm^2 V^{-1} s^{-1} along zig-zag direction[2]. (Si: ~500 cm^2/Vs; MoS_2: ~100 cm^2/Vs)
- **p-type transistor characteristics** complementary to n-type MoS_2 transistors[3].
- **Mechanically flexible**[3].
- **Highly applicable in transistors, inverters, logic circuits, photoconductive and optoelectronic devices**

[1] J. Qiao, X. Kong, Z. Hu, F Yang, and W. Ji, *Nature Communications* **5**, (2014).
[2] D. Akinwande et al., *Nature Communications* **5**, 5678 (2014).
[3] Liu, Han, et al. *arXiv preprint arXiv:1401.4133* (2014).

Theoretical Background

Density Functional Theory

- Uses electron density [n(**r**)] as basic variable instead of wave function [ψ].

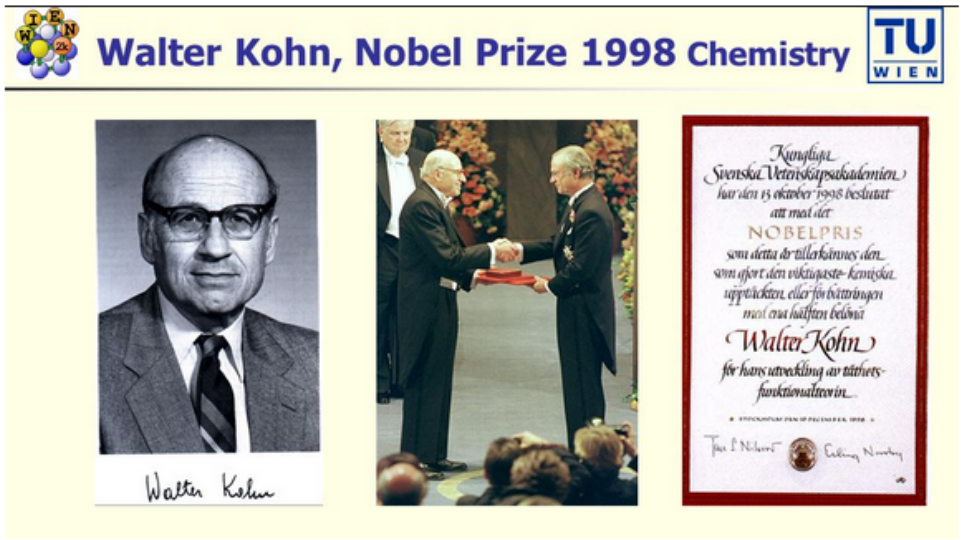


Fig. source : www.google.com (walter kohn nobel prize images)

Magnetic Moment (μ)

$\mu = m\mu_B$, m $\rightarrow$ number of unpaired electrons

$m = \int_{-\infty}^{+\infty}(D_{\uparrow}(\epsilon) - D_{\downarrow}(\epsilon))d\epsilon$

where, $D_{\uparrow}$= DOS for electrons with up spin & $D_{\downarrow}$= DOS for electrons with spin down

Computational Details

First-principles calculations based on Density Functional Theory (DFT) were carried out using Quantum-ESPRESSO

- **QUANTUM ESPRESSO:** Computational Software **Quantum** op**E**n-**S**ource **P**ackage for **R**esearch in **E**lectronic **S**tructure, **S**imulation, and **O**ptimization

- Based on plane wave basis set and Pseudopotentials.

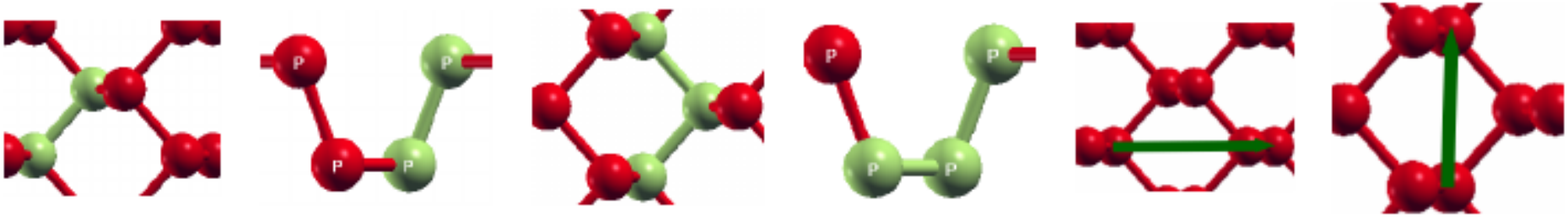
Fig. Source: `www.quantum-espresso.org`

Details of Simulation

Construction of unit cell

Experimental data used as the reference

	r_1(Å)	r_2(Å)	θ_1	θ_2	a(Å)	b(Å)
Experimental (bulk)*	2.22	2.28	96.37°	101.91 °	4.38	3.31



(a) r_1 (b) r_2 (c) θ_1 (d) θ_2 (e) **a** (f) **b**

* A. Brown et al. *Acta Cryst.* **19**, 684 (1965)

Details of Simulation

Cutoff kinetic energy (ecut) and k points

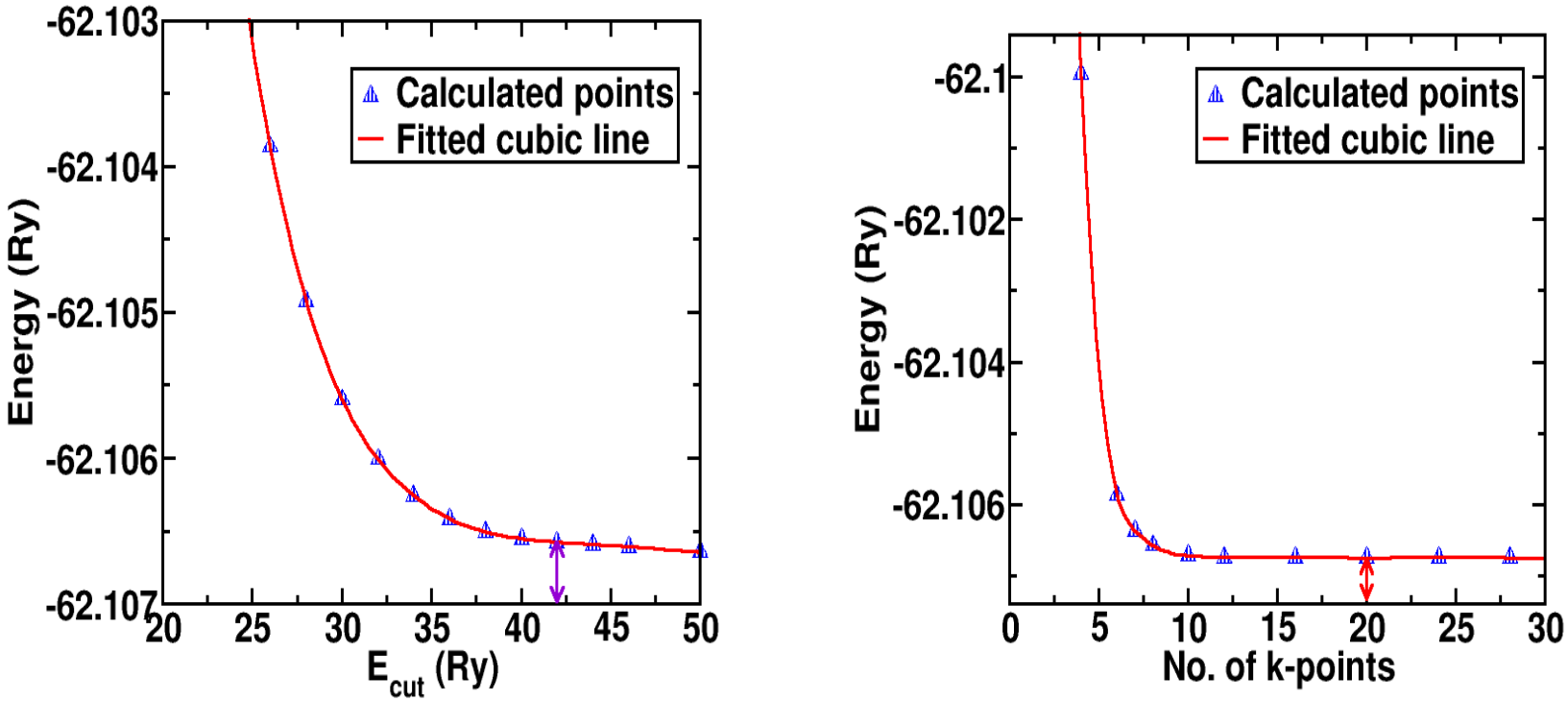


Figure: Convergence tests for ecut (left) and k points (right)

- ecut = 42 Ry
- k points = 20×20×1

Details of Simulation

Optimization of lattice parameters a & b

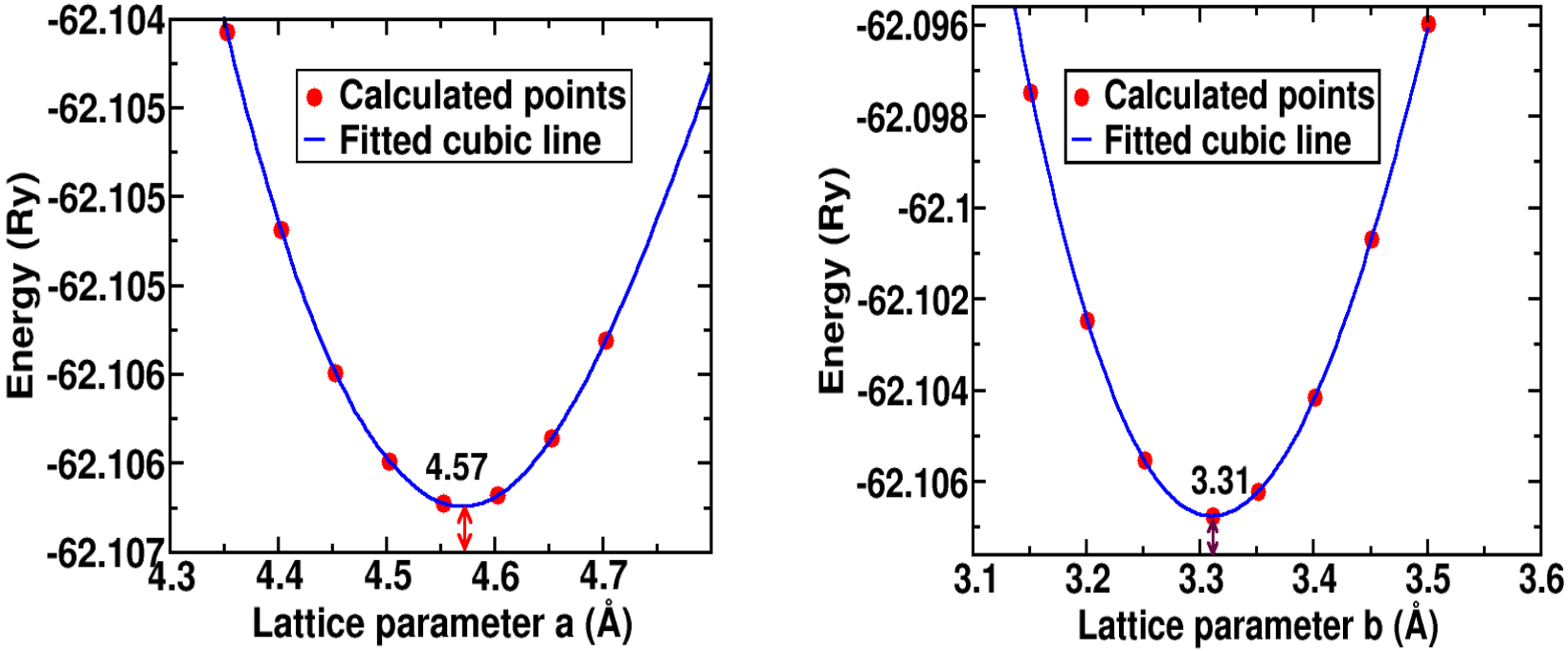
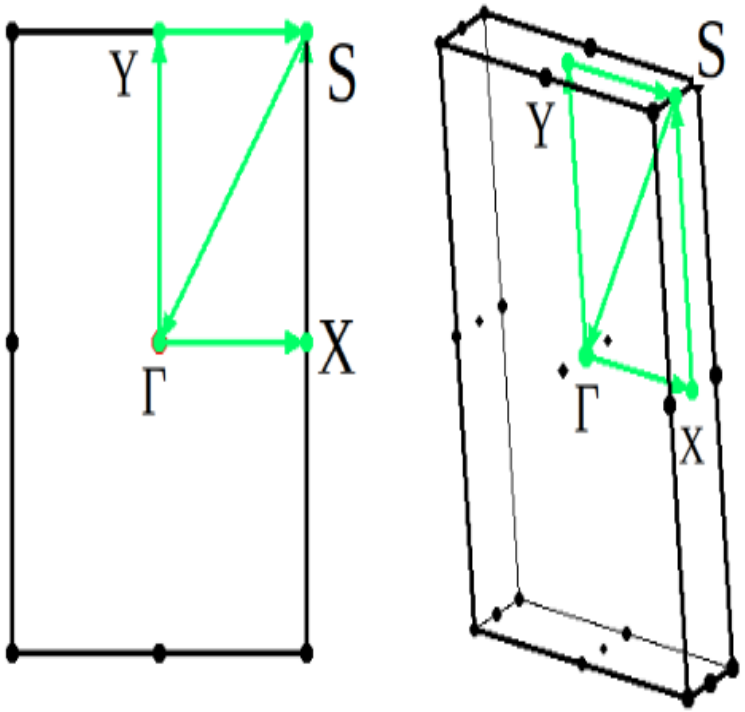


Figure: Variation of energy with lattice parameters **a** (left) and **b** (right)

- **a** = 4.57 Å
- **b** = 3.31 Å

Details of Simulation

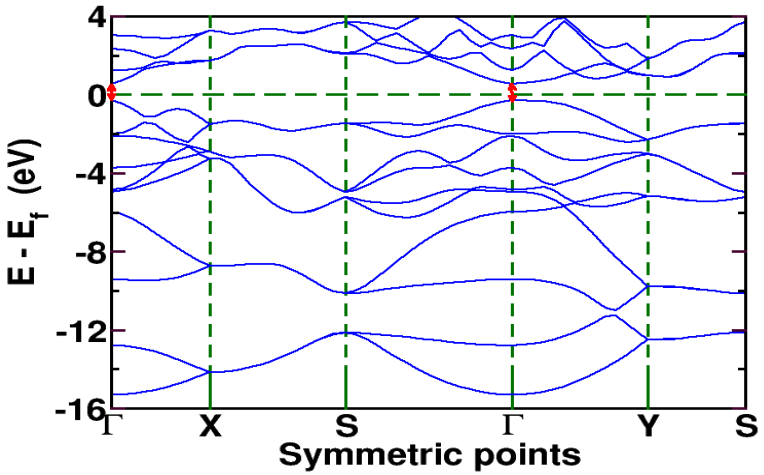
Selection of k path to study band structure



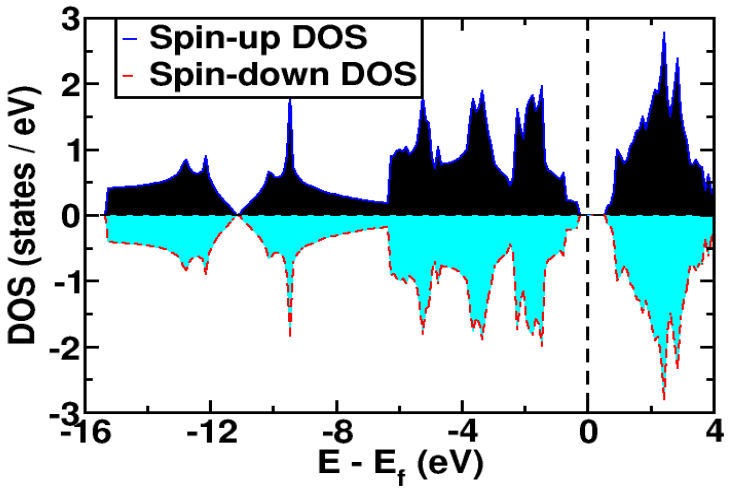
Chosen path : Γ-X-S-Γ-Y-S such that Γ-X represents zigzag direction and Γ-Y represents the armchair direction

Results and Discussion

Band Structure and Total Density of States (DOS) of Phosphorene for Unit Cell



(a) Band structure

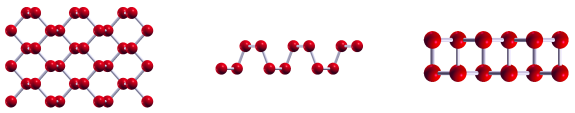


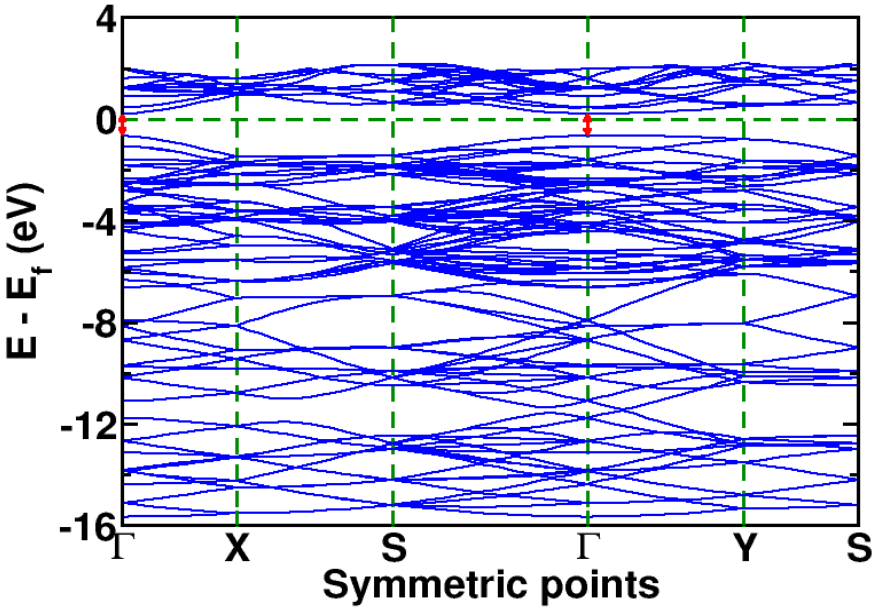
(b) Density of States

- Band Gap = 0.87 eV (Direct at Γ)
- No magnetization

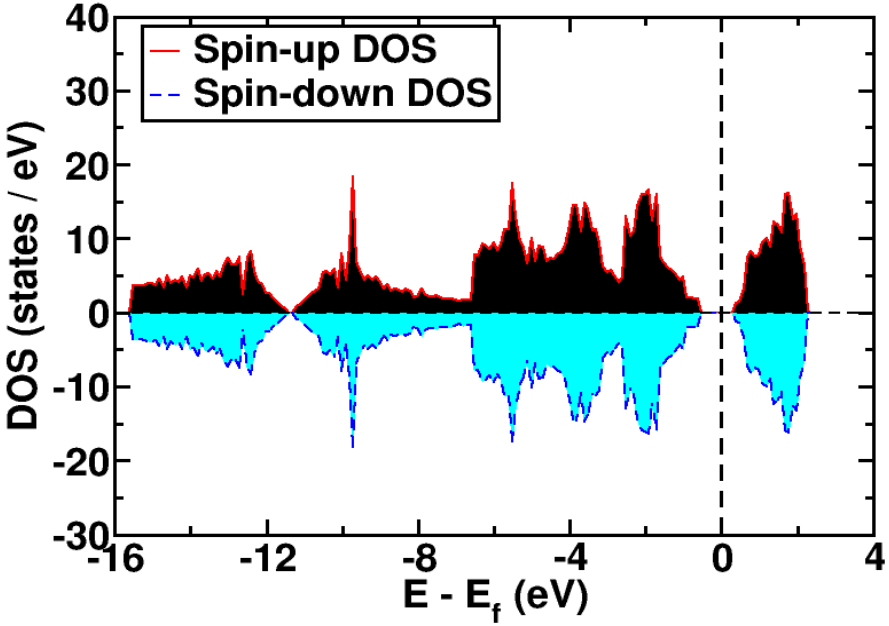
Results and Discussion

Band Structure and Total Density of States(DOS) of Phosphorene for 3x3 supercell





(a) Band structure

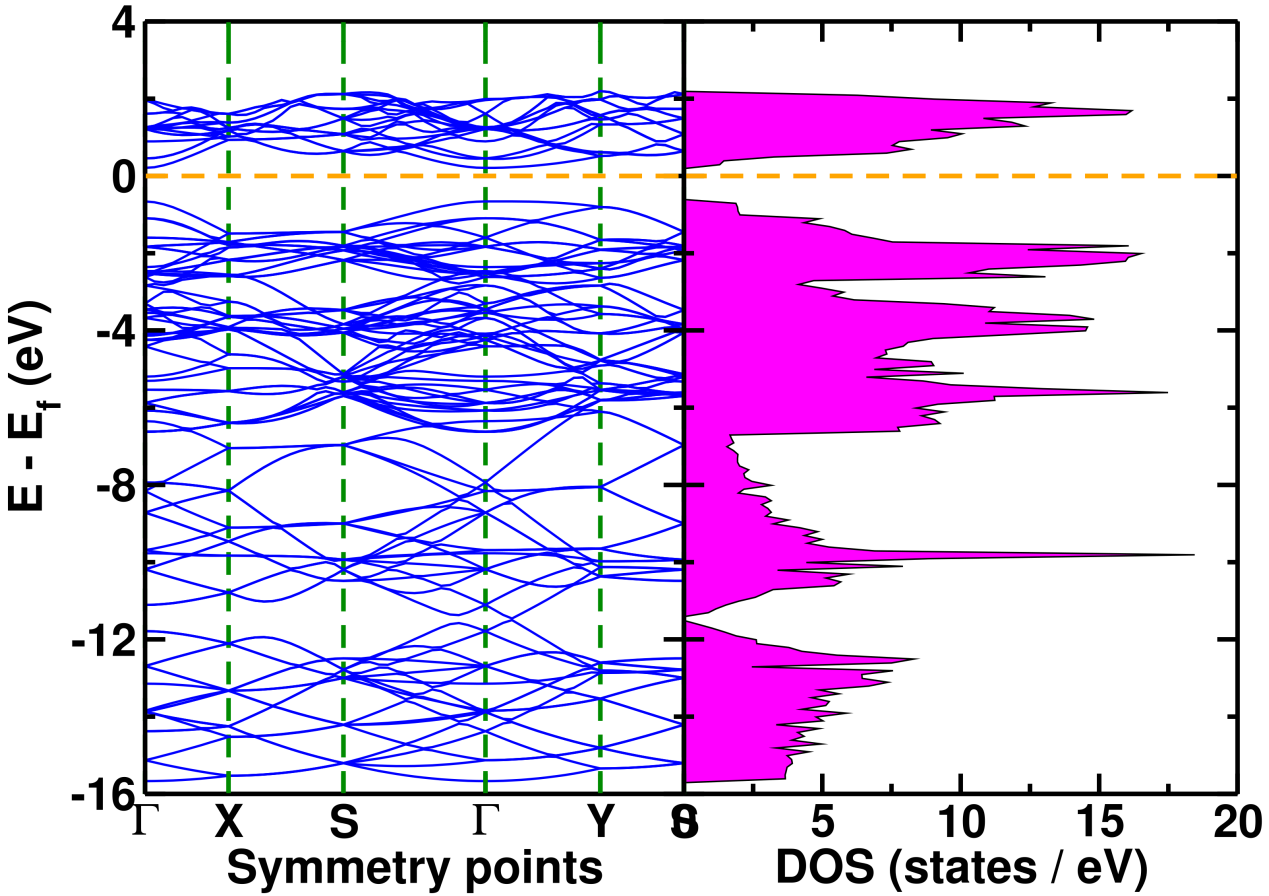


(b) Density of States

- Band Gap = 0.87 eV
- No magnetization

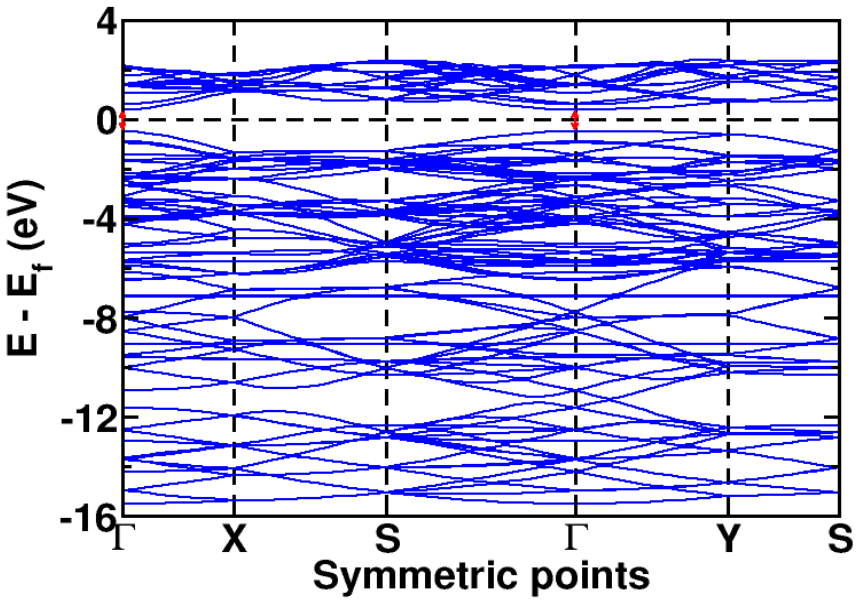
Results and Discussion

Combined form of Band Structure and DOS of pure Phosphorene for spin-up states

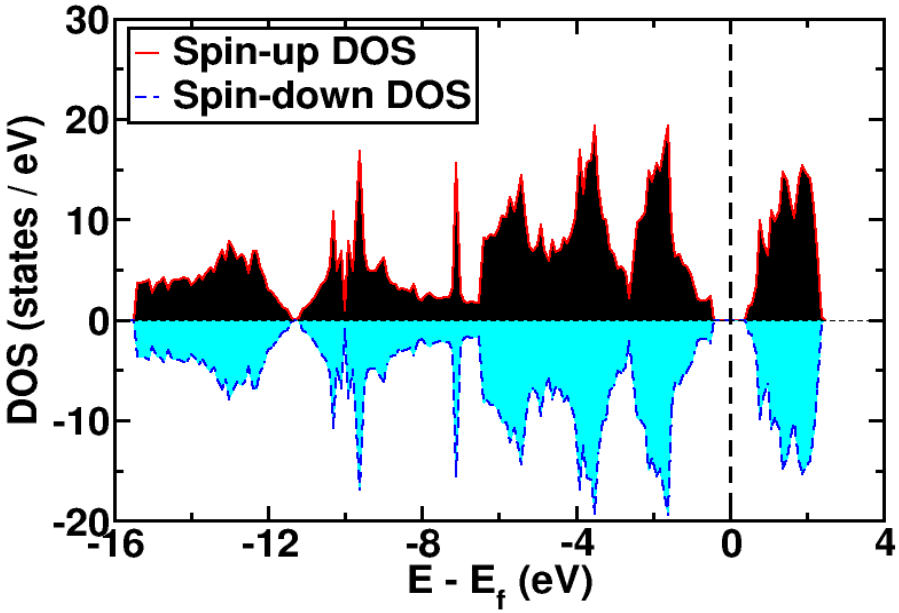


Results and Discussion

Band Structure and Total DOS of Molecular Nitrogen Adsorbed Phosphorene



(a) Band structure

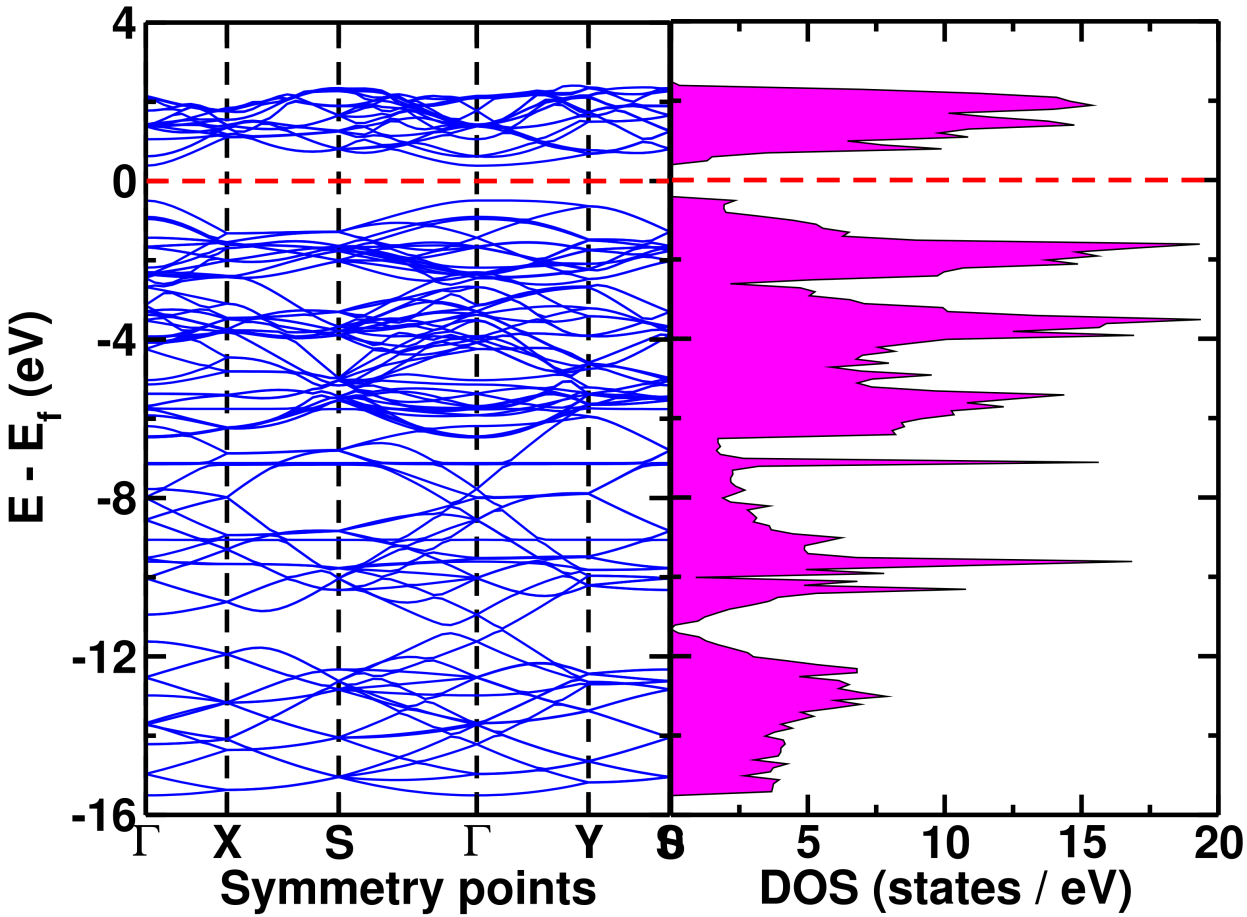


(b) Density of States

- Band Gap = 0.85 eV
- No magnetization

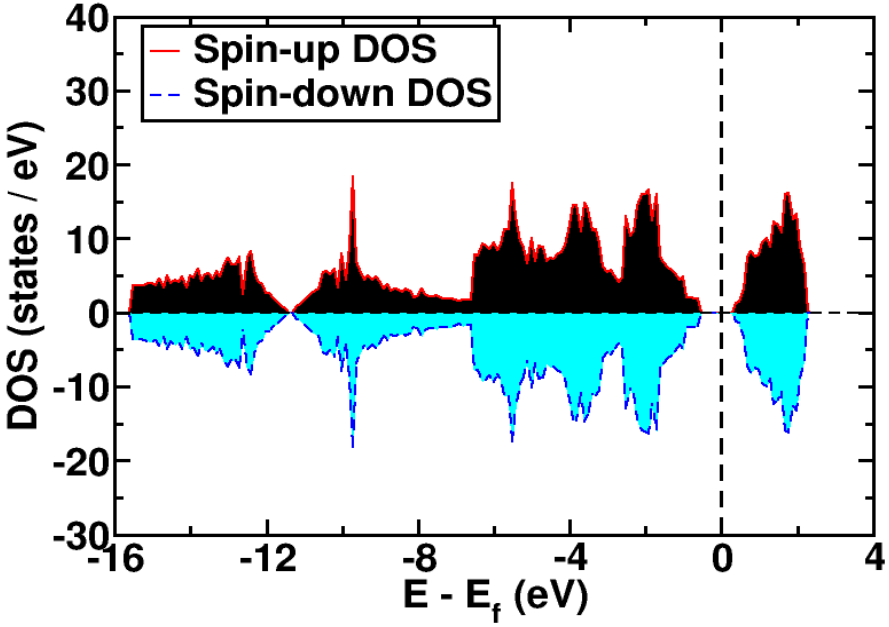
Results and Discussion

Combined form of Band Structure and DOS of N_2 adsorbed Phosphorene for spin-up states

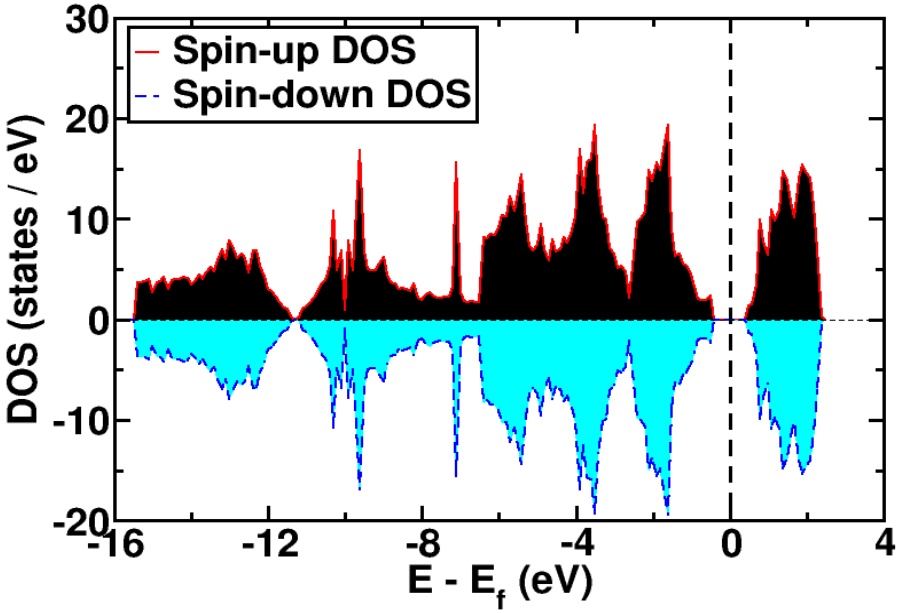


Results and Discussion

Comparison of DOS of molecular nitrogen adsorbed phosphorene with pristine phosphorene



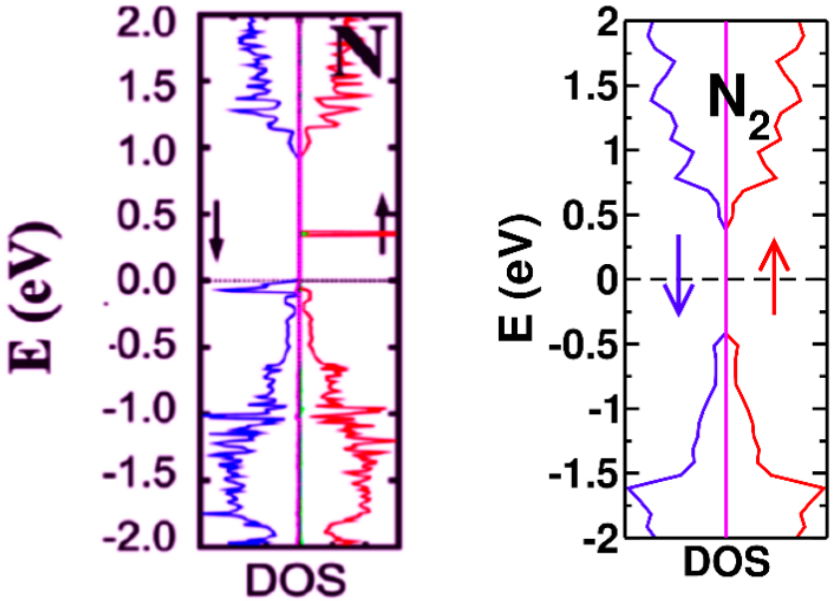
(a) Pristine



(b) N_2 adsorbed

Results and Discussion

Comparison of DOS of molecular nitrogen adsorbed phosphorene with atomic nitrogen adsorbed phosphorene



N-adsorbed* N_2-adsorbed

*P. Srivastava, K.P.S.S. Hembram, H. Mizuseki, K. Ryeol, S.S. Han, and S. Kim, *J. Phys. Chem. C* **119**, 6530-6538 (2015).

Conclusion and Concluding Remarks

- Electronic properties, magnetic properties and stability of pure and N_2 adsorped phosphorene were studied systematically.
- Adsorption of molecular nitrogen decreases band gap negligibly preserving the direct nature of band gap.
- The system under study (i.e., N_2 adsorbed phosphorene) remained non-magnetic.
- N_2 molecule adsorption behaves differently than that of N-atom adsorption on phosphorene.

One can extend this work by creating vacancies and increasing number of N_2 molecules. In addition, the optical and thermal properties can also be studied.

Acknowledgements:

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- Friends and Family

THANK YOU