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Electronic Properties and Mechanical Strength of β -Phosphorene Nano-ribbons

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Abstract: We have performed first principles calculations to find out the effect of mechanical strain on the electronic properties of zig-zag edged nano ribbons of β -phosphorene. It is found that electronic band-gap get opened-up to 2.61 eV by passivation of the edges of ribbons. Similarly, the mechanical strength is found to be increase from 1.75 GPa to 2.65 GPa on going from unpassivated nano ribbons to passivated ones along with the 2% increase in ultimate tensile strain. The band-gap value of passivated ribbon gets decreased to 0.43 eV on applying strain up to which the ribbon does not break. These tunable properties of β -phosphorene with passivation with H-atom and applying mechanical strain offer its use in tunable nano electronics.

INTRODUCTION

The existence of two-dimensional (2D) materials becomes reality after the successful exfoliation of graphene, the atomic layer of C atoms, in 2004. Graphene show exotic electronic transport and mechanical properties, but due to the lack of band gap there is limited use of graphene. Band gap plays important role for transistor technology. The band-gap limitation can be overcome by cutting graphene in the form of ribbons and that can be further tuned by applying mechanical strain and functionalized with H-atoms, which make it more valuable in the field of electronics [1].

The study of graphene was the beginning of the new era in 2D materials world. The researchers have now started to take interest in other 2D materials, which are coming recently into the picture. One of such material is phosphorene which is the 2D atomic layer of P atoms similar to graphene [2]. One of the most important properties of phosphorene is the semiconducting nature and high mobility of charge carrier which makes it good candidate in the field of semi conducting industry [3].

Phosphorene has basically two stable isotopes namely α -phosphorene and β -phosphorene [4]. α -phosphorene has been very well studied by the researcher's e.g. optical absorption spectrum and carrier conductivity of α -phosphorene is anisotropic and depends upon the strength of applied mechanical strain [5]. It has been shown recently that both zig-zag edged and armchair edged ribbons are semiconducting in nature and the band gap value decreases as the width of the ribbon is increased [6].

Here in our work we have studied the electronic and mechanical properties of low width β -phosphorene nanoribbons. We have taken zig-zag edged ribbons with two configurations i.e. unpassivated edges and passivated edges with H-atoms. The mechanical strength is calculated by obtaining stress versus strain curve.

COMPUTATIONAL METHOD

To perform first principle calculations, we have used the SIESTA (*Spanish Initiative for Electronic Simulations with Thousands of Atoms*) [7] package which performs density functional theory (DFT) calculations. A norm conserving pseudo-potential is used for the calculations. The crystal structure of ribbons was modeled using GDIS MOLECULE MODELLER. The distance between the periodic images of ribbons is kept more than 10 Å to avoid the mutual interaction. Also by make use of GGA exchange correlation functions,

we perform our calculations by choosing the reciprocal space which is sampled by grid of $10 \times 1 \times 1$ points. The fully relax coordinates are used where the forces on each atoms are less than $0.01 \text{ eV}/\text{\AA}$.

RESULTS AND DISCUSSION

We found that the minimum energy structure of β - phosphorene is buckled rather than planner like graphene, although the difference in total energy was in the order of few meV. The buckling was calculated 0.6\AA . We have taken low width of the ribbon as shown in Figure. Our optimized lattice constant for the unit cell of ribbon is 6.43\AA .

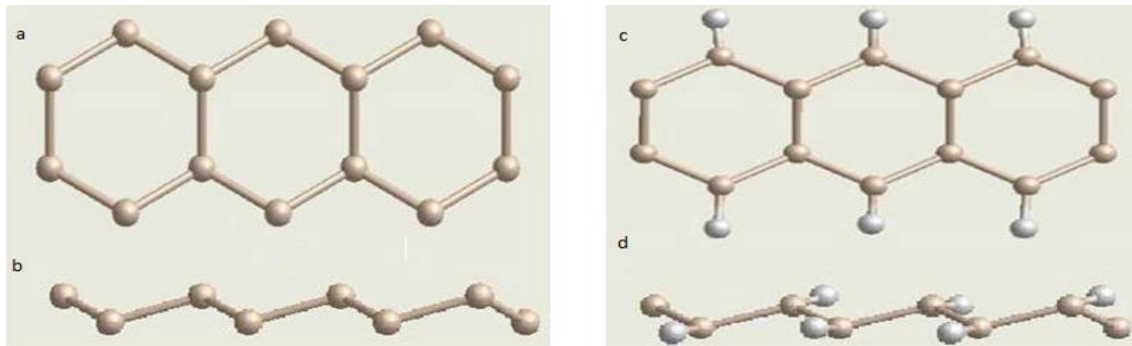


Figure 1:- Shows passivated and unpassivated top view (a, c) and side view (b, d) of β - phosphorene Nano ribbons.

We calculated the electronic band structure along the Γ -X direction of the brillouin zone. It is found that unpassivated ribbon show metallic characteristics which can be seen in electronic band structure in Figure 2 where bands are found to crossing the Fermi level. Similarly, density of states calculations further confirms the metallicity of the ribbon in terms of finite density of states at the Fermi level. The metallicity may be attributed to the unsaturated bonds presents at the edges of the ribbon. Next we saturates the edges by H-atom and found the band-gap gets open up as shown in Figure 3.

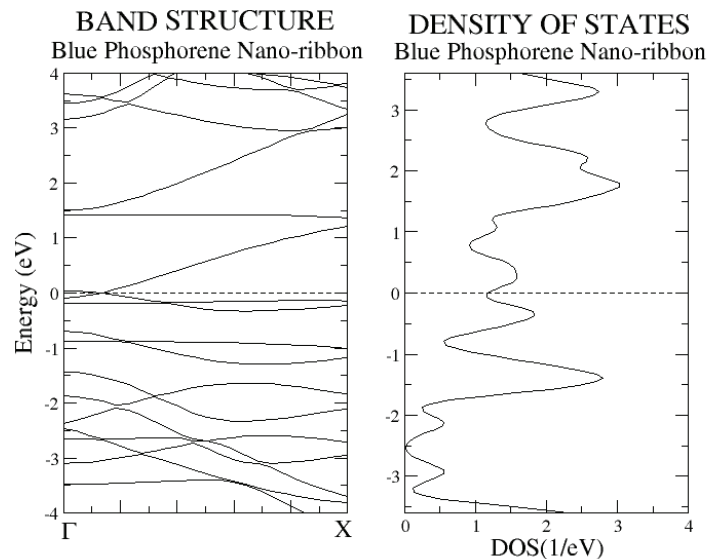


Figure 2:- Electronic band structure and density of states of unpassivated nanoribbon of β -phosphorene. Fermi level is set at 0 eV .

Mechanical Strength of β -phosphorene Nano-ribbons

Next we calculate the mechanical strength of both unpassivated and passivated nanoribbons. To study the effect of applied strain on nanoribbon, we apply the different percentage of strain by changing the lattice

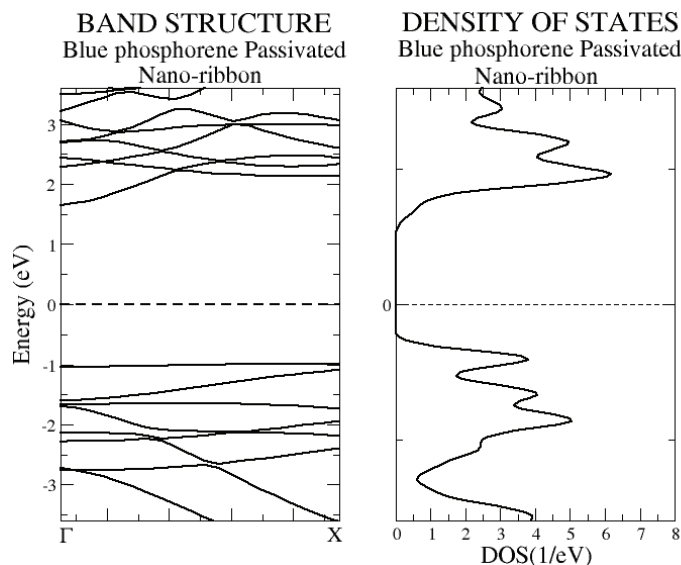


Figure 3: Electronic band structure and density of states of passivated nano-ribbon of β -phosphorene. Fermi level is set to at 0 eV.

constant value in small steps and calculating the corresponding stress in the stress tensor matrix. And the resultant results for phosphorene Nano-ribbon with and without passivation are show in the Figure 4. Note that applied strain value is the ratio of change in the lattice constant in small step to the zero-strain lattice constant. We found that the maximum strain that can be applied ribbons is 24% and 26% respectively for unpassivated and passivated ribbons before they getting broken. The calculated tensile strength was found to increase from 1.75 GPa to 2.65 GPa on passivation as can be seen in Figure 4. Therefore, it can be concluded that passivation strengthened the ribbons.

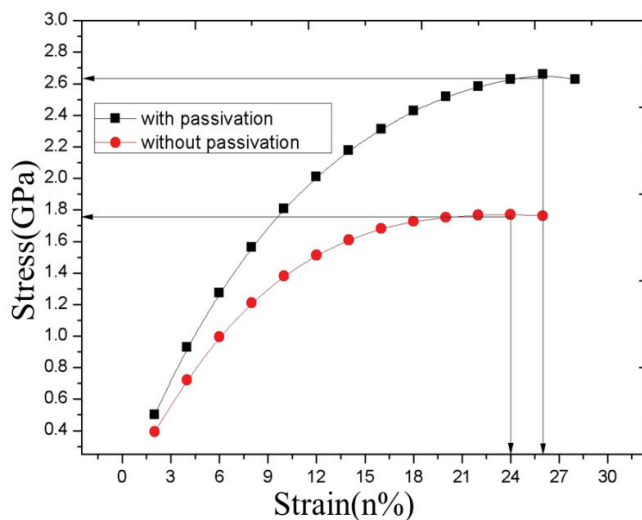


Figure: 4 Stress versus strain curves for passivated and non-passivated phosphorene nanoribbons.

Variation in Band Gap with Strain

Next we study the effect of strain on the band-gap of passivated β -phosphorene ribbons. After the Passivation when the different value of strain is applied to phosphorene nano-ribbon that the variation in the band-gap value is shown in Figure 5. It was found that band gap is increased when the passivation of the Phosphorene ribbon take place with hydrogen atom. When different values of strain are applied to the passivated Nano-ribbon, the band gap in the band structure is starts decreasing. We found that at the value of 2% strain the band gap is the 2.61eV. And when we reached up to the maximum of its mechanical strength value i.e. at 26 %, the band gap value become of 0.43eV. Therefore, the band-gap values of zigzag edged β -phosphorene passivated ribbons are tunable with applied strain that may have implications in tunable electronics and sensor applications.

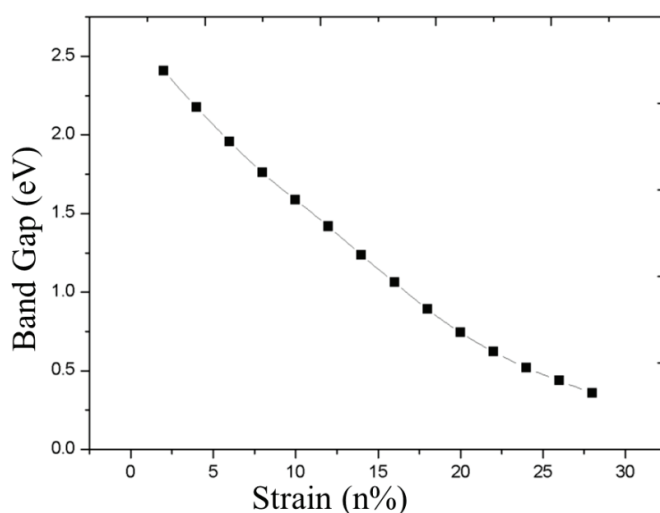


Figure 5: Shows the variation in band gap with the applied values of Strain.

the band gap value become of 0.43eV. Therefore, the band-gap values of zigzag edged β -phosphorene passivated ribbons are tunable with applied strain that may have implications in tunable electronics and sensor applications.

CONCLUSIONS

In summary, effect of the passivation and mechanical strain on the electronic properties of phosphorene nanoribbon are investigated. The applied strain changes its electronic properties in significant manner by reducing the band gap by increased value of strain. The strength of β - phosphorene ribbon is found to increase with passivation. The ultimate tensile strain also increases from 26% to 28% on passivation. These tunable properties of nanoribbons may have importance in the applications of flexible nano electronics.

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