Research Paper

Exploration of High Symmetry β -P_xSi_y Materials for 2D-Electronics

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Both the β -P and silicene have similar buckled honeycomb crystal structure and are similar in sizes, in principle, they can form alloys. Motivated by this, we explore the electronic properties of various combinations of phosphorus and silicon atoms organized in honeycomb lattice. In particular, we choose high symmetry phases P₂Si, P₃Si, P₄Si₄, P₂Si₃, P₂Si₂, and P₂Si₂ for our study. Our work reveals that the P₂Si is a Dirac semi-metal, P₃Si is an indirect bandgap semiconductor, and the other monolayers are metallic in nature. We also investigated the effect of strain and electric field on all these alloys. We find that electric field does not change the electronic properties of any of these materials. However, the compressive strain causes bandgap opening in P₄Si₄ and bandgap closing in P₂Si₃. The most important result of this study is that the tensile strain creates a perfect Dirac cone in P₂Si.

Keywords: β -Phosphorene; Silicene; 2D-Materials; First-Principle Calculations; Alloys; Bandgap Tuning; Bi-Axial Strain

Introduction

Atomically flat 2D materials (C. Tany, 2017, S. Z. Butler, 2013, K. S. Novoselov, 2016) are being investigated by several researchers for their potential applications in electronic (L. Li, 2014, V. K. Sangwan, 2018, J. Guan, 2014), plasmonic (A. N. Grigorenko, 2012, F. H. L. Koppens, 2011, A. Agarwal, 2018), and photonic devices (A. Bandyopadhyay, 2018, F. H. L. Koppens, 2014, F. Xia, 2017, Z. Sun, 2016). After the separation of monolayer of graphene from graphite, the number of 2D materials has grown exponentially, with the inclusion of many new materials such as, transition metal dichalcogenides (TMDs) (D. Sarkar, 2014), phosphorus monolayer and bilayers (buckled and puckered) (H. Liu, 2014, L. Li, 2014), and various phosphorus based compounds (G. Schusteritsch, 2016, N. Lu, 2018, N. Miao, 2017, J. Guan, 2017, Y. Jing, 2017, B. Ghosh, 2015, B. Ghosh, 2016).

- Group IV 2D materials, such as germanene and silicene (which possess a minute corrugated honeycomb lattice structure, with respect to their planar layers) have been predicted to be stable (C.-C. Liu, 2011, Q. Tang, 2013, S. Cahangirov, 2009). Both the materials have semi-metallic nature, Dirac cones and estimated Fermi velocities 10^6 (that is close to graphene) (J. Wang, 2015). After the fabrication of anisotropic 2D black phosphorene's monolayer (that has direct bandgap of ≈ 2 eV), group V 2D materials started gaining popularity (H. Liu, 2014). Several experimental and computational studies have shown that phosphorene can be used to fabricate semiconductor devices for various electronic applications (L. Li, 2014, V. K. Sangwan, 2018, J. Guan, 2014), plasmonic (L. Li, 2014, Q. Wei, 2014, V. Tran, 2014, T. Low, 2014, T. Takahashi, 1985, Y. Li, 2014, S. Das,

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2014). Following black phosphorene, various new group V 2D materials, such as blue phosphorene (indirect bandgap of 2 eV) and grey arsenene (indirect bandgap of ≈ 1.6 eV) have been predicted by computational studies (H. Liu, 2014, N. Han, 2017, Z. Zhu, 2014, S. Nahas, 2017, C. Kamal, 2015). The bi-layers and multi layers of all these group IV and V materials demonstrate some interesting electronic properties, such as the bandgap variation with the number of layers in phosphorene (D. Li, 2017). Additionally, the electronic properties of all these materials can be tuned by applying electric field and strain (S. B. Kumar, 2011, E. J. G. Santos, 2015, Z. Ni, 2012, P. Kumar, 2016, F. Liu, 2017, N. D. Drummond, 2012, D. Cakr, 2014, R. Fei, 2014, M. Ghorbani-Asl, 2013, H. Guo, 2014, P. Johari, 2012, Y. Ren, 2012, W. Zhang, 2018, Z. Guo, 2017).

Researchers have investigated, not only the mono elemental 2D materials, but also compound 2D materials, such as phosphorus compound based 2D materials. The family of phosphorus compound based 2D materials includes combination of phosphorus with group-II, III and IV elements. These 2D materials are reported to have high carrier mobility and they are easy to fabricate, because of their low exfoliation energy. A few examples of these materials are germanium triphosphide (GeP_3) (Y. Jing, 2017), phosphorous carbide (PC) (J. Guan, 2016), calcium triphosphide (CaP_3) (N. Lu, 2018), tin triphosphide (SnP_3) (B. Ghosh, 2018), and indium triphosphide (InP_3) (N. Miao, 2017). All these phosphorus based materials are predicted to possess outstanding optical absorption in the infrared to visible regime, which makes these materials probable candidates for solar applications such as photovoltaic cell and LEDs.

Atoms in the β -P and silicene are arranged in buckled honeycomb lattice (B. Ghosh, 2015, D. Jose, 2014, L. Y. V. L. C., 2017) and the covalent radius of these two materials are nearly the same, $r_{\text{Si}} = 111$ pm, and $r_{\text{P}} = 107$ pm. Due to these similarities, P and Si can form alloys in principle. Inspired by this, we study few high symmetry phases of binary compounds of P and Si, arranged in a buckled honeycomb lattice, viz., PSi , P_3Si , P_4Si_4 , PSi_3 , P_2Si , and PSi_2 . Electronic band structure calculations reveal that the P_3Si is an indirect bandgap semiconductor, P_2Si is a Dirac semi-

metal, and all other phases are metallic in nature.

Organization of this manuscript is as follows: the density functional theory (DFT) calculations' details are presented in Methodology section. In Results section, we study the structural properties, electronic band structures, and the impact of external perpendicular electric field and bi-axial strain on electronic characteristics of above-mentioned new materials. The results are outlined in the Summary.

Methodology and Simulation Details

We optimize the crystal structures and compute the electronic band structure, using DFT, as employed in QUANTUM ESPRESSO (P. Giannozzi, 2009). We use the kinetic energy cutoff of 40 Ry, with plane wave basis set and projector augmented wave pseudopotential (P. E. Blochl, 1994). To take into account the exchange-correlation, we use GGA method, suggested by Perdew-Burke-Ernzerhof (PBE) (J. P. Perdew, 1996). The dispersion forces are taken into account by using DFT-D Van der Waals correction (G. Roman Perez, 2009). We maintain minimum vacuum spacing of 15 Å, perpendicular to the monolayer plane, to avoid spurious interactions among the periodic replicas. Structures are relaxed up to the point, where the energy difference of two consecutive steps of ionic relaxation is lower than 10^{-4} Ry, and all the force components on each atom, belonging to the unit cell, are less than 10^{-3} Ry/Bohr. A κ -point mesh of $20 \times 20 \times 1$ is used for Brillouin zone integrations.

Results and Discussions

Structures Properties and Stability Analysis

In Fig. 1, we show the crystal structure and band structure of β -P and silicene. In Fig. 1 (a), r , θ , d , and h are bond length, bond angle, lattice constant, and buckling height, respectively. The calculated values of these parameters for β -P (silicene) are; $r = 2.26$ (2.27) Å, $\theta = 93.12^\circ$ (116.29°), $d = 3.28$ (3.86) Å and $h = 1.232$ (0.44) Å, which match very well with published data (B. Ghosh, 2015, D. Jose, 2014, L. Y. V. L. C., 2015). Bandgap value calculated for β -P is 1.92 eV and, silicene has a Dirac cone at the κ -point, which are also in accordance with the previous results (B. Ghosh, 2015, D. Jose, 2014, L. Y. V. L. C., 2015). This validates our simulation parameters, such as the

Fig. 1: (a) Crystal structures of β -P and silicene (hexagonal unit cell is marked in the figure). Band structures and DOS of β -P (with Brillouin zone and the high symmetry points) and silicene are shown in (b) and (c), respectively

Table 1: Structural parameters of high symmetry phase P_xSi_y , blue phosphorene and silicene structures. Here, r is bond length, b the bond angle, θ is the buckle height, and d is the lattice constant

Crystal	r (Å)	θ (°)	h (Å)	d (Å)
P	2.26	93.12	1.233	3.28
Si	2.28	116.29	0.445	3.87
PSi	2.27	104.24	0.94	3.59
P_4Si_4	2.32 (P-P)/2.27 (Si-P)/2.25 (Si-Si)	97.13 (P-P-P)/106.68 (Si-Si-Si)	0.88/1.16	7.17
PSi_3	2.26 (P-Si)/2.29 (Si-Si)	113.49 (Si-Si-Si)/105.71 (Si-P-Si)/110.04 (P-Si-Si)	0.6/0.88	7.43
P_3Si	2.25 (P-P)/2.28 (P-Si)	91.71 (P-P-P)/104.59 (P-Si-P)/98.68 (Si-P-P)	0.93/1.26	6.84
P_2Si	2.27 (P-Si)/2.26 (Si-Si)	90.06 (P-P-P)/105.08 (P-Si-P)/100.6 (P-P-Si)	1.30/0.91	6.00
PSi_2	2.25 (P-Si)/2.3 (Si-Si)	105.95 (Si-P-Si)/108.35 (P-Si-P)/110.2 (Si-Si-Si)	0.87/0.74	6.32

energy cutoff, pseudopotential and density of κ -point grid, used in the DFT calculations.

After the validation of our DFT calculation parameters, we optimize the crystal structures of the newly suggested alloys. In Fig. 2, we show the high symmetry structures of β - P_xSi_y . In these figures, phosphorus (silicon) atoms are represented by red (blue) balls. As different atomic combinations are present in our study, so we obtain different bond lengths, bond angles, and buckling heights. All the calculated structural parameters are given in Table 1. To check the stability of these structures, we calculate the formation energy (per atom) of these structures in eV. The formation energy (F.E.) is calculated as,

$$F.E. = (E_{P_xSi_y} - xE_P - yE_{Si}) / (x + y) \quad (1)$$

where, $E_{P_xSi_y}$, E_P , and E_{Si} are total energies of P_xSi_y monolayer, isolated P atom, and isolated Si atom, respectively. The formation energies of these structures are shown in Table 2. As can be seen in the Table 2, P_3Si is the most stable structure among all these structures.

Fig. 2: Crystal structures of (a) PSi, (b) P_4Si_4 , (c) P_3Si , (d) PSi_3 , (e) P_2Si , and (f) PSi_2 . The hexagonal unit cell is marked in the figure

Electronic Band Structures

The electronic band structures of all the alloys are shown in Fig. 3. Among all the alloys, PSi, P_4Si_4 , P_3Si , PSi_2 , and P_2Si are metallic in nature. Only PSi_3 is found to be an indirect bandgap semiconductor with $E_g = 0.3$ eV. However, the underestimation of

Table 2: Calculated formation energy of the relaxed structures in eV (per atom)

Crystal	Formation Energy in eV (per atom)
P	-1.015
Si	-0.455
PSi ₃	-0.101
PSi ₂	-0.654
P ₄ Si ₄	-0.683
PSi	-0.758
P ₂ Si	-0.937
P ₃ Si	-0.979

bandgap, obtained from GGA calculations, is a well-known fact. The use of more accurate hybrid functionals gives nearly two-fold increase in the bandgap (B. Ghosh, 2015, D. Kecik, 2016). In the next section, we explore the possibility of bandgap engineering by applying external vertical electric field and strain.

Impact of Electric Field

In order to study the impact of external perpendicular electric field on the electronic characteristics of these new structures, we apply external electric field, using saw tooth type potential (L. Bengtsson, 1999). We

vary the external electric field magnitude from 0.0 to 0.5 V/Å, for all the alloys. But, we do not see any significant change in the electronic band structures of these materials.

Effect of Bi-axial Strain

Application of strain, to attain favorable electronic and photonic properties of 2D materials, is known as strain engineering (Y. Sun, 2019). Extensive studies on the application of mechanical strain show that the strain significantly changes the electronic properties of 2D materials. Strain changes the overlap among atomic orbitals, leading to change of bandgap and in some cases semiconductor to metal transition or vice versa. 2D materials, being a long sheet, can sustain more strain with respect to their bulk counterparts (Z. Dai, 2018). Large amount of local strain can be easily generated in 2D materials by bending, folding, or poking. These features encouraged the researchers to study strain induced properties of 2D materials. It is very difficult to strain the free standing sheets of 2D materials by making the micro-mechanical systems. Hence, these sheets are often transferred to some substrate, and the strain in 2D sheet is regulated by the substrate deformations. In case of silicene, semi metal-metal transition caused by strain,

Fig. 3: The computed electronic dispersions and DOS of (a) PSi, (b) P₄Si₄, (c) PSi₃, (d) P₃Si, (e) P₂Si, and (f) PSi₂. These band structures reveals that P₂Si is a Dirac material, PSi₃ is a semiconductor material, and rest of the materials are metallic in nature

Dirac points and van-Hove singularities are observed (G. Liu, 2012, X. Lin, 2015, R. Qin, 2012). For graphene, strain engineering has been extensively explored by several researchers and reviewed by C. Si (C. Si, 2016). Impact of strain on electronic properties of black phosphorene is studied in (D. Cakr, 2014, R. Fei, 2014). Similar studies for TMD materials have also been reported (M. Ghorbani-Asl, 2013, H. Guo, 2014, P. Johari, 2012). A number of studies (Y. Ren, 2018, W. Zhang, 2018, Z. Guo, 2017), exploring the impact of strain on blue phosphorene nanoribbons and hetero structures have been performed.

To determine the impact of strain on the electronic properties of these newly predicted materials, we apply bi-axial strain on these structures and calculate the electronic band structures using GGA-DFT approach. The significant results, obtained from our study, are summarized below:

Impact of Bi-axial Strain on the Electronic Dispersion of P_4Si_4

We calculated the electronic band structures of P_4Si_4 for a wide range (–10 % to 10 %) of bi-axial strain. As already mentioned, pristine P_4Si_4 is a metallic compound. For the tensile strain, the valance bands and the conduction bands of P_4Si_4 do not change significantly. For compressive strain up to –6%, we do not find any significant change in the band structure of P_4Si_4 . However, under the compressive strain of –8 % and –10 % (see Fig. 4), P_4Si_4 transforms to an indirect bandgap semiconductor from its metallic state. Also, the presence of almost top flat valence band in these structures indicates the possibility that hole doping may cause doping-induced Stoner instability, which might lead to ferromagnetic ground states.

Impact of Bi-axial Strain on the Electronic Dispersion of PSi_3

We calculated the electronic band structures of PSi_3 for a wide range (–10 % to 10 %) of bi-axial strain. As already mentioned, pristine PSi_3 is an indirect bandgap semiconductor. When tensile strain is applied on PSi_3 , valence bands do not shift significantly but the conduction bands move downwards. However, we do not observe any semiconductor to metal transition up to 10% of tensile strain. Application of compressive strain beyond –4% (see Fig. 5), reduces

Fig. 4: Opening of the bandgap observed in P_4Si_4 (that is originally a metal), under the applied bi-axial strain –10 % and –8 %

the bandgap and, hence, converts the PSi_3 to a metallic compound. The transition from semiconductor to metal occurs at compressive strain of –3%.

Impact of Bi-axial Strain on the Electronic Dispersion of P_2Si

We calculated the electronic band structures of P_2Si for a wide range (–10 % to 10 %) of bi-axial strain. As already mentioned, pristine P_2Si is a metallic compound. When tensile strain (2-8 %) is applied on P_2Si , it is converted to a Dirac semi-metal. As can be

Fig. 5: Closing of the bandgap observed in PSi_3 (that is originally a semiconductor material), under the bi-axial compressive strain -10% to -4%

seen in the Fig. 6, the valence and conduction bands touch each other at 2% or more tensile strain. Under compressive strain, the material remains metallic.

Summary

In summary, we explore the high symmetry $\beta\text{-P}_x\text{Si}_y$ based 2D materials using DFT calculations. We find that out of 6 structures, PSi , PSi_3 , P_4Si_4 , and PSi_2 are metallic, P_3Si is indirect bandgap semiconductor, and most importantly P_2Si is Dirac semi-metal. We have done the stability analysis of these structures based on their formation energy. We find that among all these structures, P_3Si is the most stable one. We also study

Fig. 6: Observation of the perfect Dirac cone in P_2Si structure, under the bi-axial tensile strain 2% to 8%

the effect of external perpendicular electric field on electronic band structures of these materials, but we do not observe any significant change in any of the material. Finally, we studied the effect of bi-axial strain on electronic dispersions of these materials. We observe bandgap opening in P_4Si_4 and bandgap closing in PSi_3 , for compressive strain. In case of P_2Si , perfect Dirac cone is obtained for tensile strain.

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