Phonon dispersions and electronic structures of two-dimensional IV-V compounds

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Abstract

One novel family of two-dimensional IV-V compounds have been proposed, whose dynamical stabilities and electronic properties have been systematically investigated using the density functional theory. Extending from our previous work, two phases of carbon phosphorus bilayers α-C2P2 and β-C2P2 have been proposed. The results indicate both of them are dynamically stable, and are broad band gap insulators with intrinsic HSE gaps of 2.70 eV and 2.67 eV, respectively. More similar α- and β- C2Y2 (Y= As, Sb, and Bi) can be obtained if the phosphorus atoms in the α- and β-C2P2 replaced by other pnictogens, respectively. If the C atoms in the α- and β-C2Y2 (Y= P, As, Sb, and Bi) bilayers are further replaced by other group IV elements X (X=Si, Ge, Sn, and Pb), respectively, more derivatives of α- and β-X2Y2 (X=Si, Ge, Sn, and Pb; Y=N, P, As, Sb, and Bi) also can be obtained. The dynamical stabilities and the electronic properties of all the proposed bilayers have been systematically investigated. It was found that the majority of the two-dimensional IV-V compounds are dynamically stable due to the absence of imaginary modes in their Brillouin zone. The proposed bilayers range from metal to broad gap insulators depending on their constitutions. All insulated bilayers can undergo a transition from insulator to metal under the biaxial strain. Amazingly, some of them can undergo a transition from indirect bandgap to direct bandgap. These new IV-V compounds can become candidates as photovoltaic device, thermoelectric material field as well as lamellated superconductors.

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Introduction

Since the discovery of graphene by the mechanical exfoliation in experiment 1, the research on this fantastic two-dimensional (2D) materials has become a focus due to its superior electronic 2 and transport properties 3-5. Similarly, some other 2D materials comprised of IV group atoms, such as silicene, 2D germanium 6, stanene 7, and plumbene 8-9, have been proposed by the theoretical method. All of them can exhibit topological properties under certain conditions 7-12, and some phases have been realized in experiment 13-16. On the other hand, various 2D monolayers comprised of V atoms also have been widely investigated both theoretically 17-20 and experimentally 21-23. Particularly, the few-layer phosphorene has an impressive potential application due to its high mobility 24-25 and novel transport properties 26. As large tunable bandgap insulators, the nitrogen atomic monolayers 27-31 perhaps be applied in the straintronics field 32. Following the astonishing superconductivity and correlated property have been detected in the bilayer twisted graphene 33-39, the investigation of bilayer twisted materials enriched the potential application of 2D materials 40-43.

Besides the exploration of the 2D materials comprised of only one element in group IV or V, various binary compounds also received significant attention in recent years. For example, three phases of carbon nitride bilayers have been introduced in our previous work 44, which exhibit novel electronic and mechanical properties 45, 46. As the nearest neighbor of nitrogen in group V, the phosphorus can also form various binaries with the carbon. The study on organophosphorus compounds contain both carbon and phosphorus is an active field in material science. The phosphorus-carbon binary compounds, which are referred to as phosphorus carbides (PCs), with various stoichiometries have been studied both experimentally and theoretically 47. Recently, various 2D carbon-phosphorus (CPs) monolayers have been predicted by the first principle investigations 48, 49, 50-53. The α-CP, β-CP, and γ-CP are promising 2D materials in optoelectronics as well as electronics 48, and the black phosphorus carbide (α-CP) monolayers is a potential material of gas sensors 54. Furthermore, the few-layer black carbide phosphorus (α-CP) has a bright application of the field-effect transistor in experiment 55. The stable phosphorus carbide (β0-PC) monolayer 49 can exhibit robust superconducting behavior 56. It has been found that the Phosphorus-carbon bond could enhance the performance of battery anodes 57. The carbon can also form monolayers with the other elements in group V, the 2D material M2C3 (M = As, Sb, and Bi) with high carrier mobility have potential applications in the photovoltaic field 58.
This work begins with two phases of carbon phosphorus monolayers, named \(\alpha\)-C\(_2\)P\(_2\) and \(\beta\)-C\(_2\)P\(_2\), respectively. Based on the structures of two monolayers, a family monolayers \(\alpha\)-C\(_2\)Y\(_2\) and \(\beta\)-C\(_2\)Y\(_2\) (Y = As, Sb, and Bi) have been proposed by replacing the phosphorus atoms with the others in group V. All the \(\alpha\)-C\(_2\)Y\(_2\) and \(\beta\)-C\(_2\)Y\(_2\) (Y = P, As, Sb, and Bi) have been systematically investigated. These 2D materials are dynamically stable, and range from insulators to metals, in which the insulators can occur insulator-metal transition under strains. Furthermore, as the carbon in \(\alpha\)- and \(\beta\)-C\(_2\)Y\(_2\) (Y = P, As, Sb, and Bi) replaced by the other elements X (X = Si, Ge, Sn, and Pb) in group IV, more monolayers have been proposed, and the dynamical stabilities, as well as the electronic properties, have been systematically investigated.

**Calculation methods**

The projector augmented wave and Perdew-Burke-Ernzerhof (PBE) functional exchange-correlation 59 have been used to optimize the crystal structures and calculate the electronic structures by the Vienna Ab initio Simulation Package (VASP) code 60. A screened Coulomb potential has been used in the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional calculation 61 62. A vacuum no less than 20 Å has been inserted to the bilayers. The structures have been relaxed until all the components of the net forces on the ions are no more than \(10^{-4}\) eV/Å, and the convergence criterion in the electronic iteration is \(10^{-8}\) eV. The Brillouin zone was sampled by the 20×20×1 \(\Gamma\)-centered grid. The finite displacement method has been used to calculate the phonon dispersions by VASP + Phonopy 63. The cut-off energy and the size of the supercells for calculations of the force constants are available in the Supplementary Material (SM).

**Results and discussion**

Enlightened by the previously predicated carbon nitride bilayers 64, we proposed two types of carbon phosphorus (C\(_2\)P\(_2\)) bilayers in this work. As the nitrogen (N) atoms in the \(\alpha\)- and \(\beta\)-C\(_2\)N\(_2\) replaced by the phosphorus (P) atoms, two similar bilayers can be obtained, named \(\alpha\)-C\(_2\)P\(_2\) and \(\beta\)-C\(_2\)P\(_2\), respectively. The lattice structures of the 2D materials in the equilibrium state are shown in Figure 1(a-b), which are consisted of two carbon phosphorus monolayers through the C-C bonds. Both phases are hexagonal structures with the same crystal lattice parameters, the lattice constants \(a\), the length of interlayer C-P band \(l_{C-P}\), and the thickness \(\delta\)
Figure 1. Top view and side view of (a) $\alpha$-C$_2$P$_2$ and (b) $\beta$-C$_2$P$_2$ bilayer, respectively. The grey and light-yellow spheres denote carbon and phosphorus atoms, respectively. (c) The first Brillouin zone of the two phases.

Table 1. The crystal lattice parameters of C$_2$Y$_2$ (Y=N, P, As, Sb, and Bi) (Unit in Å)

| Phase   | $a$  | $l_{C-C}$ | $l_{C-Y}$ | $\delta$ |
|---------|------|-----------|-----------|----------|
| $\alpha$-C$_2$N$_2$ | 2.35 | 1.62      | 1.44      | 2.60     |
| $\beta$-C$_2$N$_2$ | 2.35 | 1.62      | 1.44      | 2.60     |
| $\alpha$-C$_2$P$_2$ | 2.90 | 1.55      | 1.89      | 3.30     |
| $\beta$-C$_2$P$_2$ | 2.90 | 1.55      | 1.89      | 3.30     |
| $\alpha$-C$_2$As$_2$ | 3.11 | 1.53      | 2.04      | 3.46     |
| $\beta$-C$_2$As$_2$ | 3.11 | 1.53      | 2.04      | 3.46     |
| $\alpha$-C$_2$Sb$_2$ | 3.41 | 1.53      | 2.25      | 3.71     |
| $\beta$-C$_2$Sb$_2$ | 3.41 | 1.53      | 2.25      | 3.71     |
| $\alpha$-C$_2$Bi$_2$ | 3.60 | 1.49      | 2.38      | 3.79     |
| $\beta$-C$_2$Bi$_2$ | 3.60 | 1.49      | 2.38      | 3.79     |

of them are 2.90 Å, 1.89 Å, and 3.30 Å, respectively, which are larger than the $\alpha$- and $\beta$-C$_2$N$_2$
Figure 2. Phonon dispersions of the C$_2$Y$_2$ (Y = P, As, Sb, and Bi) bilayers. (a)–(b) are the phonon dispersions of $\alpha$-C$_2$P$_2$, $\beta$-C$_2$P$_2$, $\alpha$-C$_2$As$_2$, $\beta$-C$_2$As$_2$, $\alpha$-C$_2$Sb$_2$, $\beta$-C$_2$Sb$_2$, $\alpha$-C$_2$Bi$_2$, and $\beta$-C$_2$Bi$_2$, respectively.

44, as shown in Table 1. While the length of C-C bonds $l_{C-C}$ between layers is 1.55 Å, which is shorter than the C$_2$N$_2$ bilayers, but 0.13 Å longer than C-C bonds in the graphene. Both C-C bonding and C-P bonding are sp$^3$ hybridized. Furthermore, more similar bilayers C$_2$Y$_2$ (Y = As, Sb, and Bi) can be obtained as the P atoms in the $\alpha$- and $\beta$-C$_2$P$_2$ replaced by the Y (Y = As, Sb, and Bi) atoms in group V, which have the similar lattice structures and bonding characteristic of C$_2$P$_2$ bilayers. The fully optimized crystal lattice parameters of C$_2$Y$_2$ (Y = N, P, As, Sb, and Bi) in Table 1 indicate that as the atomic number of Y (Y = N, P, As, Sb, and Bi) atom increases, the lattice constant $a$, the length of interlayer C-Y bond $l_{C-Y}$, and the thickness of the bilayers $\delta$ are monotonously increasing, while the distance between the nearest carbon atoms $l_{C-C}$ is monotonously decreasing. This trend is consistent with the periodic law of the elements. Similar 2D materials can be obtained if the carbon atoms in C$_2$Y$_2$ (Y = N, P, As, Sb, and Bi) bilayers are replaced by the Group-V elements (Si, Ge, Sn, and Pb), which denoted as X$_2$Y$_2$ (X = Si, Ge, Sn, and Pb; Y = N, P, As, Sb, and Bi). These derivatives have similar lattice structures and symmetry as $\alpha$- or $\beta$-C$_2$P$_2$, as shown in Figure 1. The fully optimized crystal lattice parameters of the derivatives are available in Table S (1-4) of the SM. The crystal lattice parameters indicate that, for each particular X (X = Si, Ge, Sn, and Pb) element, as the atomic number of Y atom increases, the lattice constant $a$, the X-Y bond length $l_{X-Y}$, and the thickness of the bilayers $\delta$ are monotonously increasing, while the distances between the two nearest atoms in group IV $l_{X-X}$ are monotonously decreasing. All the X$_2$Y$_2$ (X = C, Si, Ge, Sn, and Pb;
Figure 3. Band structure of $\alpha$-C$_2$P$_2$ (a) and $\beta$-C$_2$P$_2$ (b), the solid blue lines denote results from PBE, and the red dash lines denote results from HSE06.

Y=N, P, As, Sb, and Bi) bilayers are hexagonal structures, and the point group of both $\alpha$ and $\beta$ types are D$_{3h}$ and D$_{3d}$, respectively. In each layer, the X (X=C, Si, Ge, Sn, and Pb) atoms and Y (Y=P, As, Sb, and Bi) atoms are sp$^3$ hybridized instead of coplanar. The Brillouin zone (BZ) of them are regular hexagons, as shown in Figure 1(c).

To study the dynamical stabilities of all the 46 phases proposed bilayers, their phonon dispersions have been calculated by the first principle theory. The phonon dispersions of the $\alpha$- and $\beta$-C$_2$Y$_2$ (Y=P, As, Sb, and Bi) bilayers, as shown in Figure 2(a-h), exhibit no imaginary frequencies in the BZ, which means all of them are dynamically stable. The greater atomic mass of the Y (Y=P, As, Sb, Bi) atoms results in smaller acoustic velocities, higher optical frequencies, and broader frequency gaps. Furthermore, for $\alpha$-Si$_2$P$_2$, $\beta$-Si$_2$P$_2$, $\alpha$-Si$_2$As$_2$, $\beta$-Si$_2$As$_2$, $\beta$-Ge$_2$P$_2$, $\alpha$-Ge$_2$As$_2$, $\beta$-Ge$_2$As$_2$, $\beta$-Sn$_2$N$_2$, $\beta$-Sn$_2$P$_2$, $\beta$-Sn$_2$As$_2$, and $\alpha$-Sn$_2$Bi$_2$, small imaginary frequency modes are present at the vicinity of $\Gamma$. All other derivatives of X$_2$Y$_2$ (X=Si, Ge, Sn, and Pb; Y=N, P, As, Sb, and Bi) bilayers are dynamically stable. The phonon dispersions of these materials are available in Figure S of SM. The lowest acoustic modes of $\alpha$-Pb$_2$N$_2$, $\beta$-Pb$_2$N$_2$, $\alpha$-Pb$_2$Bi$_2$, and $\beta$-Pb$_2$Bi$_2$ exhibit visible imaginary frequencies around K points or along the $\Gamma$-K line in the BZ, as shown in Figure S(15, and 19) of the SM, which means these bilayers may not be dynamically stable in the free state.

The $\alpha$- and $\beta$-C$_2$P$_2$ bilayers are indirect insulators with a gap of 1.79 eV and 1.77 eV on the PBE level, respectively, as shown in Figure 3. On the HSE level, their band gaps become
The blue solid and broken red line curve denotes calculated by PBE and PBE+SOC, respectively. 2.70 eV and 2.67 eV, respectively, which are much narrower than the α- and β-C2N2. The conducting minimums (CBM) of the α- and β-C2P2 at the M and K point in the BZ, respectively. And the valence band maximum (VBM) of both at the Γ points. The spin-orbital coupling (SOC) had not been included in the calculation of α- and β-C2P2, while for C2Y2 (Y=As, Sb, and Bi), the SOC have been included in the electronic structure calculation.

As shown in Figure 4(a-c), all the α-C2As2, β-C2As2, and α-C2Sb2 are indirect gap insulators with or without SOC. The calculated gaps of the three phases from PBE are 1.18 eV, 1.02 eV, and 0.22 eV, respectively. And the ones from PBE+SOC calculations are 1.09 eV, 0.95 eV, and 0.07 eV, respectively. As the SOC breaks the degeneracy of the bands in the BZ, the gaps have been decreased by 0.09 eV, 0.07 eV, and 0.15 eV, respectively. The other three phases, β-C2Sb2, α-C2Bi2, and β-C2Bi2, are metals with or without SOC. Interestingly, for both α- and β-C2Bi2, there are four crossbands near the Γ points without the SOC, which disappear if the SOC is included. These results imply the possible topological superconductivity under some specific conditions. The values of the bandgaps, the positions of CBM, and VBM are listed in Table 2. From Table 2, we can conclude that for a particular α or β type lattice structure, as the atomic number of group V increases, the band gaps monotonously decrease, while the effect of SOC in the bands increases. Furthermore, the electronic bands of the derivatives X2Y2.
The electronic band parameters of C$_2$Y$_2$ (Y=N, P, As, Sb, and Bi) in the PBE background.

| Phase   | PBE   | PBE+SOC | $\Delta$ | $\varepsilon_C$ (%) |
|---------|-------|---------|----------|---------------------|
|         | Gap1 (eV) | CBM position | VBM position | Gap2 (eV) | CBM position | VBM position |          |
| $\alpha$-C$_2$N$_2$ | 3.76 | M | K-\Gamma | / | / | / | / | 27$^\dagger$ 44 |
| $\beta$-C$_2$N$_2$ | 4.23 | M | K-\Gamma | / | / | / | / | 22$^\dagger$ 44 |
| $\alpha$-C$_2$P$_2$ | 1.79$^i$ | K | $\Gamma$ | / | / | / | / | 19$^\dagger$ |
| $\beta$-C$_2$P$_2$ | 1.77$^i$ | M | $\Gamma$ | / | / | / | / | 24$^\dagger$ |
| $\alpha$-C$_2$As$_2$ | 1.18$^i$ | K | $\Gamma$ | 1.09$^i$ | K | $\Gamma$ | -0.09 | 14$^\dagger$ |
| $\beta$-C$_2$As$_2$ | 1.02$^i$ | M | $\Gamma$ | 0.95$^i$ | M | $\Gamma$ | -0.07 | -16$^\dagger$ |
| $\alpha$-C$_2$Sb$_2$ | 0.22$^i$ | K | $\Gamma$ | 0.07$^i$ | K | $\Gamma$ | -0.15 | 10$^\dagger$ |
| $\beta$-C$_2$Sb$_2$ | 0 | M | $\Gamma$ | 0 | M | $\Gamma$ | 0 | 16$^\dagger$ |
| $\alpha$-C$_2$Bi$_2$ | 0 | / | / | 0 | M-K | $\Gamma$ | 0 | / |
| $\beta$-C$_2$Bi$_2$ | 0 | / | / | 0 | M | $\Gamma$ | 0 | / |

The superscript $d$ represents the direct gap, and $i$ represents the indirect gap. Gap1 and Gap2 represent the band gaps calculated by PBE and PBE+SOC, respectively, $\Delta$ = Gap2-Gap1. $\varepsilon_C$ represents the critical strain from insulativity to metallicity. $^*$ represents the critical strain in the PBE background, $^\dagger$ represents the critical strain in the PBE+SOC background. / represents blank.

(X=Si, Ge, Sn, and Pb; Y= N, P, As, Sb, and Bi) also have been calculated, whose electronic band parameters (the gap value, the CBM, and the VBM positions) listed in Table S (5-8) of the SM.

In the actual applications, the 2D materials are usually attached to the particular substrates, and they are subjected to inevitable lattice mismatch, in which the lattice is either strained or compressed. In other words, the bandgap can be tuned by strain, which is a useful method in the nano materials research field 65-68. Because the crystal lattices are regular hexagons, the biaxial strain has been applied to tune the bandgap. As shown in Figure 6(a), as the biaxial strain increase, both bandgap of $\alpha$- and $\beta$-C$_2$P$_2$ monotonically decrease and exhibit linear relations in the range 2-12% and 4-13%, respectively. The gaps of $\alpha$- and $\beta$-C$_2$P$_2$ close as the strain reach 19% and 24%, respectively. Because of the realignment of bands in the strain, there are two maxima at 2% and 3-4%, respectively. From the PBE+SOC calculation, the CBM of $\alpha$-C$_2$As$_2$ at the K point in the free state, as shown in Figure 4(a). As the strain increases, the CBM shifts from K point to $\Gamma$ point, which induces the indirect gap turns to a direct one, as shown in Figure 5(a). The gap will close at strain 14%, if the strain increases further, the conducting band and valence band will cross the Fermi level, as shown in Figure 5(b). Similar
Figure 5. Band structure of $\alpha$-C$_2$As$_2$ under the strain of (a) 12% and (b) 18%, $\beta$-C$_2$As$_2$ under the strain of (c) 14%, and (d) 18% calculated by PBE+SOC.

to $\alpha$-C$_2$As$_2$, the CBM of $\beta$-C$_2$As$_2$ at M points in the free state, as shown in Figure 4(b). As the strain increases, the CBM shifts from K point to $\Gamma$ point, which also induces the transition from the indirect gap to a direct gap, as shown in Figure 5(c). The $\beta$-C$_2$As$_2$ bilayer will become a semimetal with zero gap at 16% strain, whose CBM and VBM degenerate at $\Gamma$ point. Amusingly, the band gap will reopen if the strain increases further, as shown in Figure 5(d).

There are also two maxima at 2% and 6% in the gap-strain relations of $\alpha$-C$_2$As$_2$ and $\beta$-C$_2$As$_2$, as shown in Figure 6(b), respectively. The band gaps of $\alpha$-C$_2$Sb$_2$ and $\beta$-C$_2$Sb$_2$ also close as the strain reach 10% and 16%, respectively. There are two maximum points at 2% and 5%, respectively, as shown in Figure 6(c). Each total energies of the $\alpha$- and $\beta$-C$_2$Y$_2$ (Y=P, As, and Sb) monotonically increase as the strain increases, as shown in Figure 6(d), and the total energy of each $\beta$ phase is a bit lower than the $\alpha$ one for any strains. Furthermore, the other insulators, $\alpha$-Si$_2$P$_2$, $\beta$-Si$_2$P$_2$, $\alpha$-Si$_2$As$_2$, $\beta$-Si$_2$As$_2$, $\alpha$-Si$_2$Sb$_2$, $\beta$-Si$_2$Sb$_2$, $\alpha$-Si$_2$Bi$_2$, $\beta$-Si$_2$Bi$_2$, $\alpha$-Ge$_2$N$_2$, $\beta$-Ge$_2$N$_2$, $\alpha$-Ge$_2$P$_2$, $\beta$-Ge$_2$P$_2$, $\alpha$-Ge$_2$As$_2$, $\beta$-Ge$_2$As$_2$, $\alpha$-Ge$_2$Sb$_2$, $\beta$-Ge$_2$Sb$_2$, $\alpha$-Sn$_2$P$_2$, $\beta$-Sn$_2$P$_2$, $\alpha$-Sn$_2$As$_2$, $\beta$-Sn$_2$As$_2$, $\alpha$-Sn$_2$Sb$_2$, $\beta$-Sn$_2$Sb$_2$, $\alpha$-Pb$_2$P$_2$, $\beta$-Pb$_2$P$_2$, $\alpha$-Pb$_2$As$_2$, and $\beta$-Pb$_2$As$_2$ also can undergo insulator-metal transition by the biaxial strain, as shown in Figure S(39-51), and the critical strains of the bilayers listed in Table S(5-9).
Figure 6. Dependence of energy gaps on the strain of (a) C$_2$P$_2$, (b) C$_2$As$_2$, (c) C$_2$Sb$_2$, and (d) the total energies of them.

Conclusions

Forty-six phases of 2D IV-V compounds have been proposed as an extension of our previous work. The dynamical stabilities and electronic properties have been investigated using the density functional theory. The fully optimized structural parameters of the bilayers exhibit trends that are consistent with the periodic law of elements. The phonon dispersions indicate the majority of the bilayers are dynamically stable in the free state. From the phonon dispersions of the 2D IV-V compounds, one can find that, as the atomic number in the bilayers increases, the highest optical frequency of the phonon decreases. The greater atomic mass of the bilayers implies stronger stability. The calculated electronic structures indicate that the bilayers range from insulators to metals with various band gaps, depending on the components. Usually, the bilayers containing lighter elements in group IV and lighter elements in group V exhibit broader bandgaps. With a higher atomic number, the SOC effect on the electronic band becomes more significant. For a particular element in group IV, the bilayers own familiar band structures, and the band gap decreases as the atomic number increases. The band gap of the majority bilayers can decrease under strain, even closes, and exhibit transition from insulator
to metal. Besides, the band gap of some special bilayers will increase in the beginning, and then decrease and eventually close under the biaxial stain. The wide-gap bilayers may have potential applications in the photovoltaic devices, and the narrow bandgap ones may become thermoelectric materials. Furthermore, the superconductivity can be investigated by analyzing the electroacoustic coupling effect of the gapless bilayers. In a word, the new 2D materials proposed in this work perhaps become competent candidates in the spintronics and straintronics field.

We find a parallel work of α-C2P2 published 69.

Conflicts of interest

The authors declare no competing interests.

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Supplementary Material for
Phonon dispersions and electronic structures of two-dimensional IV-V compounds

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I. Crystal lattice parameters

The lattice constants and the distance between the nearest carbon atoms $l_{Si-Y}$, the Si-Y bond, and the thick of the bilayers $\delta$ can be obtained by fully optimized.

Table S1. Crystal lattice parameters of Si$_2$Y$_2$ (Y=N, P, As, Sb, Bi) (Unit in Å)

| Phase    | $a$  | $l_{X-X}$ | $l_{X-Y}$ | $\delta$ |
|----------|------|-----------|-----------|----------|
| $\alpha$-Si$_2$N$_2$ [1] | 2.90 | 2.43      | 1.76      | 3.54     |
| $\beta$-Si$_2$N$_2$ [1]  | 2.90 | 2.43      | 1.76      | 3.54     |
| $\alpha$-Si$_2$P$_2$     | 3.53 | 2.37      | 2.28      | 4.41     |
| $\beta$-Si$_2$P$_2$      | 3.53 | 2.37      | 2.28      | 4.41     |
| $\alpha$-Si$_2$As$_2$    | 3.69 | 2.36      | 2.40      | 4.58     |
| $\beta$-Si$_2$As$_2$     | 3.69 | 2.36      | 2.40      | 4.58     |
| $\alpha$-Si$_2$Sb$_2$    | 4.02 | 2.36      | 2.62      | 4.82     |
| $\beta$-Si$_2$Sb$_2$     | 4.02 | 2.36      | 2.62      | 4.82     |
| $\alpha$-Si$_2$Bi$_2$    | 4.17 | 2.35      | 2.73      | 4.92     |
| $\beta$-Si$_2$Bi$_2$     | 4.17 | 2.35      | 2.73      | 4.92     |

Table S2. Crystal lattice parameters of Ge$_2$Y$_2$ (Y=N, P, As, Sb, Bi) (Unit in Å)

| Phase    | $a$  | $l_{X-X}$ | $l_{X-Y}$ | $\delta$ |
|----------|------|-----------|-----------|----------|
| $\alpha$-Ge$_2$N$_2$ | 3.10 | 2.57      | 1.91      | 3.90     |
| $\beta$-Ge$_2$N$_2$  | 3.10 | 2.57      | 1.91      | 3.90     |
| $\alpha$-Ge$_2$P$_2$ | 3.66 | 2.51      | 2.37      | 4.65     |
| $\beta$-Ge$_2$P$_2$  | 3.66 | 2.51      | 2.37      | 4.65     |
| $\alpha$-Ge$_2$As$_2$ | 3.82 | 2.50      | 2.49      | 4.80     |
| $\beta$-Ge$_2$As$_2$ | 3.82 | 2.50      | 2.49      | 4.80     |
| $\alpha$-Ge$_2$Sb$_2$ | 4.12 | 2.50      | 2.69      | 5.01     |
| $\beta$-Ge$_2$Sb$_2$ | 4.12 | 2.50      | 2.69      | 5.01     |
| $\alpha$-Ge$_2$Bi$_2$ | 4.26 | 2.49      | 2.78      | 5.09     |
| $\beta$-Ge$_2$Bi$_2$ | 4.26 | 2.49      | 2.78      | 5.09     |

Table S3. Crystal lattice parameters of Sn$_2$Y$_2$ (Y=N, P, As, Sb, Bi) (Unit in Å)

| Phase    | $a$  | $l_{X-X}$ | $l_{X-Y}$ | $\delta$ |
|----------|------|-----------|-----------|----------|
| $\alpha$-Sn$_2$N$_2$ | 3.42 | 2.98      | 2.11      | 4.44     |
| $\beta$-Sn$_2$N$_2$  | 3.42 | 2.98      | 2.11      | 4.44     |
| $\alpha$-Sn$_2$P$_2$ | 3.95 | 2.89      | 2.56      | 5.22     |
| $\beta$-Sn$_2$P$_2$  | 3.95 | 2.89      | 2.56      | 5.22     |
| $\alpha$-Sn$_2$As$_2$ | 4.09 | 2.88      | 2.67      | 5.36     |
| $\beta$-Sn$_2$As$_2$ | 4.09 | 2.88      | 2.67      | 5.36     |
| $\alpha$-Sn$_2$Sb$_2$ | 4.38 | 2.87      | 2.87      | 5.58     |
| $\beta$-Sn$_2$Sb$_2$ | 4.38 | 2.87      | 2.87      | 5.58     |
| $\alpha$-Sn$_2$Bi$_2$ | 4.51 | 2.86      | 2.96      | 5.66     |
| $\beta$-Sn$_2$Bi$_2$ | 4.51 | 2.86      | 2.96      | 5.66     |
Table S4. Crystal lattice parameters of Pb$_2$Y$_2$ (Y=N, P, As, Sb, Bi) (Unit in Å)

| Phase   | $a$  | $l_{X-X}$ | $l_{X-Y}$ | $\delta$ |
|---------|------|-----------|-----------|----------|
| $\alpha$-Pb$_2$N$_2$ | 3.64 | 3.17      | 2.24      | 4.75     |
| $\beta$-Pb$_2$N$_2$  | 3.64 | 3.17      | 2.24      | 4.75     |
| $\alpha$-Pb$_2$P$_2$  | 4.12 | 3.06      | 2.67      | 5.49     |
| $\beta$-Pb$_2$P$_2$  | 3.64 | 3.17      | 2.24      | 4.75     |
| $\alpha$-Pb$_2$As$_2$ | 4.25 | 3.05      | 2.77      | 5.62     |
| $\beta$-Pb$_2$As$_2$ | 4.25 | 3.05      | 2.77      | 5.62     |
| $\alpha$-Pb$_2$Sb$_2$ | 4.53 | 3.04      | 2.96      | 5.81     |
| $\beta$-Pb$_2$Sb$_2$ | 4.53 | 3.04      | 2.96      | 5.81     |
| $\alpha$-Pb$_2$Bi$_2$ | 4.63 | 3.02      | 3.03      | 5.89     |
| $\beta$-Pb$_2$Bi$_2$ | 4.63 | 3.02      | 3.03      | 5.89     |
II. Phonon dispersions

Figure S1

Figure S2

Figure S3
Figure S4

Figure S5

Figure S6
Figure S10

Figure S11

Figure S12
Figure S16

Figure S17

Figure S18
Figure S19

Phonon dispersion of $\alpha$-$\text{Pb}_2\text{Bi}_2$

Phonon dispersion of $\beta$-$\text{Pb}_2\text{Bi}_2$
III. Electronic bands

Figure S20. Electronic band of \(\alpha\)-Si\(_2\)P\(_2\) (left) and \(\beta\)-Si\(_2\)P\(_2\) (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.

Figure S21. Electronic band of \(\alpha\)-Si\(_2\)As\(_2\) (left) and \(\beta\)-Si\(_2\)As\(_2\) (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.
Figure S22. Electronic band of $\alpha$-Si$_2$Sb$_2$ (left) and $\beta$-Si$_2$Sb$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.

Figure S23. Electronic band of $\alpha$-Si$_2$Bi$_2$ (left) and $\beta$-Si$_2$Bi$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.

Figure S24. Electronic band of $\alpha$-Ge$_2$N$_2$ (left) and $\beta$-Ge$_2$N$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.
Figure S25. Electronic band of $\alpha$-Ge$_2$P$_2$ (left) and $\beta$-Ge$_2$P$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.

Figure S26. Electronic band of $\alpha$-Ge$_2$As$_2$ (left) and $\beta$-Ge$_2$As$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.

Figure S27. Electronic band of $\alpha$-Ge$_2$Sb$_2$ (left) and $\beta$-Ge$_2$Sb$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.
Figure S28. Electronic band of $\alpha$-Ge$_2$Bi$_2$ (left) and $\beta$-Ge$_2$Bi$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.

Figure S29. Electronic band of $\alpha$-Sn$_2$N$_2$ (left) and $\beta$-Sn$_2$N$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.

Figure S30. Electronic band of $\alpha$-Sn$_2$P$_2$ (left) and $\beta$-Sn$_2$P$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.
Figure S31. Electronic band of $\alpha$-Sn$_2$As$_2$ (left) and $\beta$-Sn$_2$As$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.

Figure S32. Electronic band of $\alpha$-Sn$_2$Sb$_2$ (left) and $\beta$-Sn$_2$Sb$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.

Figure S33. Electronic band of $\alpha$-Sn$_2$Bi$_2$ (left) and $\beta$-Sn$_2$Bi$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.
Figure S34. Electronic band of $\alpha$-Pb$_2$N$_2$ (left) and $\beta$-Pb$_2$N$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.

Figure S35. Electronic band of $\alpha$-Pb$_2$P$_2$ (left) and $\beta$-Pb$_2$P$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.

Figure S36. Electronic band of $\alpha$-Pb$_2$As$_2$ (left) and $\beta$-Pb$_2$As$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.
Figure S37. Electronic band of α-Pb$_2$Sb$_2$ (left) and β-Pb$_2$Sb$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.

Figure S38. Electronic band of α-Pb$_2$Bi$_2$ (left) and β-Pb$_2$Bi$_2$ (right), the solid blue line represents the results calculated by PBE, the red dot line represents the results calculated by PBE+SOC.
IV. Dependence of energy gap on the strain

Figure S39. Dependence of energy gap on the strain of $\alpha$-$\text{Si}_2\text{P}_2$ and $\beta$-$\text{Si}_2\text{P}_2$.

Figure S40. Dependence of energy gap on the strain of $\alpha$-$\text{Si}_2\text{As}_2$ and $\beta$-$\text{Si}_2\text{As}_2$.

Figure S41. Dependence of energy gap on the strain of $\alpha$-$\text{Si}_2\text{Sb}_2$ and $\beta$-$\text{Si}_2\text{Sb}_2$.

Figure S42. Dependence of energy gap on the strain of $\alpha$-$\text{Si}_2\text{Bi}_2$ and $\beta$-$\text{Si}_2\text{Bi}_2$. 
Figure S43. Dependence of energy gap on the strain of $\alpha$-Ge$_2$N$_2$ and $\beta$-Ge$_2$N.

Figure S44. Dependence of energy gap on the strain of $\alpha$-Ge$_2$P$_2$ and $\beta$-Ge$_2$P$_2$.

Figure S45. Dependence of energy gap on the strain of $\alpha$-Ge$_2$As$_2$ and $\beta$-Ge$_2$As$_2$.

Figure S46. Dependence of energy gap on the strain of $\alpha$-Ge$_2$Sb$_2$ and $\beta$-Ge$_2$Sb.
Figure S47. Dependence of energy gap on the strain of $\alpha$-Sn$_2$P$_2$ and $\beta$-Sn$_2$P$_2$.

Figure S48. Dependence of energy gap on the strain of $\alpha$-Sn$_2$As$_2$ and $\beta$-Sn$_2$As$_2$.

Figure S49. Dependence of energy gap on the strain of $\alpha$-Sn$_2$Sb$_2$ and $\beta$-Sn$_2$Sb$_2$.

Figure S50. Dependence of energy gap on the strain of $\alpha$-Pb$_2$P$_2$ and $\beta$-Pb$_2$P$_2$. 
Figure S51. Dependence of energy gap on the strain of $\alpha$-Pb$_2$As$_2$ and $\beta$-Pb$_2$As$_2$. 
V. Electronic band parameters

Table S5. Electronic band parameters of Si$_2$Y$_2$(Y=N, P, As, Sb, and Bi) in the PBE background.

| Phase      | PBE         | PBE+SOC     | $\Delta$ | $\varepsilon_C$ (%) |
|------------|-------------|-------------|----------|---------------------|
|            | Gap1 (eV)  | CBM position | VBM position | Gap2 (eV) | CBM position | VBM position |          |            |
| $\alpha$-Si$_2$N$_2$ [1] | 1.73$^i$ | M | K-$\Gamma$ | / | / | / | 17$^*$ |
| $\beta$-Si$_2$N$_2$ [1] | 1.89$^i$ | M | K-$\Gamma$ | / | / | / | 16$^*$ |
| $\alpha$-Si$_2$P$_2$ | 1.489$^i$ | M | $\Gamma$-$K$ | 1.486$^i$ | M | $\Gamma$-$K$ | -0.003 | 18 |
| $\beta$-Si$_2$P$_2$ | 1.820$^i$ | M | $\Gamma$-$K$ | 1.822$^i$ | M | $\Gamma$-$K$ | 0.002 | 14 |
| $\alpha$-Si$_2$As$_2$ | 1.60$^i$ | M | $\Gamma$ | 1.52$^i$ | M | $\Gamma$ | -0.08 | 18 |
| $\beta$-Si$_2$As$_2$ | 1.86$^i$ | M | $\Gamma$ | 1.77$^i$ | M | $\Gamma$ | -0.09 | 13 |
| $\alpha$-Si$_2$Sb$_2$ | 1.19$^i$ | M | $\Gamma$ | 0.99$^i$ | M | $\Gamma$ | -0.2 | 20 |
| $\beta$-Si$_2$Sb$_2$ | 1.04$^i$ | M | $\Gamma$ | 0.86$^i$ | M | $\Gamma$ | -0.18 | 20 |
| $\alpha$-Si$_2$Bi$_2$ | 0.61$^d$ | $\Gamma$ | $\Gamma$ | 0.23$^d$ | $\Gamma$ | $\Gamma$ | -0.38 | 20 |
| $\beta$-Si$_2$Bi$_2$ | 0.73$^d$ | $\Gamma$ | $\Gamma$ | 0.33$^d$ | $\Gamma$ | $\Gamma$ | 0.4 | 16 |

The superscript $i$ represents the direct gap, and $d$ represents the indirect gap. Gap1 and Gap2 represent the band gaps calculated by PBE and PBE+SOC, respectively, $\Delta$=Gap2-Gap1. $\varepsilon_C$ denotes the critical strain from insulativity to metallicity. * represents the critical stain in the PBE background, the others are in the PBE+SOC background. / represents blank.

Table S6. Electronic band parameters of Ge$_2$Y$_2$(Y=N, P, As, Sb, and Bi) in the PBE background.

| Phase      | PBE         | PBE+SOC     | $\Delta$ | $\varepsilon_C$ (%) |
|------------|-------------|-------------|----------|---------------------|
|            | Gap1 (eV)  | CBM position | VBM position | Gap2 (eV) | CBM position | VBM position |          |            |
| $\alpha$-Ge$_2$N$_2$ | 1.172$^i$ | $\Gamma$ | $\Gamma$-$K$ | 1.174$^i$ | $\Gamma$ | $\Gamma$-$K$ | 0.002 | 5 |
| $\beta$-Ge$_2$N$_2$ | 1.062$^i$ | $\Gamma$ | $\Gamma$-$K$ | 1.067$^i$ | $\Gamma$ | $\Gamma$-$K$ | 0.005 | 5 |
| $\alpha$-Ge$_2$P$_2$ | 1.34$^i$ | M | $\Gamma$-$K$ | 1.32$^i$ | M | $\Gamma$-$K$ | -0.02 | 11 |
| $\beta$-Ge$_2$P$_2$ | 1.201$^i$ | M | $\Gamma$-$K$ | 1.185$^i$ | M | $\Gamma$-$K$ | -0.016 | 9 |
| $\alpha$-Ge$_2$As$_2$ | 1.195$^i$ | M | $\Gamma$ | 1.062$^i$ | M | $\Gamma$ | -0.133 | 10 |
| $\beta$-Ge$_2$As$_2$ | 1.091$^i$ | M | $\Gamma$ | 0.956$^i$ | M | $\Gamma$ | -0.135 | 9 |
| $\alpha$-Ge$_2$Sb$_2$ | 0.656$^i$ | M | $\Gamma$ | 0.426$^i$ | M | $\Gamma$ | -0.23 | 14 |
| $\beta$-Ge$_2$Sb$_2$ | 0.495$^i$ | M | $\Gamma$ | 0.273$^i$ | M | $\Gamma$ | -0.222 | 11 |
| $\alpha$-Ge$_2$Bi$_2$ | 0.224$^d$ | $\Gamma$ | $\Gamma$ | 0 | / | / | -0.224 | / |
| $\beta$-Ge$_2$Bi$_2$ | 0.284$^d$ | M | $\Gamma$ | 0 | / | / | -0.284 | / |

The superscript $i$ represents the direct gap, and $d$ represents the indirect gap. Gap1 and Gap2 represent the band gaps calculated by PBE and PBE+SOC, respectively, $\Delta$=Gap2-Gap1. $\varepsilon_C$ denotes the critical strain from insulativity to metallicity. / represents blank.
Table S7. Electronic band parameters of Sn$_2$Y$_2$(Y=N, P, As, Sb, and Bi) in the PBE background.

| Phase      | PBE           | PBE+SOC       | Δ    | $\varepsilon_C$ (%) |
|------------|---------------|---------------|------|---------------------|
|            | Gap1 (eV)    | CBM position | VBM position | Gap2 (eV) | CBM position | VBM position |
| $\alpha$-Sn$_2$N$_2$ | 0.125$^t$ | $\Gamma$ | $\Gamma$-$K$ | 0.123$^i$ | $\Gamma$ | $\Gamma$-$K$ | -0.002 | 1 |
| $\beta$-Sn$_2$N$_2$ | 0.050$^i$ | $\Gamma$ | $\Gamma$-$K$ | 0.058$^i$ | $\Gamma$ | $\Gamma$-$K$ | 0.008 | 1 |
| $\alpha$-Sn$_2$P$_2$ | 1.280$^i$ | M | $\Gamma$-$K$ | 1.255$^i$ | M | $\Gamma$-$K$ | -0.025 | 8 |
| $\beta$-Sn$_2$P$_2$ | 1.196$^i$ | M | $\Gamma$-$K$ | 1.175$^i$ | M | $\Gamma$-$K$ | -0.021 | 7 |
| $\alpha$-Sn$_2$As$_2$ | 1.128$^d$ | $\Gamma$ | $\Gamma$ | 1.027$^d$ | $\Gamma$ | $\Gamma$ | -0.101 | 8 |
| $\beta$-Sn$_2$As$_2$ | 1.075$^d$ | $\Gamma$ | $\Gamma$ | 0.975$^i$ | $\Gamma$ | $\Gamma$ | -0.1 | 7 |
| $\alpha$-Sn$_2$Sb$_2$ | 0.289$^i$ | M | $\Gamma$ | 0.057$^i$ | M-$K$ | $\Gamma$ | -0.232 | 8 |
| $\beta$-Sn$_2$Sb$_2$ | 0.151$^i$ | M | $\Gamma$ | 0 | / | / | -0.151 | 4 |
| $\alpha$-Sn$_2$Bi$_2$ | 0.475$^d$ | $\Gamma$ | $\Gamma$ | 0 | / | / | -0.475 | / |
| $\beta$-Sn$_2$Bi$_2$ | 0.493$^d$ | $\Gamma$ | $\Gamma$ | 0 | / | / | -0.493 | / |

The superscript $t$ represents the direct gap, and $d$ represents the indirect gap. Gap1 and Gap2 represent the band gaps calculated by PBE and PBE+SOC, respectively, $\Delta=$Gap2-Gap1. $\varepsilon_C$ denotes the critical strain from insulativity to metallicity. / represents blank.

Table S8. Electronic band parameters of Pb$_2$Y$_2$(Y=N, P, As, Sb, and Bi) in the PBE background.

| Phase      | PBE           | PBE+SOC       | Δ    | $\varepsilon_C$ (%) |
|------------|---------------|---------------|------|---------------------|
|            | Gap1 (eV)    | CBM position | VBM position | Gap2 (eV) | CBM position | VBM position |
| $\alpha$-Pb$_2$N$_2$ | 0 | / | / | 0 | / | / | 0 | / |
| $\beta$-Pb$_2$N$_2$ | 0 | / | / | 0 | / | / | 0 | / |
| $\alpha$-Pb$_2$P$_2$ | 0.400$^i$ | M | $\Gamma$-$M$ | 0.313$^i$ | M | $\Gamma$ | -0.087 | 4 |
| $\beta$-Pb$_2$P$_2$ | 0.315$^i$ | M | $\Gamma$-$M$ | 0.260$^i$ | M | $\Gamma$ | -0.055 | 3 |
| $\alpha$-Pb$_2$As$_2$ | 0.363$^i$ | M | $\Gamma$-$M$ | 0.166$^i$ | M | $\Gamma$ | -0.197 | 3 |
| $\beta$-Pb$_2$As$_2$ | 0.261$^i$ | M | $\Gamma$ | 0.098$^i$ | M | $\Gamma$ | -0.163 | 3 |
| $\alpha$-Pb$_2$Sb$_2$ | 0.23$^i$ | M | $\Gamma$ | 0 | / | / | -0.23 | / |
| $\beta$-Pb$_2$Sb$_2$ | 0.120$^i$ | M | $\Gamma$ | 0 | / | / | -0.12 | / |
| $\alpha$-Pb$_2$Bi$_2$ | 0.064$^d$ | $\Gamma$ | $\Gamma$ | 0 | / | / | -0.064 | / |
| $\beta$-Pb$_2$Bi$_2$ | 0 | / | / | 0 | / | / | 0 | / |

The superscript $i$ represents the direct gap, and $d$ represents the indirect gap. Gap1 and Gap2 represent the band gaps calculated by PBE and PBE+SOC, respectively, $\Delta=$Gap2-Gap1. $\varepsilon_C$ denotes the critical strain from insulativity to metallicity. / represents blank.
VI. Computational details

In the calculation of the force constants for phonon dispersions, the cut-off energy and the size of supercells are shown in Table 9.

Table S9. The cut-off energy and the size of the supercells

| phase      | cut-off energy (eV) | size of the supercell | phase      | cut-off energy (eV) | size of the supercell | phase      | cut-off energy (eV) | size of the supercell |
|------------|---------------------|-----------------------|------------|---------------------|-----------------------|------------|---------------------|-----------------------|
| α-C2P2     | 520                 | 6x6x1                 | α-Si2Bi2   | 350                 | 4x4x1                 | α-Sn2As2   | 280                 | 4x4x1                 |
| β-C2P2     | 520                 | 6x6x1                 | β-Si2Bi2   | 350                 | 4x4x1                 | β-Sn2As2   | 280                 | 5x5x1                 |
| α-C2As2    | 520                 | 5x5x1                 | α-Ge2N2    | 520                 | 4x4x1                 | α-Sn2Sb2   | 230                 | 4x4x1                 |
| β-C2As2    | 520                 | 5x5x1                 | β-Ge2N2    | 520                 | 4x4x1                 | β-Sn2Sb2   | 230                 | 4x4x1                 |
| α-C2Sb2    | 520                 | 6x6x1                 | α-Ge2P2    | 335                 | 4x4x1                 | α-Sn2Bi2   | 600                 | 4x4x1                 |
| β-C2Sb2    | 520                 | 6x6x1                 | β-Ge2P2    | 335                 | 5x5x1                 | β-Sn2Bi2   | 600                 | 5x5x1                 |
| α-C2Bi2    | 600                 | 5x5x1                 | α-Ge2As2   | 280                 | 4x4x1                 | α-Pb2N2    | 520                 | 4x4x1                 |
| β-C2Bi2    | 600                 | 5x5x1                 | β-Ge2As2   | 280                 | 5x5x1                 | β-Pb2N2    | 520                 | 5x5x1                 |
| α-Si2N2    | 450                 | 4x4x1                 | α-Ge2Sb2   | 230                 | 5x5x1                 | α-Pb2P2    | 335                 | 5x5x1                 |
| β-Si2N2    | 450                 | 4x4x1                 | β-Ge2Sb2   | 230                 | 5x5x1                 | β-Pb2P2    | 335                 | 5x5x1                 |
| α-Si2P2    | 335                 | 5x5x1                 | α-Ge2Bi2   | 230                 | 5x5x1                 | α-Pb2As2   | 280                 | 4x4x1                 |
| β-Si2P2    | 335                 | 5x5x1                 | β-Ge2Bi2   | 230                 | 5x5x1                 | β-Pb2As2   | 280                 | 5x5x1                 |
| α-Si2As2   | 320                 | 5x5x1                 | α-Sn2N2    | 600                 | 4x4x1                 | α-Pb2Sb2   | 230                 | 4x4x1                 |
| β-Si2As2   | 320                 | 5x5x1                 | β-Sn2N2    | 600                 | 4x4x1                 | β-Pb2Sb2   | 230                 | 5x5x1                 |
| α-Si2Sb2   | 320                 | 5x5x1                 | α-Sn2P2    | 335                 | 4x4x1                 | α-Pb2Bi2   | 138                 | 4x4x1                 |
| β-Si2Sb2   | 320                 | 5x5x1                 | β-Sn2P2    | 335                 | 4x4x1                 | β-Pb2Bi2   | 138                 | 4x4x1                 |

VII. References

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