Supporting information for:

Atomically thin binary V-V compound semiconductor: a first-principles study

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ENERGY-STRAIN RELATION IN α- (β-) AsP MONOLAYERS

In the main manuscript, we have shown that the basic band gap values of AsP depend sensitively on the in-layer strain, which indicates that strain mechanism is an effective way to mediate the electronic properties. To make this realizable, the desirable strains should be available in the elastic regime and at a low energy penalty. The relationships of energy and strains in Fig. S1 indicate that it is exact the case, because both α - and β - AsP are very flexible and require about ~0.20 eV/atom to be stretched or compressed by ~8%, giving rise to dramatic changed electronic properties. In the strain-stress relationship, we also find that the anisotropy in the α -AsP structure, leading to the xdirection normal to the ridges softer than the y-direction along the ridges. We observe an harmonic behavior in both α - and β - AsP for compressive or tensile strain values exceeding ~8%, whether applying uniaxial or biaxial strain.



Fig. S1. (Color online) Energy change in (a) α -AsP and (b) β -AsP monolayers as a function of the in-layer strain, from -10% to 10%, with an interval scale of 2%. The dot line are guides to the eye.

BAND STRUCTURE AND STRAIN RELATIONSHIPS IN α- AND β- Asp MONOLAYERS

As described in the main manuscript, we found that the

band structures of α - and β - AsP depend sensitively on the biaxial or uniform strain, as shown in Fig. S2.



Fig. S2. Band structures of (a) α -AsP and (b) β -AsP with different strains, from -10% to 10%, with an interval scale of 2%. Minus is for the compression, oppositely for the stretch. The Fermi level is set at zero.



Fig. S3. (Color online) Optimum geometry and electronic band structure of (a-d) two different in-layer heterostructures of α -SbNP₂ and (e-h) two different in-layer heterostructures of β -SbNP₂. The heterostructures differ in the arrangement of P atoms.

LATERAL HETEROSTRUCTURES OF SbNP₂

Since both SbN and phosphorene are rather flexible, they may adjust to each other and form in-laver heterostructures at little or no energy penalty. The geometric and electronic structures of the constructed two types of SbNP₂ heterostructures have been shown in Fig. S3. One type of heterostructure, as presented in Fig. S3 (a) and (e), contains P-P and Sb-N atom pairs completely separated from like atom pairs. Another type of heterostructure, as shown in Fig. S3 (c) and (g), contains alternating, contiguous SbN and phosphorus chains. These structures maintain a rectangular lattice with four atoms per unit cell. Generally speaking, we find the in-layer heterostructures to be less stable than pure phosphorene and SbN monolayers. The least stable heterostructures among these are those with isolated P-P or Sb-N atom pairs, as shown in Fig. S3 (a) and (e), which are ~0.02 eV/atom less stable than SbN and phosphorene monolayers due to their highly frustrated geometries. The heterostructures with contiguous phosphorus and SbN chains, as seen in Fig. S3 (c) and (g), may better optimize the nearest neighbor environment. This causes less frustration, making these systems only ~0.01 eV/atom less stable than isolated SbN and phosphorene monolayers. We find all the three in-layer heterostructures to be indirect band gap semiconductors. As in the vertical heterostructures, we find the fundamental band gaps to be substantially smaller than that of isolated SbN and phosphorene monolayers. As seen in Fig. S3 (a), (b), and (e), (f), the fundamental band gap Eg is close to 0.5 eV in the less stable heterostructures with isolated Sb-N and P-P pairs. We find larger band gap values in the more stable heterostructures with contiguous SbN and P chains (*Eg*=0.98eV) in α -SbNP₂ presented in Fig. S3 (c) and (d). The direct band gap Eg=0.37 eV in β -SbNP₂, as shown in Fig. S3 (g) and (h), leading to an infrared shift of absorption spectrum. These findings indicate an interesting possibility

of isoelectronic doping as an effective way to mediate the electronic properties of $SbNP_n$ systems.