Supporting On-Line Information for:
Designing Isoelectronic Counterparts to Layered Group V Semiconductors

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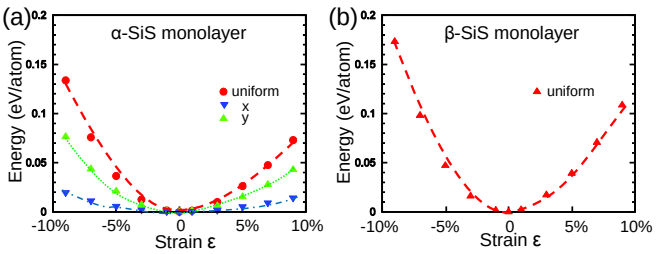

FIG. S1. (Color online) Energy change in (a) α-SiS and (b) β-SiS monolayers as a function of the in-layer strain ϵ. The energy zero corresponds to the optimized, unstrained geometry.

ENERGY-STRAIN RELATION IN α- AND β-SiS MONOLAYERS

We have shown in the main manuscript that the fundamental band gap value of SiS depends sensitively on the in-layer tensile strain, which suggests strain engineering as an effective way to tune the electronic properties. To make this practicable, the desirable strains should be achievable in the elastic regime and at a low energy penalty. Our results in Fig. S1 suggest that this is indeed the case, since both α- and β-SiS are very flexible and require less than 0.05 eV/atom to be stretched or compressed by 5%, which would change their electronic properties significantly. We also find that the anisotropy in the α-SiS structure is also seen in the strain-stress relationship, rendering the x-direction normal to the ridges softer than the y-direction along the ridges. Whether applying uniaxial or uniform strain, we observe anharmonic behavior in both α- and β-SiS for compressive or tensile strain values exceeding ≈5%.

FRONTIER STATES IN SiS/P VERTICAL HETEROSTRUCTURES

As stated in the main manuscript, we found that the interlayer interaction in vertical SiS/P heterostructures, in particular in bilayers, is not purely dispersive. We found evidence for a weak overlap of electronic states in neighboring layers, which cause a significant change in the electronic band structure and the fundamental band

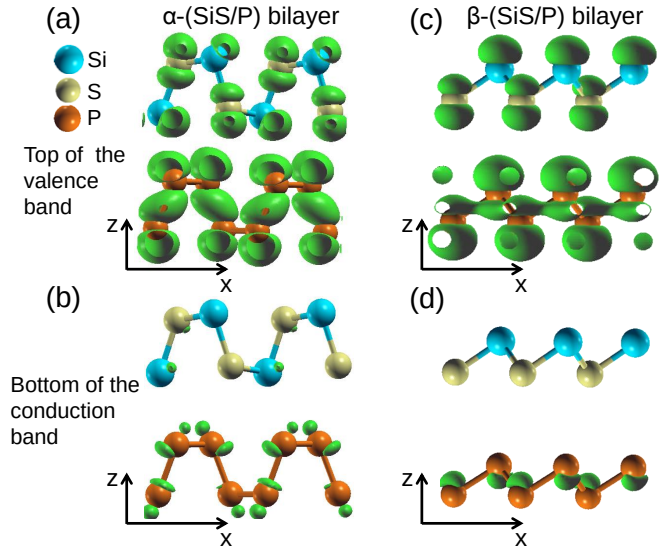

FIG. S2. (Color online) Frontier states in the valence and conduction band range of SiS/P bilayers, presented as ρ =const. isosurfaces superposed to ball-and-stick models of the structure. The energy range represented extends from the mid-gap to 0.1 eV below the top of the valence band (vb) for the valence frontier states and from the mid-gap to 0.1 eV above the bottom of the conduction band (cb) for the conduction frontier states. The isosurface values for α-(SiS/P) are $\rho_{vb} = 6\times10^{-5}$ e/Å^3 in (a) and $\rho_{cb} = 6\times10^{-5}$ e/Å^3 in (b). The isosurface values for β-(SiS/P) are $\rho_{vb} = 9\times10^{-4}$ e/Å^3 in (c) and $\rho_{cb} = 9\times10^{-4}$ e/Å^3 in (d).

gap. As seen in Fig. S2, the frontier states both in the valence and the conduction band region are dominated by phosphorus. Whereas the SiS layers essentially do not contribute at all to the frontier states in the conduction band region, depicted in Fig. S2(b) and S2(d), their contribution to the frontier valence states, shown in Fig. S2(a) and S2(c), is much smaller that that of phosphorene.

STABILITY AND VIBRATIONAL SPECTRA OF α- AND β-SiS

To check the stability of α- and β-SiS monolayers, we calculated the vibration spectra of these structures and display them in Fig. S3. Both spectra lack soft vibration modes or imaginary frequencies, confirming their resistance to spontaneous collapse. The "U" shape feature in the β-SiS spectrum near the Γ-point is a signature of the

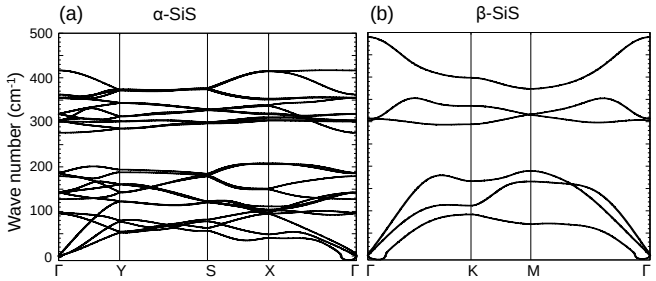

FIG. S3. (Color online) Vibrational spectra of (a) α-SiS and (b) β-SiS monolayers. A super-cell containing 8 atoms has been used for α-SiS and the primitive unit cell has been used for β-SiS.

flexural acoustic mode, which is usually hard to converge in 2D layers. Further stabilization of the monolayers is expected to occur upon deposition on a substrate.

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