Supplementary Material

Band alignment and optoelectronic characteristics of blue phosphorene/SbN van der Waals heterostructures

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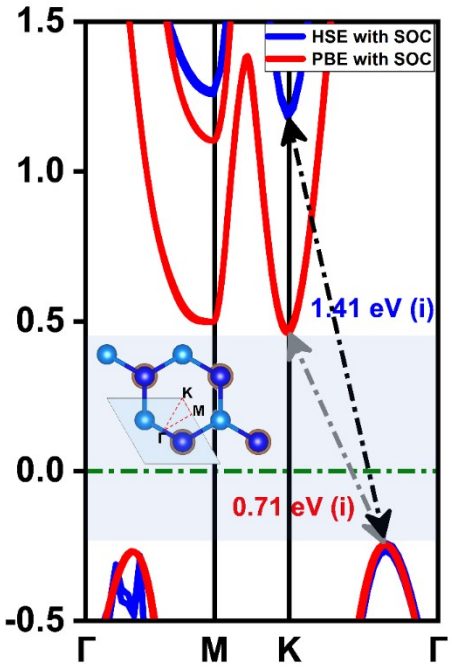

Figure S1 The band structures of the most stable configuration (hcp-top) of Blue-P/SbN vdWHs were calculated using both PBE+SOC and HSE06+SOC methods.

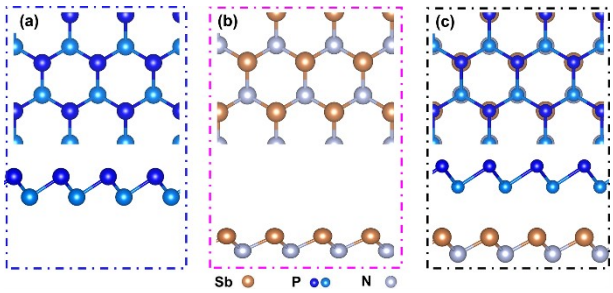

Figure S2 (a)-(c)The geometric structures of Blue-P monolayer, SbN monolayer, and the most stable configurations of Blue-P/SbN vdWHs, respectively.

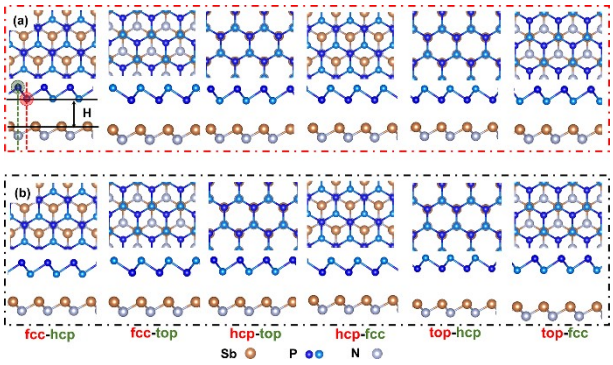

Figure S3 Top and side views of six high symmetry structures of Blue-P/SbN vdWHs. (a) Initial structures and (b) optimized structures, respectively. The yellow, dark (light) blue, and gray balls represent Sb, P and N atoms, respectively.

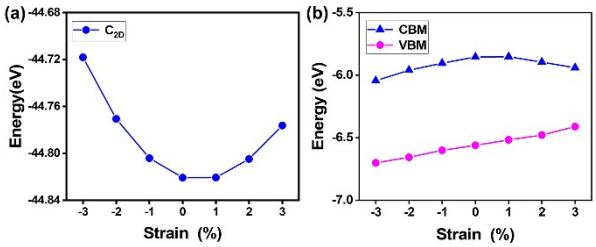

Figure S4 (a) Total energy variation curves of heterostructure under different strains, (b) Change curve of CBM and VBM under different strains.

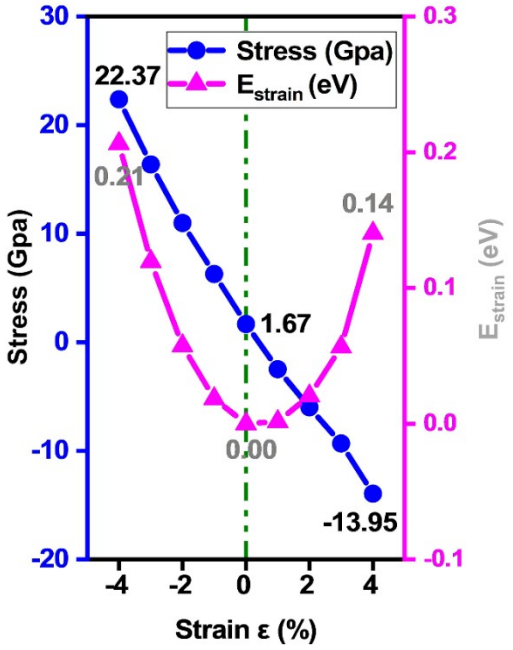

Figure S5 Strain energy (E_{strain})and stress-strain curves of Blue-P/SbN vdWHs were calculated. The blue line represents the change of stress-strain, the pink line represents the change of strain energy.

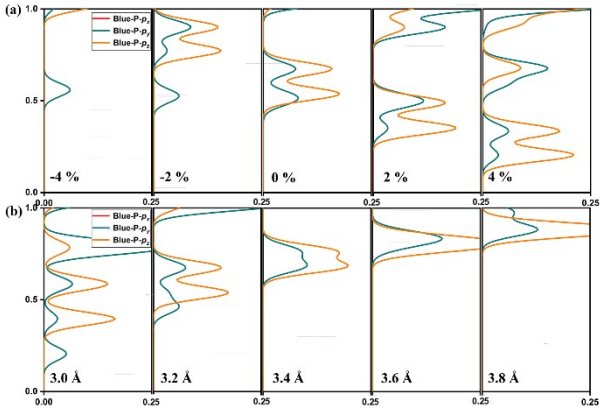

Figure S6 The contributions of each *p* orbital sub-orbital to the CBM of the Blue-P monolayer in Blue-P/SbN vdWHs under (a) Different biaxial strains, and (b) Different interlayer distances.

Table S1. Binding energy (E_b), interlayer distances (H_{-FS}), P-P bond lengths (R_{-FS}) of Blue-P/SbN vdWHs.

	Type-	fcc-hcp	fcc-top	**hcp-top**	hcp-fcc	top-hcp	top-fcc
Blue-P/ SbN	**E_b(eV)**	-0.195	-0.230	**-0.241**	-0.233	-0.105	-0.109
	H_{-FS}(Å)	3.29	3.22	**3.22**	3.21	4.02	3.89
	R_{-FS}(Å)	2.25	2.25	**2.25**	2.25	2.25	2.25

Table S2 P-P bond and Sb-N bond lengths and the interlayer distances (d) of vdWHs lengths under different strains.

Strain(%)	-4	-2	0	2	4
$R_{(P-P)}$ (Å)	2.21	2.24	2.26	2.28	2.32
$R_{(Sb-N)}$ (Å)	2.10	2.12	2.14	2.16	2.18
$d_{(interlayer)}$ (Å)	3.33	3.28	3.23	3.18	3.13