Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Ideal inert substrates for planar antimonene: h-BN and hydrogenated SiC(0001)

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Table S1 Detailed informations for PA/substrate.

Configuration	Supercell	Lattice(Å)	Lattice mismatch	Interlayer distance/(Å)	Binding energy/(eV)
Ag(111)	$(\sqrt{3}\times\sqrt{3})/(1\times1)$	5.11	0.8%	2.41	2.55
monolayer-BN	$(2\times2)/(1\times1)$	5.02	0.6%	3.48	1.09
bilayer-BN	$(2\times2)/(1\times1)$	5.02	0.6%	3.49	0.61
C-SiC	$(\sqrt{3}\times\sqrt{3})/(1\times1)$	5.32	5.3%	2.70	0.48
Si-SiC	$(\sqrt{3}\times\sqrt{3})/(1\times1)$	5.32	5.3%	3.02	0.42

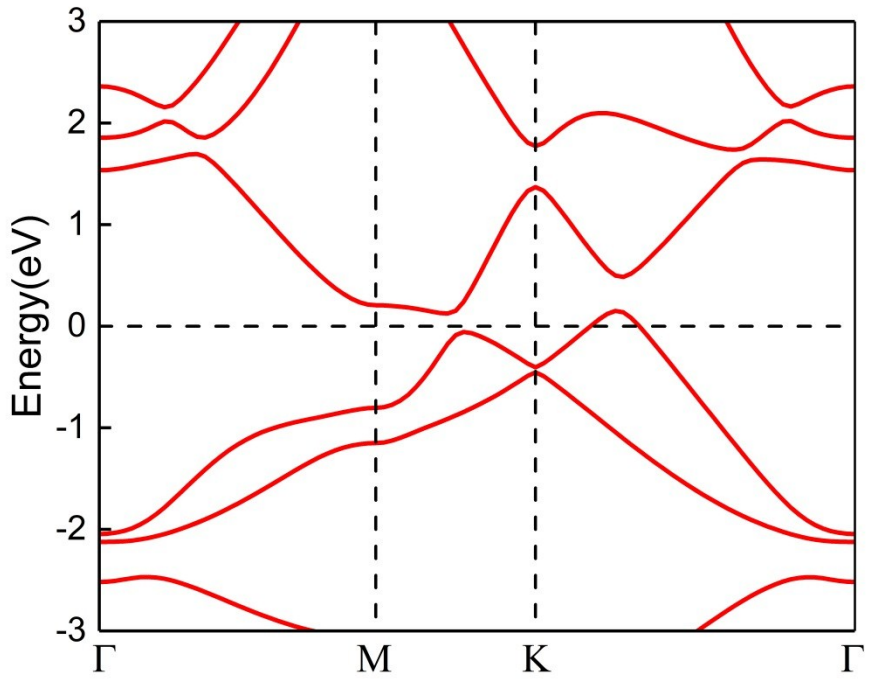

Fig. S1 Band structure of PA with SOC.

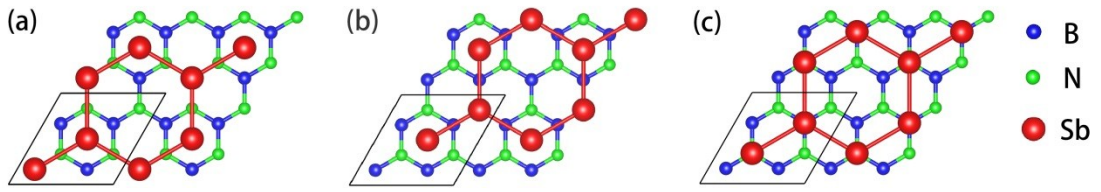

Fig. S2 Different configurations for PA/BN. The black rhombus denotes the unit cell. The total energies of three configurations are (a) -78.402, (b) -78.416, (c) -78.421 eV, respectively.

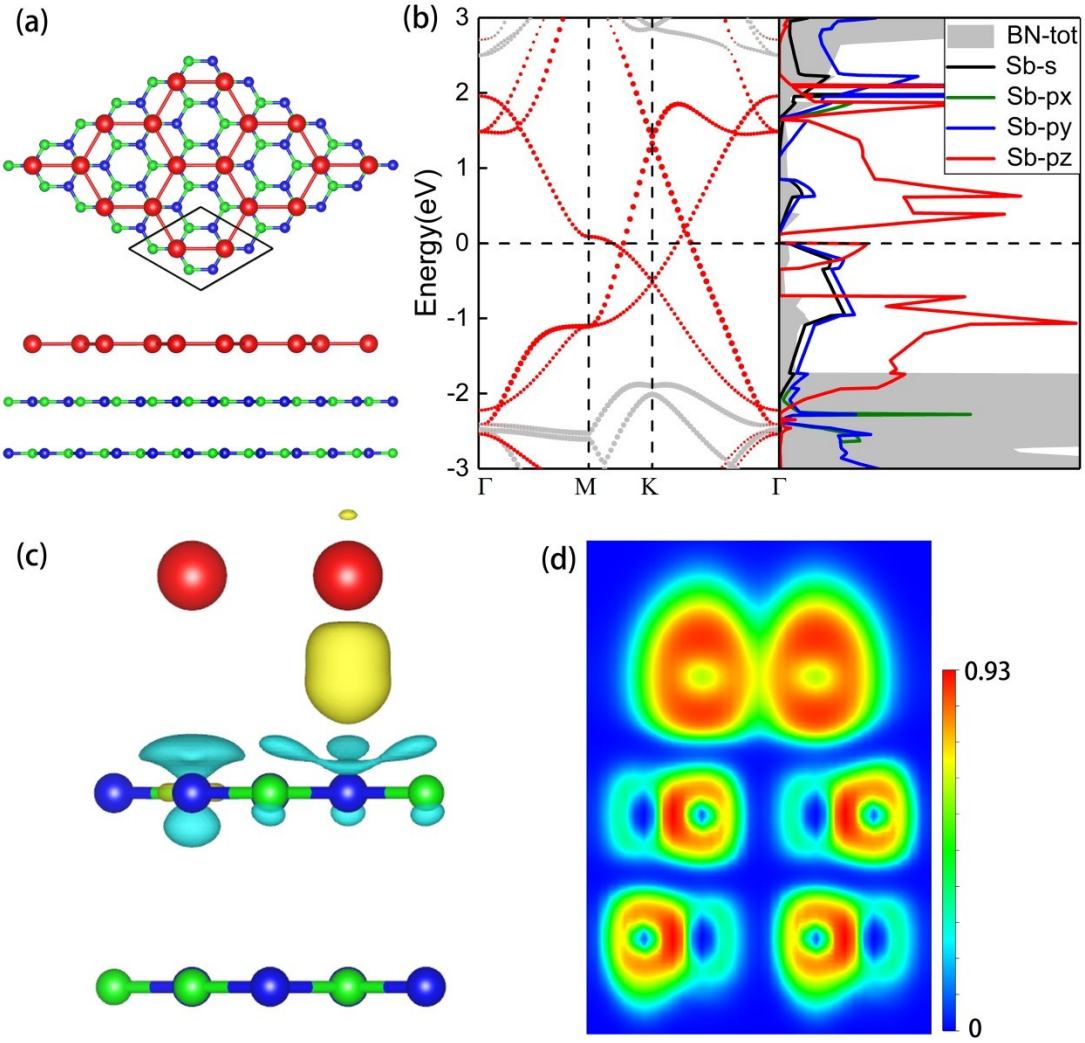

Fig. S3 (a) Top and side views of PA/bilayer BN. The black rhombus marks the unit cell. (b) Band structure and PDOS of PA/bilayer BN. The red and grey dots represent the contribution from PA and bilayer BN, respectively. (c) Charge density difference of PA/bilayer-BN, the yellow and blue clouds correspond to electron accumulation and depletion, respectively. The isosurface value is 0.0005 eÅ^{-3}. (d) ELF of PA/bilayer BN.

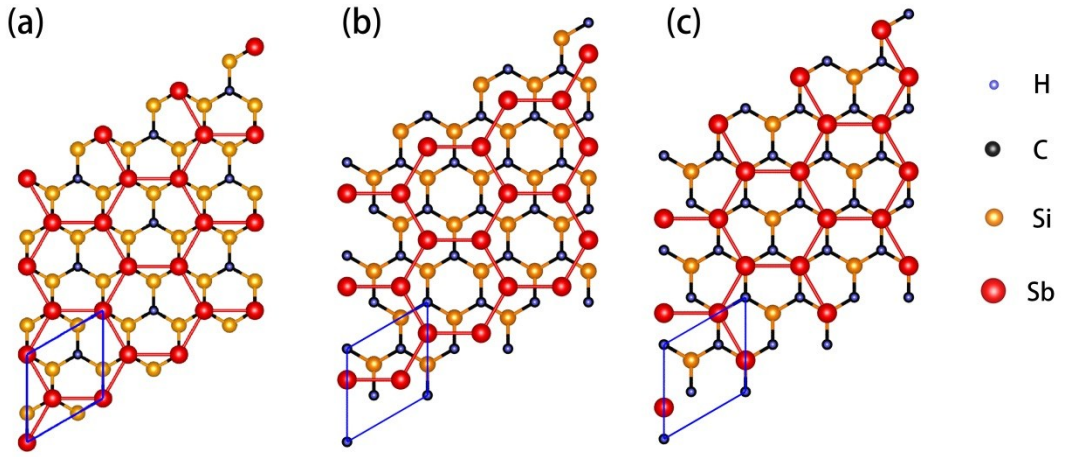

Fig. S4 Different configutions for PA/C-SiC. For simplification, we only show the PA and the upper surface of SiC contacting the PA. The blue rhombus marks the unit cell. The total energy of three models of PA/C-SiC is (a) -260.048, (b) -260.082, (c) -260.078 eV, respectively.

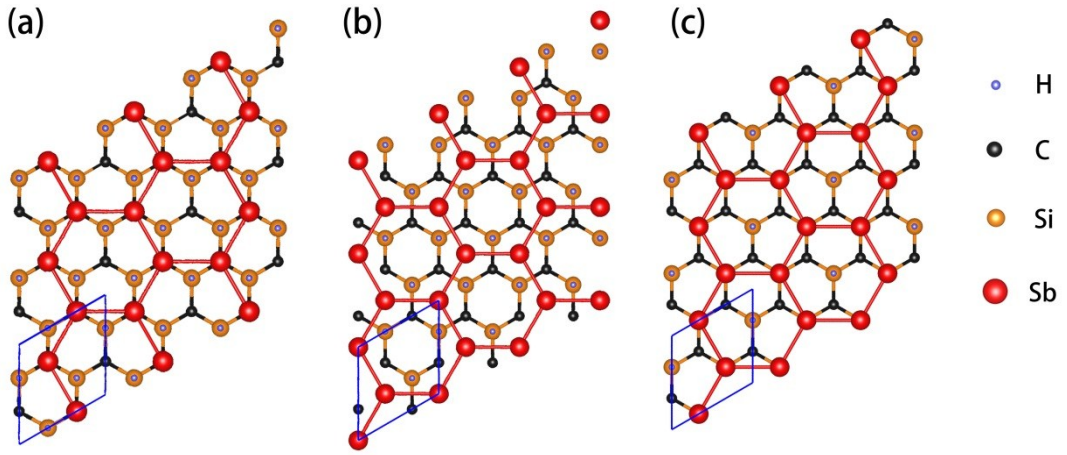

Fig. S5 Different configutions for PA/Si-SiC. For simplification, we only show the PA and the upper surface of SiC contacting the PA. The blue rhombus marks the unit cell.

The total energy of three models of PA/Si-SiC is (d) -260.082, (e) -260.083, (f) -260.083 eV, respectively.

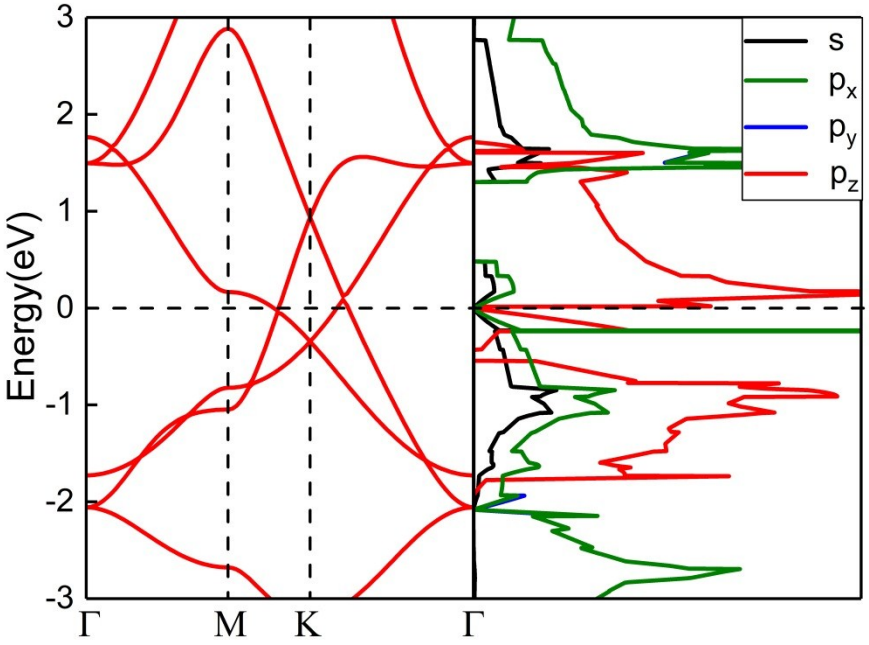

Fig. S6 Band structure and PDOS of PA with 5.3% tension strain.