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

Supporting Information

First principles study on the electronic structures and contact properties of graphene/XC (X = P, As, Sb, Bi) van der Waals heterostructures

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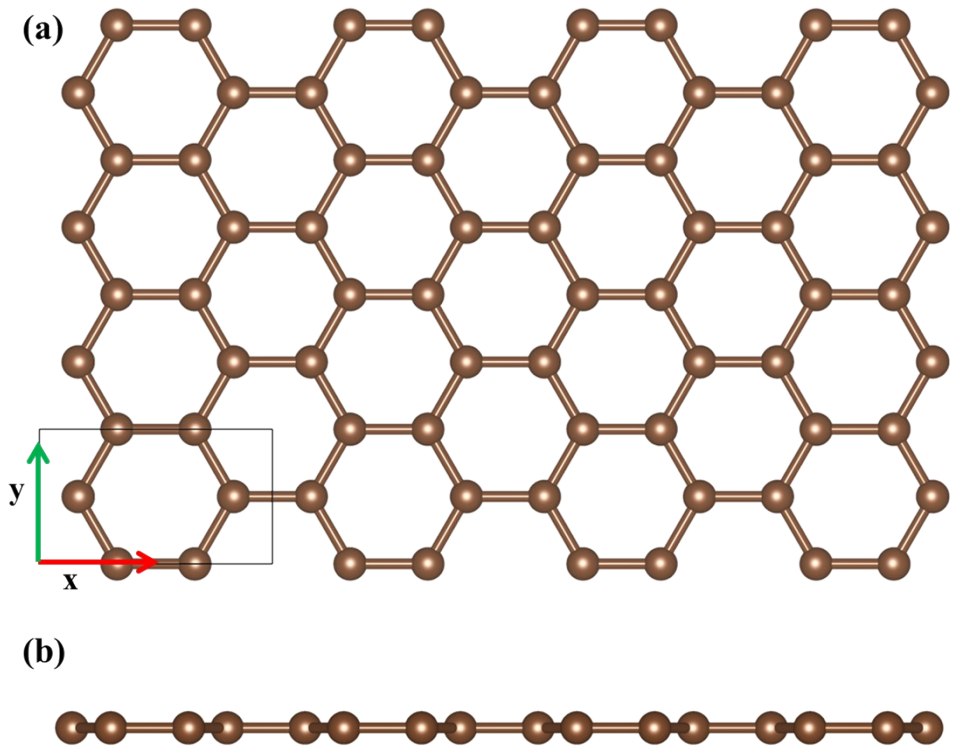

Fig. S1 (a) Top and (b) side views of the optimized graphene (Gr) monolayer.

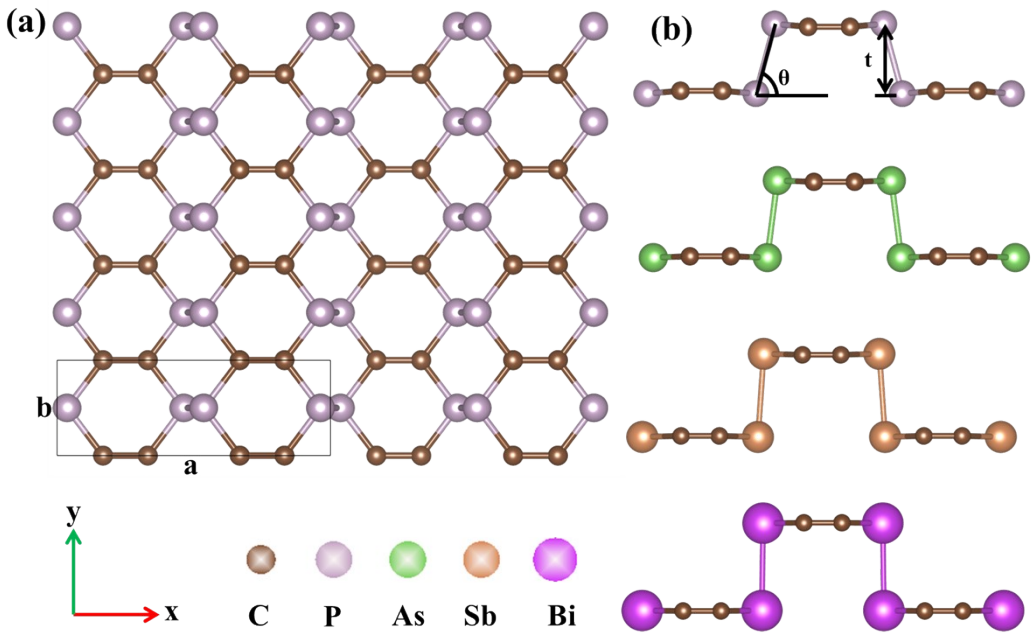

Fig. S2 (a) Top and (b) side views of the optimized atomic structures of XC (X = P, As, Sb, Bi) monolayers.

Table S1 Optimized geometric parameters of XC (X = P, As, Sb, Bi) monolayers: bonding length (X-C, C-C and X-X), inclination (θ) of X-X bond and vertical distance (t) between two adjacent X atoms.

	X-C (Å)	C-C (Å)	X-X (Å)	θ (◦)	t (Å)
PC	1.82	1.36	2.35	74.94	2.27
AsC	1.98	1.35	2.57	82.64	2.54
SbC	2.20	1.34	2.92	86.02	2.91
BiC	2.32	1.33	3.06	89.28	3.05

Table S2 Optimized lattice constants of Gr and XC monolayers (X = P, As, Sb, Bi).

Lattice constants	Gr	PC	AsC	SbC	BiC
a (Å)	4.27	8.56	8.19	8.50	8.47
b (Å)	2.47	2.92	3.13	3.47	3.66

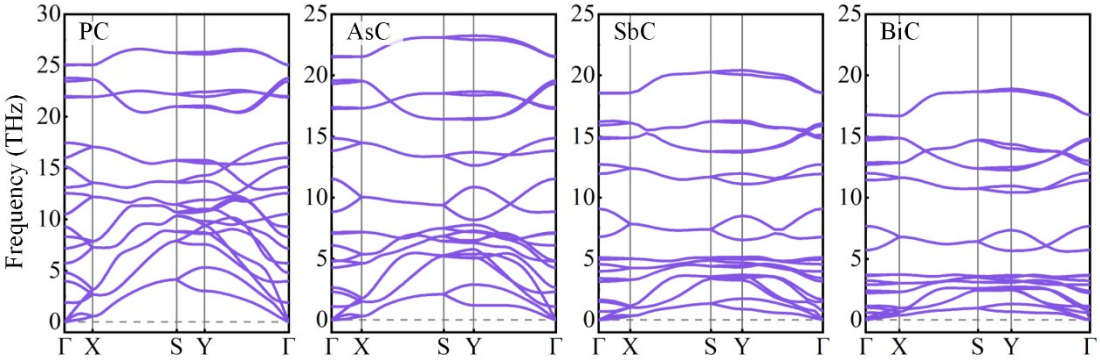

Fig. S3 Phonon spectra of isolated XC monolayers (X = P, As, Sb, Bi).

Table S3 Lattice mismatches of Gr/XC (X = P, As, Sb, Bi) heterostructures.

Lattice mismatch	Gr/PC	Gr/AsC	Gr/SbC	Gr/BiC
x direction	0.06%	2.12%	0.28%	0.48%
y direction	0.75%	2.48%	-2.63%	0.63%

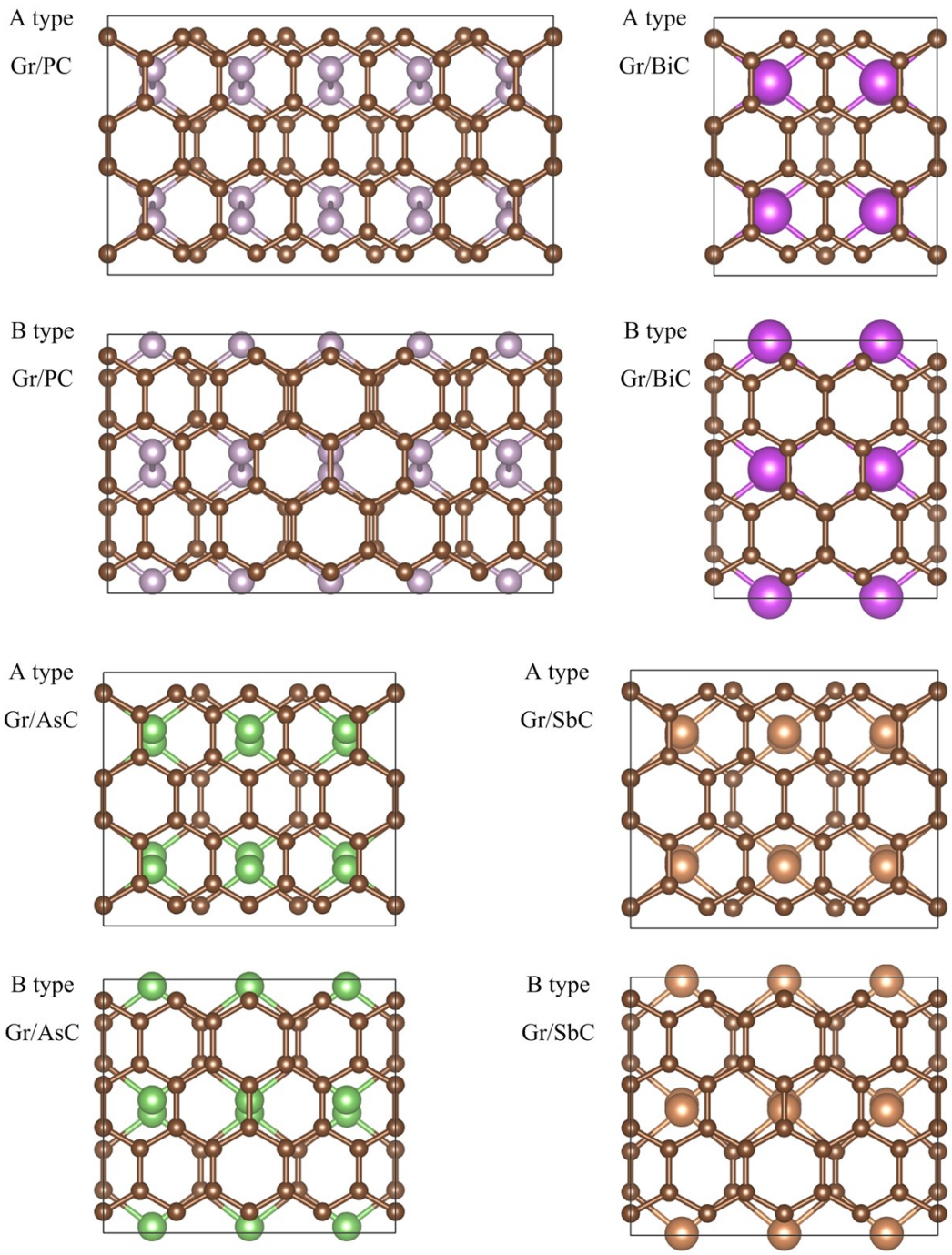

Fig. S4 Geometry configurations for Gr/XC heterostructures (X = P, As, Sb, Bi) with two different stacking types.

Table S4 Total energies (E_{tot}) of Gr/XC heterostructures (X = P, As, Sb, Bi) with different stacking types.

Gr/XC	type	E_{tot} (eV)
Gr/PC	A	-723.9904
	B	-723.9883
Gr/AsC	A	-449.2705
	B	-446.6225
Gr/SbC	A	-438.4028
	B	-435.3700
Gr/BiC	A	-313.7318
	B	-313.7298

Table S5 The bond lengths and bond angles of Gr/XC heterostructures.

Gr/XC	X-C (Å)	C-C (Å)	X-X (Å)	C-X-X (°)
Gr/PC	1.83	1.36	2.30	97.09
Gr/AsC	2.01	1.35	2.54	93.48
Gr/SbC	2.18	1.34	2.92	91.18
Gr/BiC	2.33	1.33	3.04	90.77

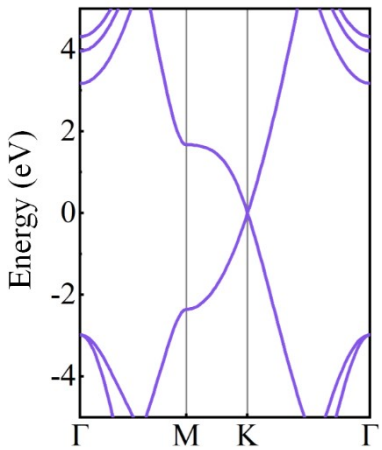

Fig. S5 The band structure of pristine graphene.

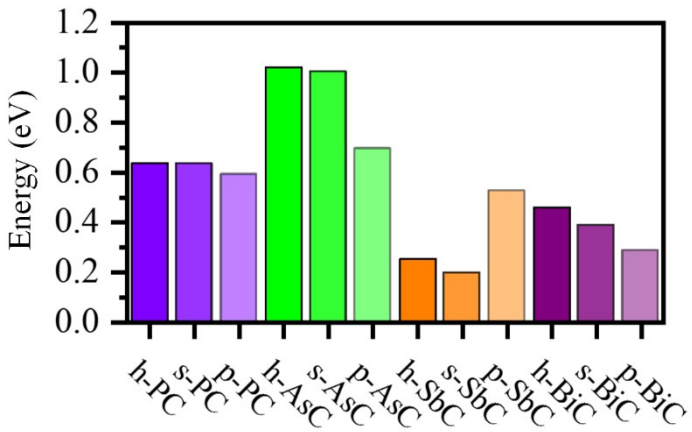

Fig. S6 The comparison of the band gaps of XC in the Gr/XC heterostructures (h-XC), isolated XC with strained supercell sizes of heterostructures (s-XC) and pristine XC without strains (p-XC).