Supplementary Information

The sp^2 character of B doped arsenene with tunable electronic properties predicted by theoretical studies

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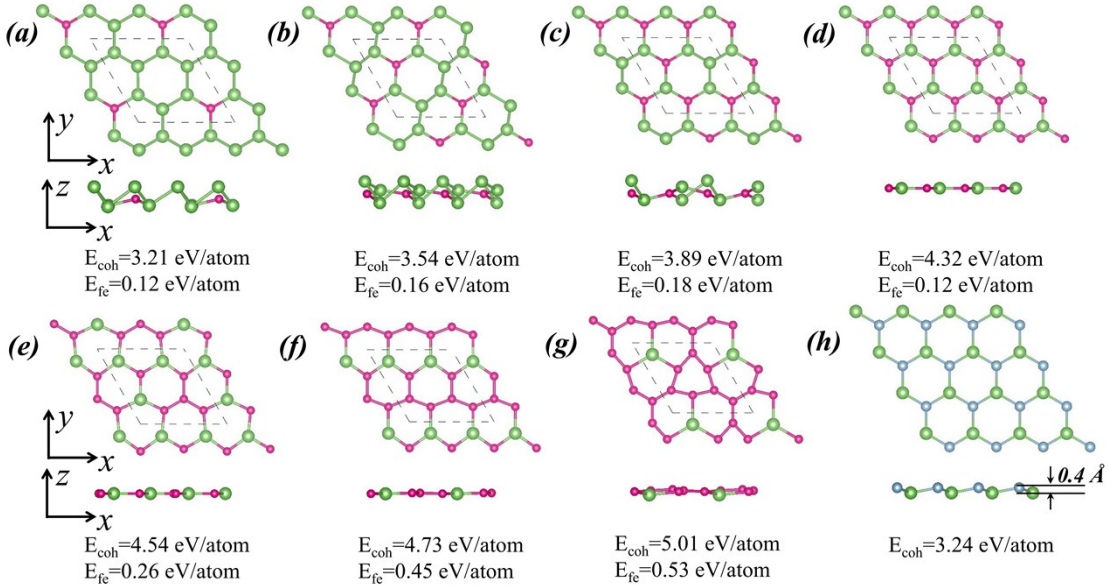

Figure S1 Top- and side-view of optimized structures for B doped arsenene: (a) As_7B, (b) As_6B_2, (c) As_5B_3, (d) As_4B_4, (e) As_3B_5, (f) As_2B_6, and (g) AsB_7. The supercell is outlined by the dot line. (h) is the structure of AsAl. The corresponding cohesive energy (E_{coh}) and formation energy (E_{fe}) are also indicated.

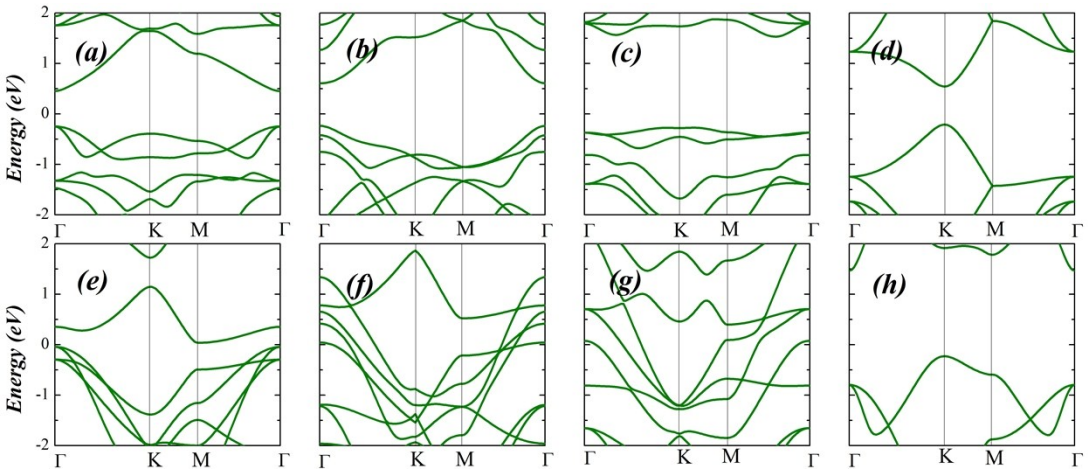

Figure S2 Band structures of (a) As_7B, (b) As_6B_2, (c) As_5B_3, (d) As_4B_4, (e) As_3B_5, (f) As_2B_6, (g) AsB_7 and (h) AsAl.

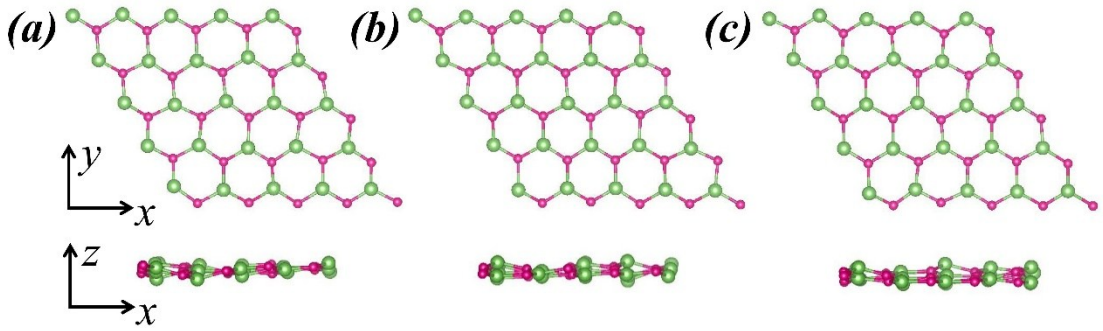

Figure S3 Snapshots of the final structure at (a) 500 K, (b) 700 K and (c) 1000 K after 10 ps of molecular dynamics simulation. The upper and lower panels are top- and side-view, respectively.

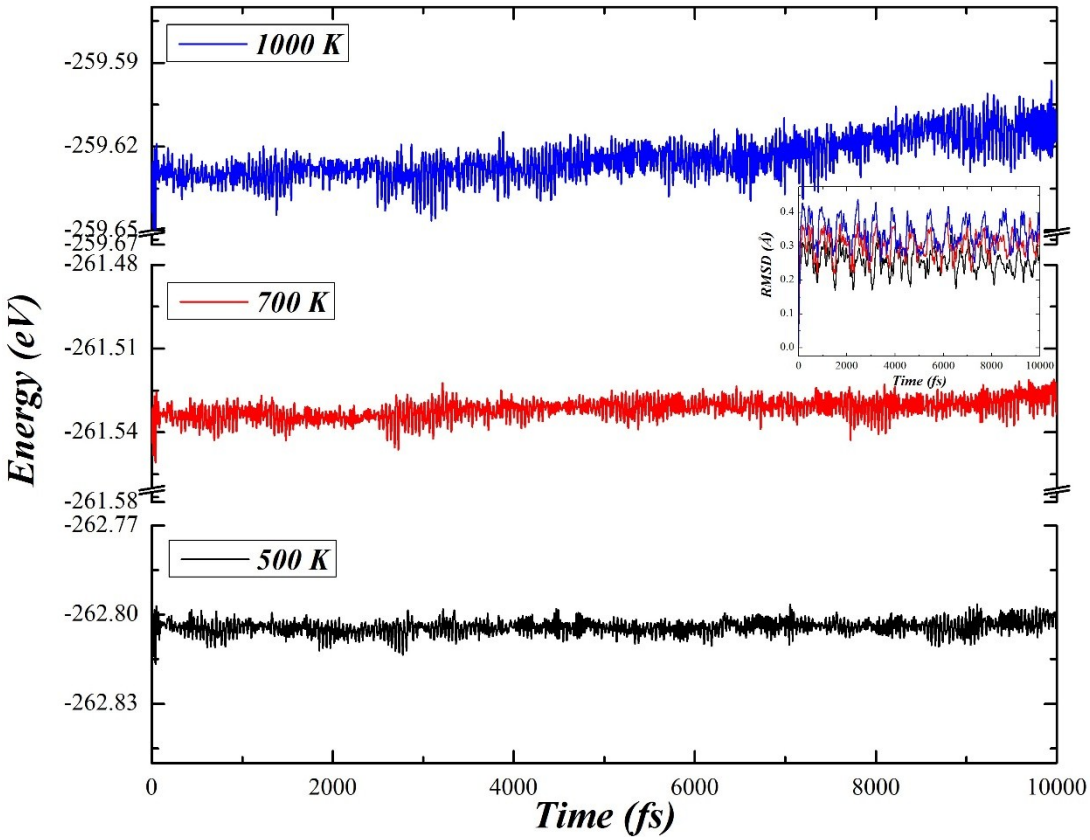

Figure S4 The variation of total energy and mean squared displacement with simulation time for AsB monolayer.

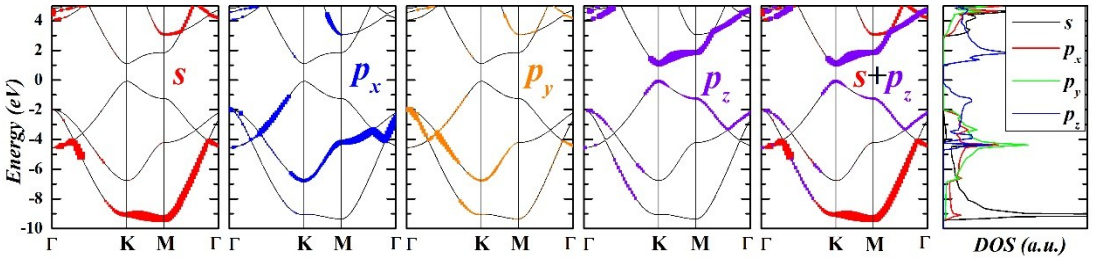

Figure S5 The s, p_x, p_y, p_z and s+p_z orbitals decomposed band structure and partial density of states of B atom for AsB monolayer.

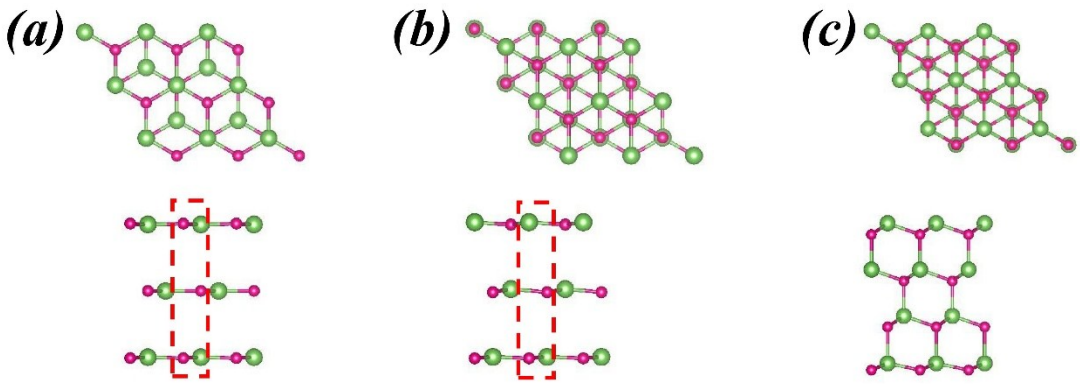

Figure S6 (a) ABA-, (b) ABC- and (c) ABCA-stacking atomic structure of AsB.

Table S1 Structural parameters for layered AsB obtained by using optB86b-vdW functional.

Thickness	stacking order	a_1=a_2 (Å)	$l_{\text{As-B}}$ (Å)	d-spacing (Å)
1	\	3.39	1.96	\
2	AB	3.39	1.96	3.57
3	ABA	3.39	1.96	3.66
	ABC	3.39	1.96	3.48/3.50
4	ABAB	3.39	1.96	3.64/3.77/3.58
	ABCA	Non-layer structure	\	\
5	ABABA	3.39	1.96	3.63/3.71
	ABCAB	Non-layer structure	\	\

Table S2 Work functions (W_F) of AsB as a function of layer thickness.

Thickness	1	2	3	4	5
W_F (eV)	5.61	5.50	5.60	5.53	5.59

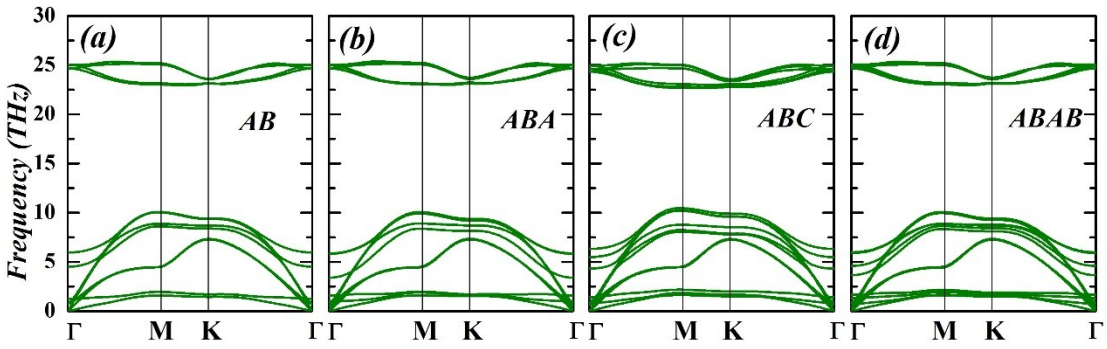

Figure S7 The phonon spectra of (a) AB stacked, (b) ABA stacked, (c) ABC stacked and (d) ABAB stacked AsB. No imaginary mode confirms the lattice dynamic stability of thicker AsB.

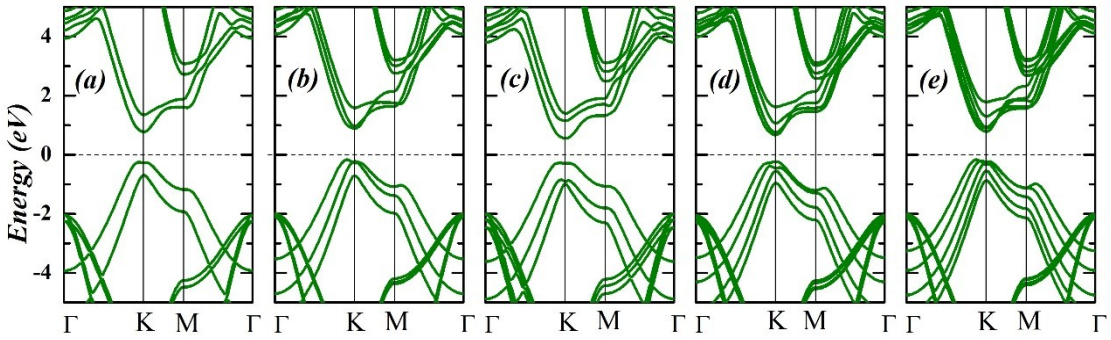

Figure S8 HSE06 band structures of (a) AB stacked, (b) ABA stacked, (c) ABC stacked, (d) ABAB stacked and (e) ABABA stacked AsB.

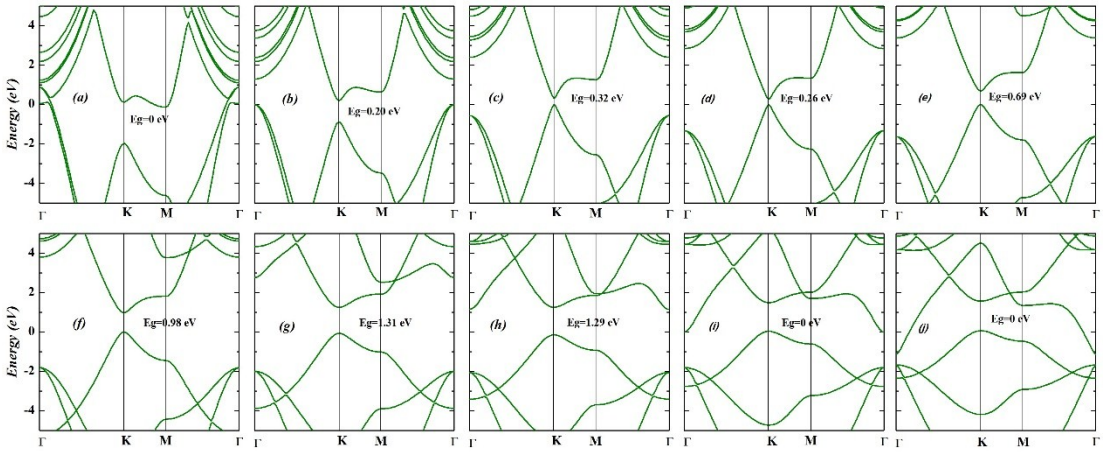

Figure S9 HSE06 band structure of AsB monolayer at strain of (a) −30%, (b) −25%, (c) −20%, (d) −15%, (e) −10%, (f) −5%, (g) 5%, (h) 10%, (i) 15% and (j) 20%.