Supporting Information

Strain–induced Band Structure Modulation in Hexagonal Boron Phosphide/Blue Phosphorene vdW Heterostructure

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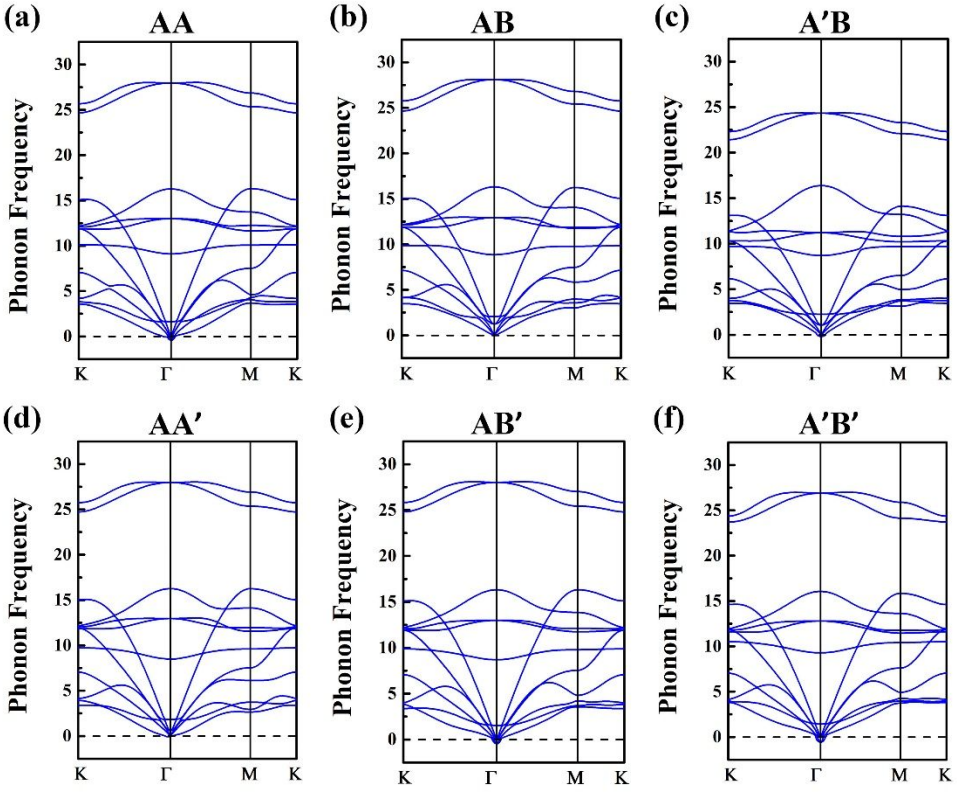

Figure S1. The phonon frequency for each stacking pattern.

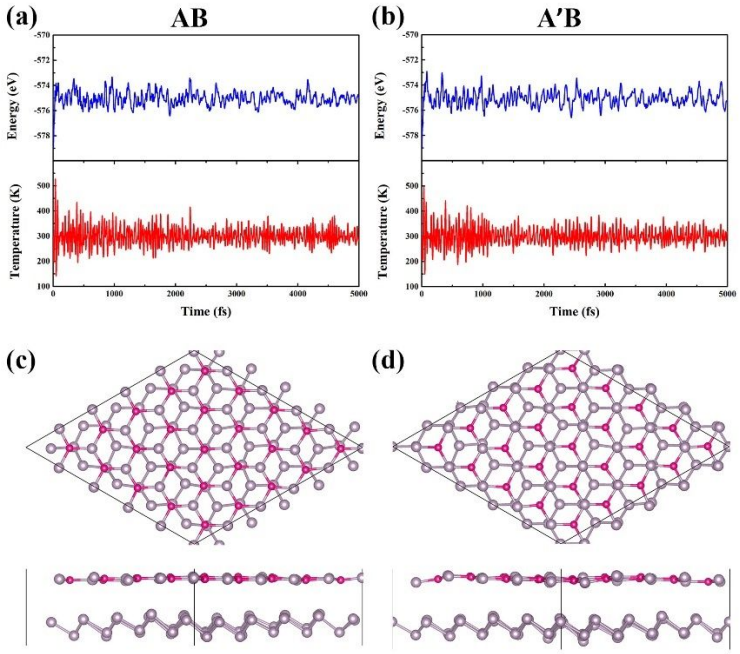

Figure S2. Total energy and temperature fluctuations with respect to molecular dynamic (MD) steps at 300K for AB (a), A'B (b) stacking patterns of the *h*-BP/BlueP heterostructure. After 5000 steps, supercell structures for AB (c) and A'B (d) stacking patterns of the *h*-BP/BlueP heterostructure.

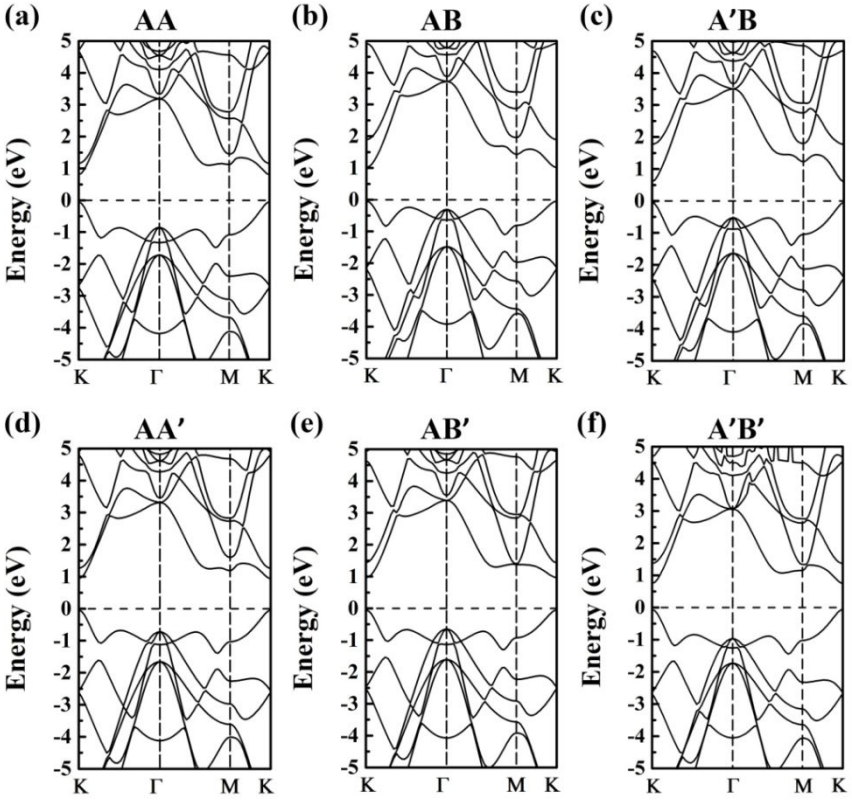

Figure S3. Band structures of AA (a), AB (b), A'B (c), A'A (d), AB' (e) and A'B' (f) stacking patterns for the *h*-BP/BlueP heterostructure by PBE functional.

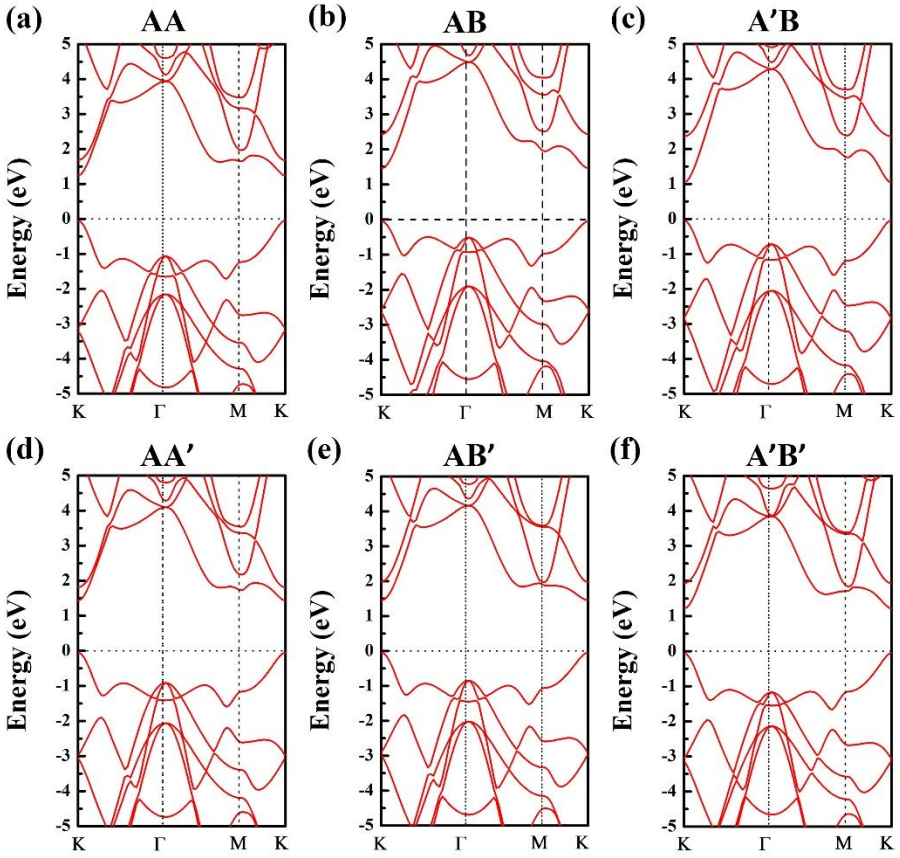

Figure S4. Band structures of AA (a), AB (b), A'B (c), A'A (d), AB' (e) and A'B' (f) stacking patterns for the *h*-BP/BlueP heterostructure by HSE06 functional.

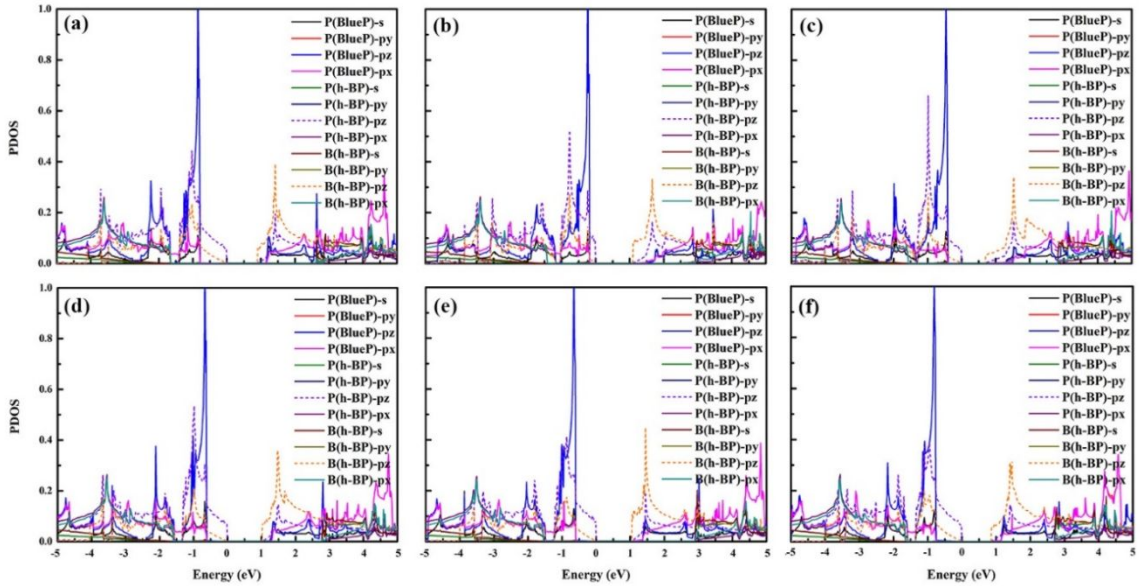

Figure S5. Partial density of states of AA (a), AB (b), A'B (c), A'A (d), AB' (e) and A'B' (f) stacking patterns for the *h*-BP/BlueP heterostructure by PBE functional.

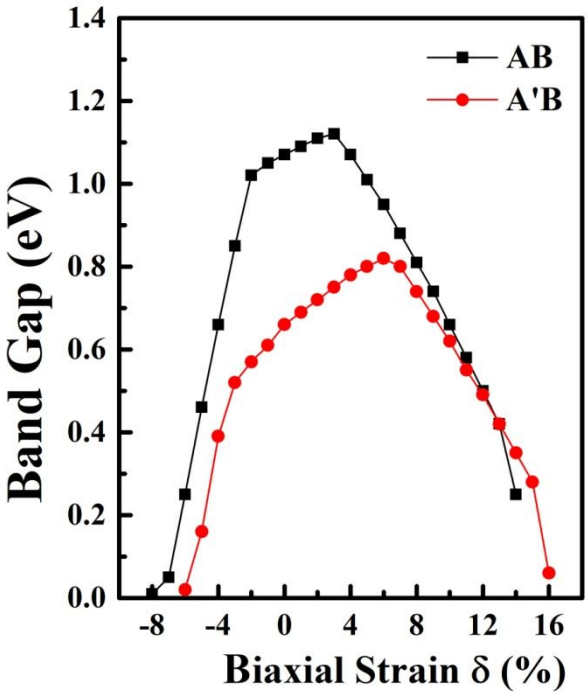

Figure S6. Energy band gap as a function of biaxial strain δ.