

Supporting Information

Strain enhanced visible-ultraviolet absorption of blue phosphorene/MoX₂ (X=S,Se) heterolayers

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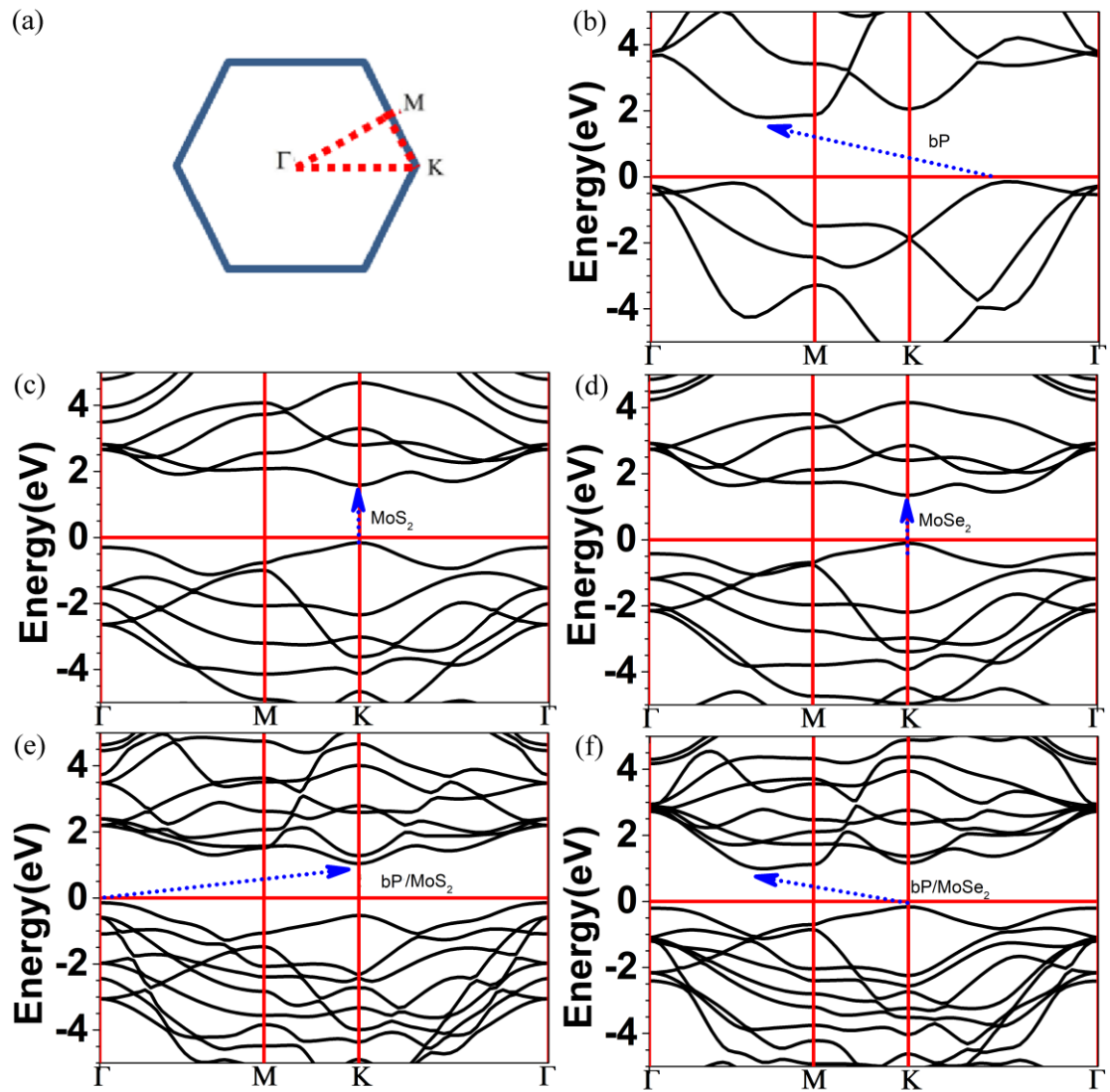


Figure S1. (a) Brillouin zone with high-symmetry points labeled. Band structures (PBE) of (b) bP monolayer, (c) MoS₂ monolayer, (d) MoSe₂ monolayer, (e) bP/MoS₂ vdW heterostructure and (f) bP/MoSe₂ vdW heterostructure.

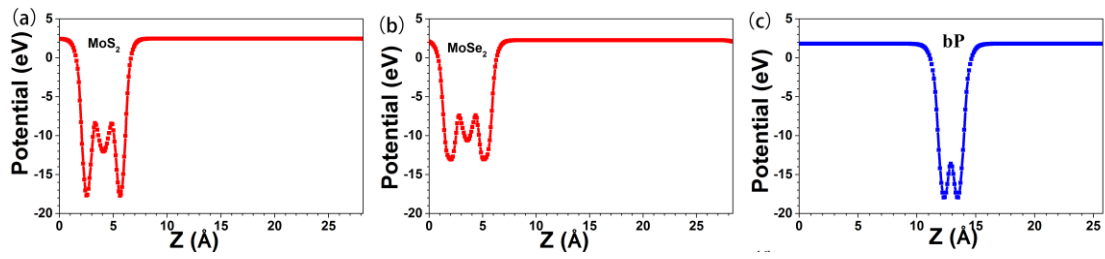


Figure S2. The planar average potential of (a) MoS₂, (b) MoSe₂ and (c) bP.

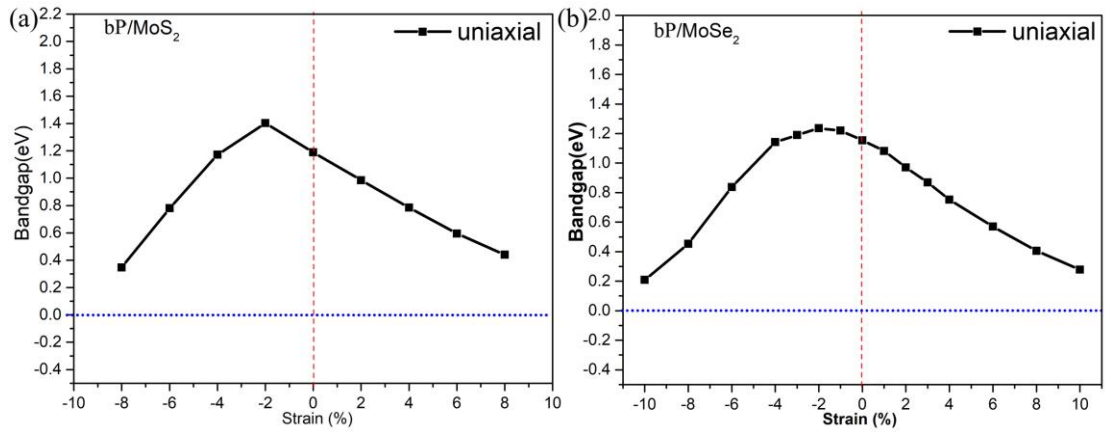


Figure 3S. (a) The band gap (PBE) of (a) bP/MoS₂ and (b) bP/MoSe₂ vdW heterostructure as a function of uniaxial strain.

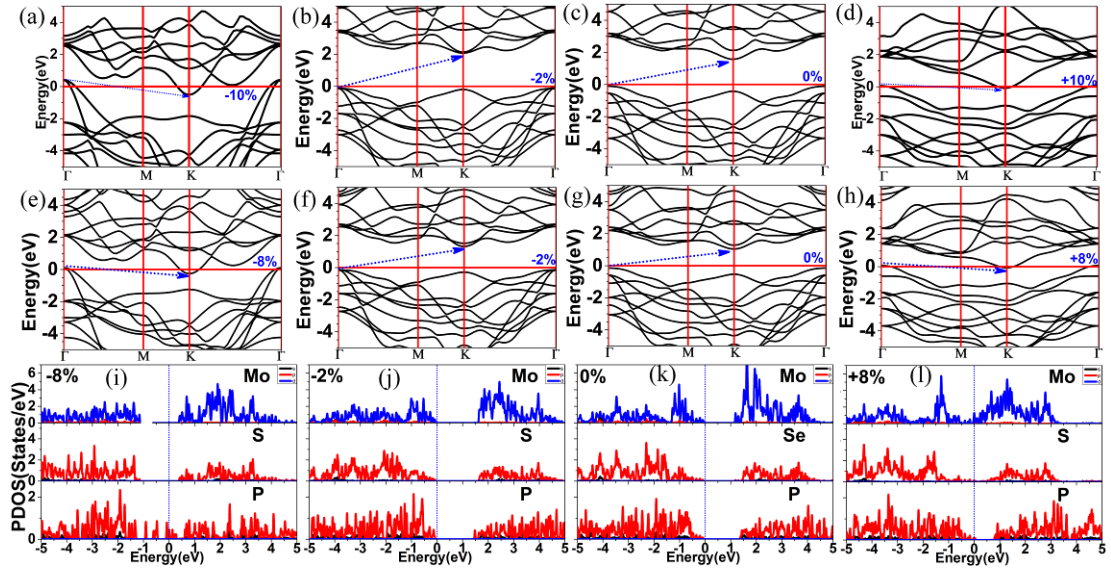


Figure S4. Band structures (HSE06) of bP/MoS₂ vdW heterostructure: at (a) -10%, (b) -2%, (c) 0% and (d) +10% biaxial strain, respectively. Band structures (PBE) and PDOS (PBE) of bP/MoS₂ vdW heterostructure: at (e)(i)-8%, (f)(j) -2%, (g)(k)0% and (h)(l) +8% biaxial strain, respectively.

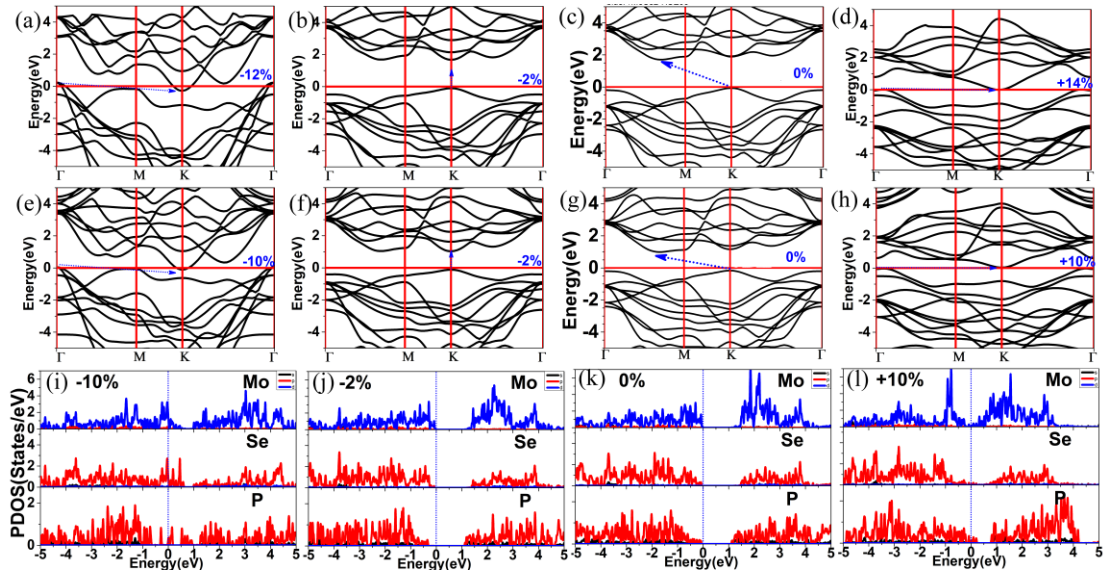


Figure S5. Band structures (HSE06) of bP/MoSe₂ vdW heterostructure: at (a) -12%, (b) -2%, (c) 0% and (d) +14% biaxial strain, respectively. Band structures (PBE) and PDOS (PBE) of bP/MoSe₂ vdW heterostructure: at (e)(i)-10%, (f)(j) -2%, (g)(k)0% and (h)(l) +10% biaxial strain, respectively.