

Supporting information

Electronic structure and interface contact of twodimensional van der Waals Boron Phosphide/Ga₂SSe heterostructure

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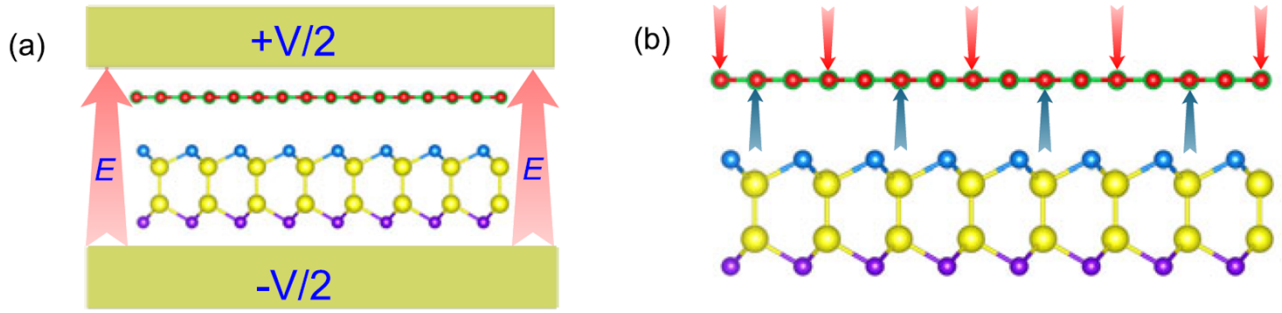


Fig. S1. The schematic models of (a) electric fields and (b) strains, applying to the heterostructure.

Fig. S1 shows the schematic models of electric fields and strains along the z direction of the heterostructure. The directions of the electric field, pointing from the Ga₂SSe layer to BP layer is defined as the positive direction. The compressive and tensile strains are applied perpendicularly to the heterostructure surface across the z direction.

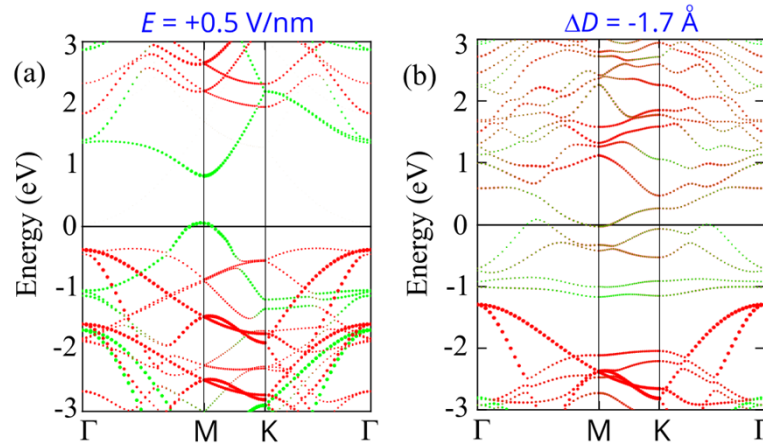


Fig. S2. Projected band structures of BP/SGa₂Se vdWH under (a) $E = +0.5$ V/nm and (b) $\Delta D = -1.7$ Å. Red and green lines represent the contributions of Ga₂SSe and BP layers, respectively.

XCRYSDEN XSF file

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0.0000000000000000	0.0000000000000000	39.9999847412000022

Direct

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BP/SeGa2S vdWH

XCrySDen XSF file

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0.0000000000000000 0.0000000000000000 39.9999847412000022

S Ga Se B P

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