Supplementary Information

Strain-mediated Type-I/Type-II Transition in MXene/Blue Phosphorene van der Waals Heterostructures for Flexible Optical/Electronic Devices

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Figure S1

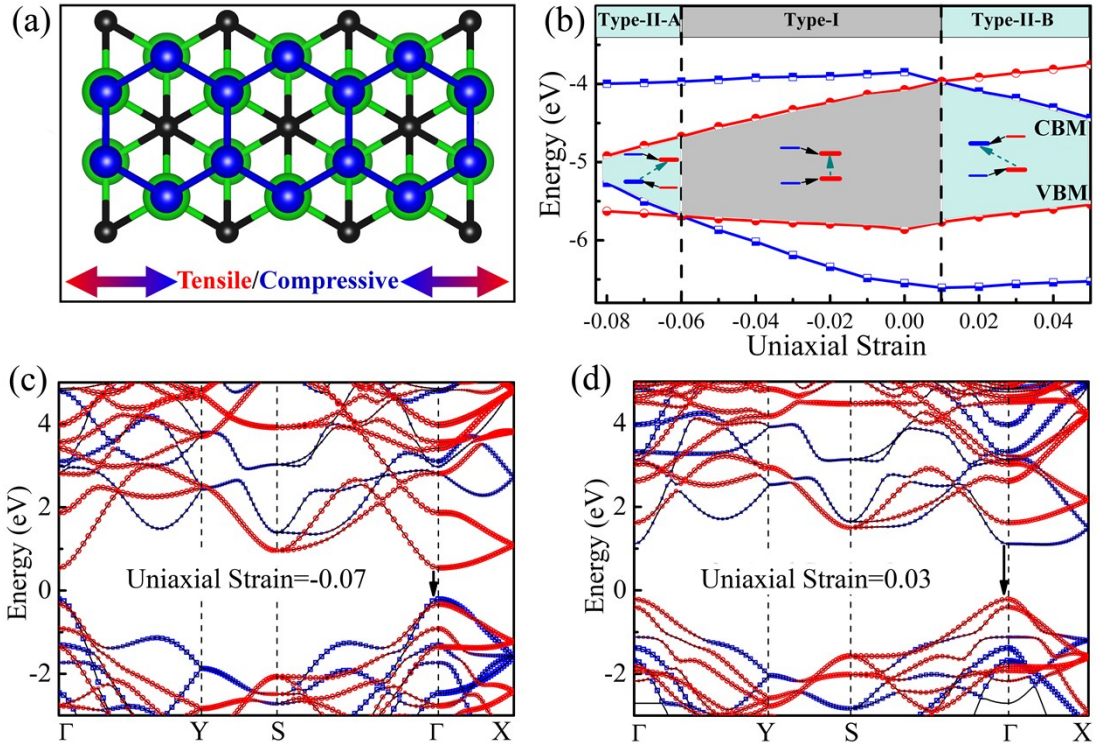

Figure S1 (a) Schematic drawing of the application of uniaxial strain. (b) The band edge positions of Zr_2CO_2 and BlueP under various uniaxial strains ranging from -0.08 to 0.05, which are illustrated by the red half circle and blue half square, respectively. Calculated band structures of Zr_2CO_2/BlueP vdW heterostructure under uniaxial strains of (c) -0.05 and (d) 0.03 by HSE06, where the size of the red circles and blue squares in Figure S1c and d illustrate the projected weight of Zr_2CO_2 and BlueP respectively.

It can be seen that the application of uniaxial strains can also realize the transition from type-I to type-II heterostructures and reverse the band edge positions of the modulated type-II heterostructures, which are consistent with the modulation effect of biaxial strain discussed in Figure 3 of the main text.