Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Broken-gap Energy Alignment in Two-dimensional van der Waals Heterostructures for Multifunctional Tunnel Diodes

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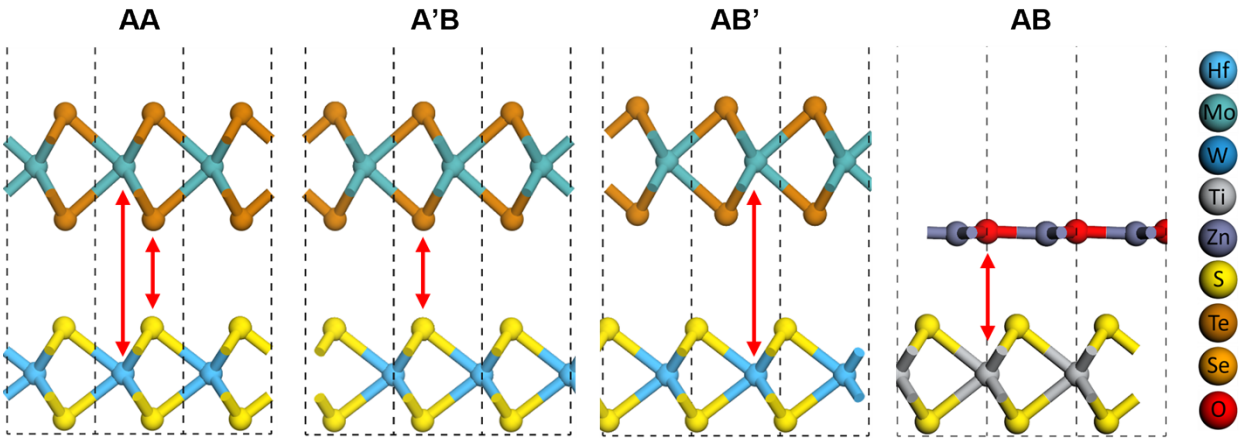

Figure S1. The 3 high symmetry stacking patterns, AA, A'B and AB', considered for $HfS_2/MoTe_2$, HfS_2/WTe_2, TiS_2/WSe_2 and $TiSe_2/WTe_2$, and AA, AB' and AB, considered for 1T-HfS_2/WTe_2 and TiS_2/ZnO.

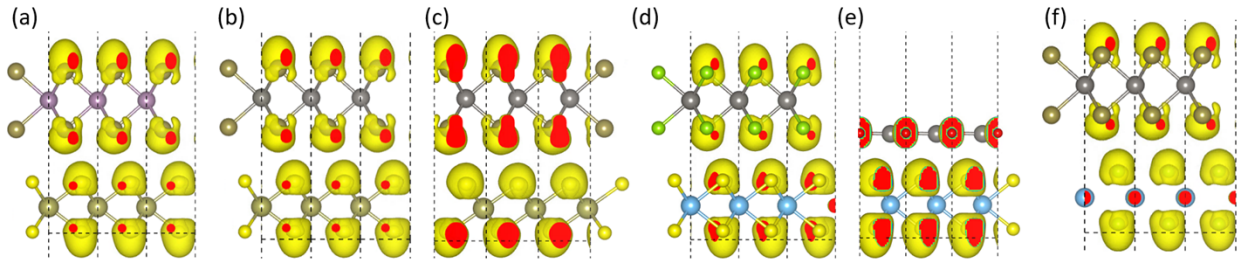

Figure S2. Electron localisation function isosurface plots of (a) $HfS_2/MoTe_2$, (b) HfS_2/WTe_2, (c) 1T-HfS_2/WTe_2, (d) TiS_2/WSe_2, (e) TiS_2/ZnO and (f) $TiSe_2/WTe_2$.

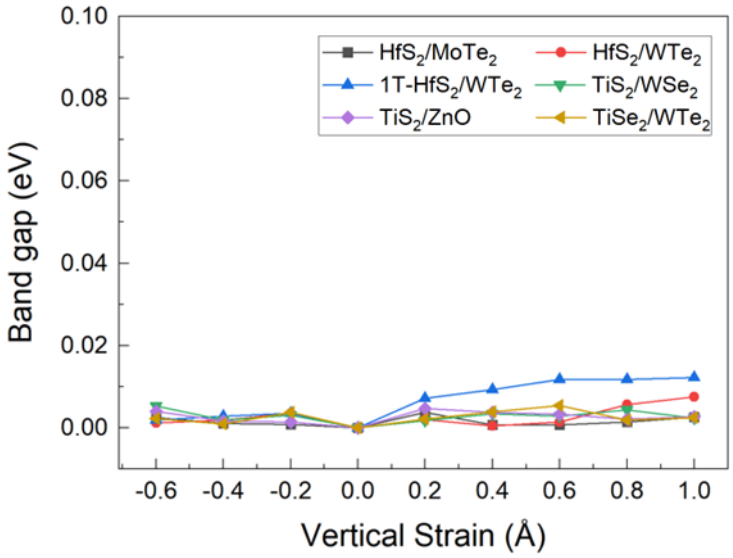

Figure S3. Calculated band gap as a function of vertical strain for the 6 heterostructures.