

Supporting Information for:

ZnO/WSe₂ vdW heterostructure for Photocatalytic Water Splitting

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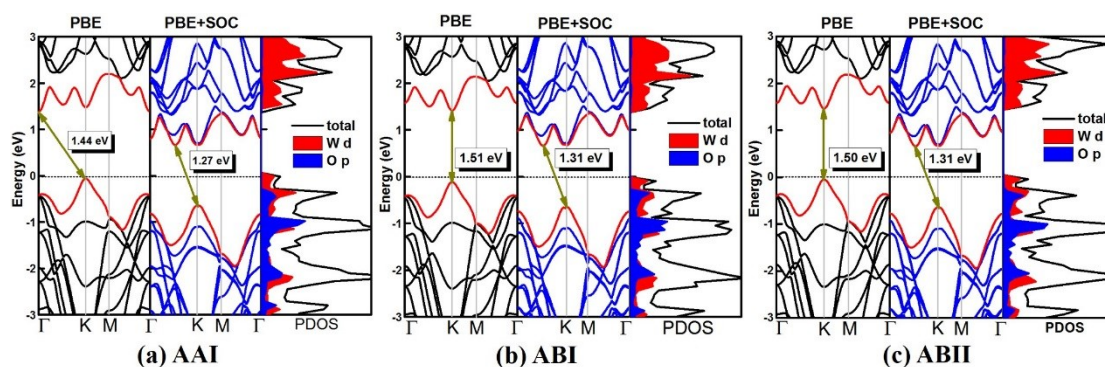


Fig. S1 (a), (b) and (c) The band gap and PDOS of AAI, ABI and ABII patterns at the PBE level without and with SOC.

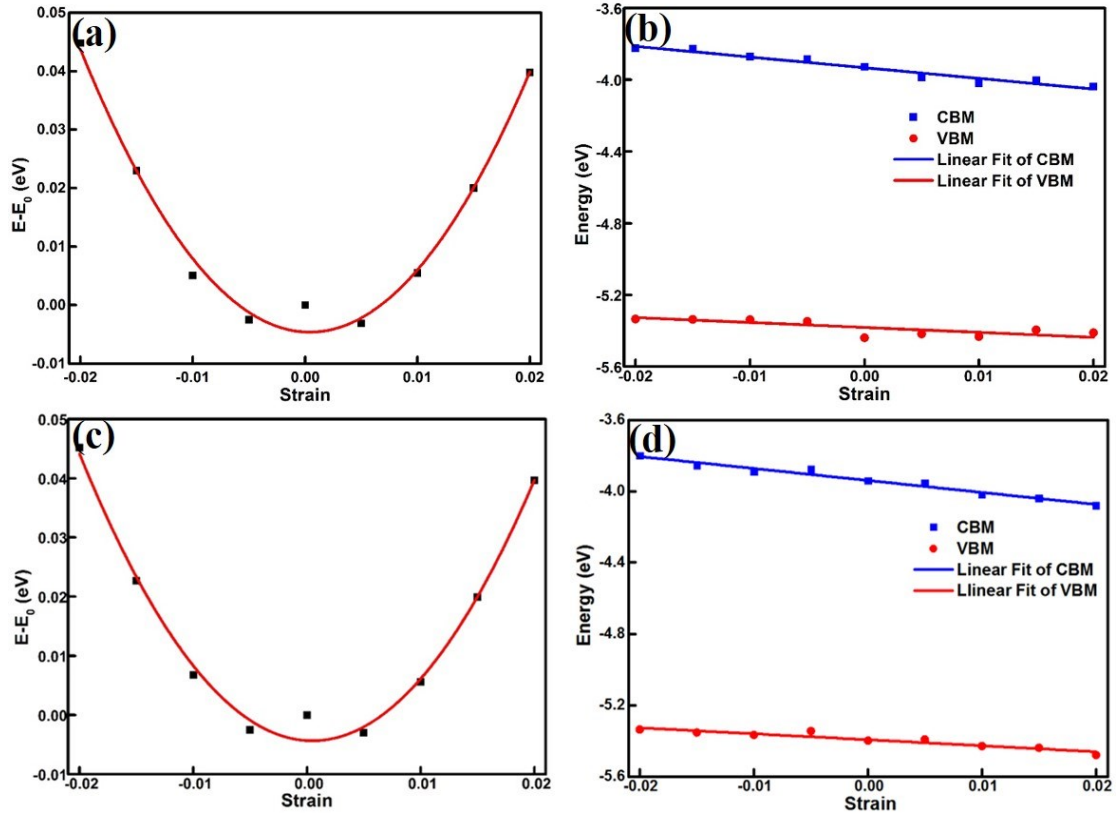


Fig. S2 Band edge positions and total energy as a function of the uniaxial strain for (a,b) along the armchair (x) and (c,d) along the zigzag (y) direction.

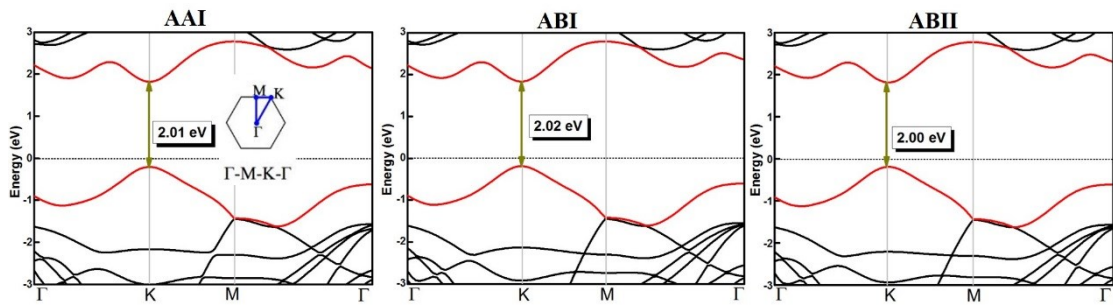


Fig. S3 The band gaps of patterns AAI, ABI and ABII at the HSE06 level.

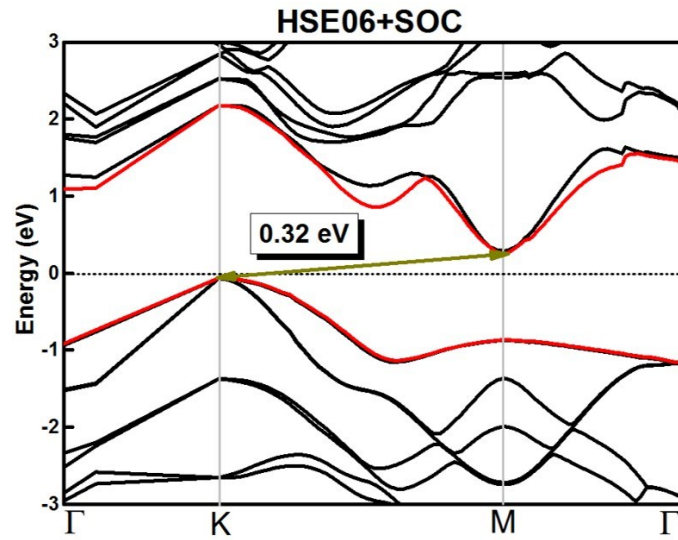


Fig. S4 The band gap of pattern AAIL at the HSE06 with SOC level.

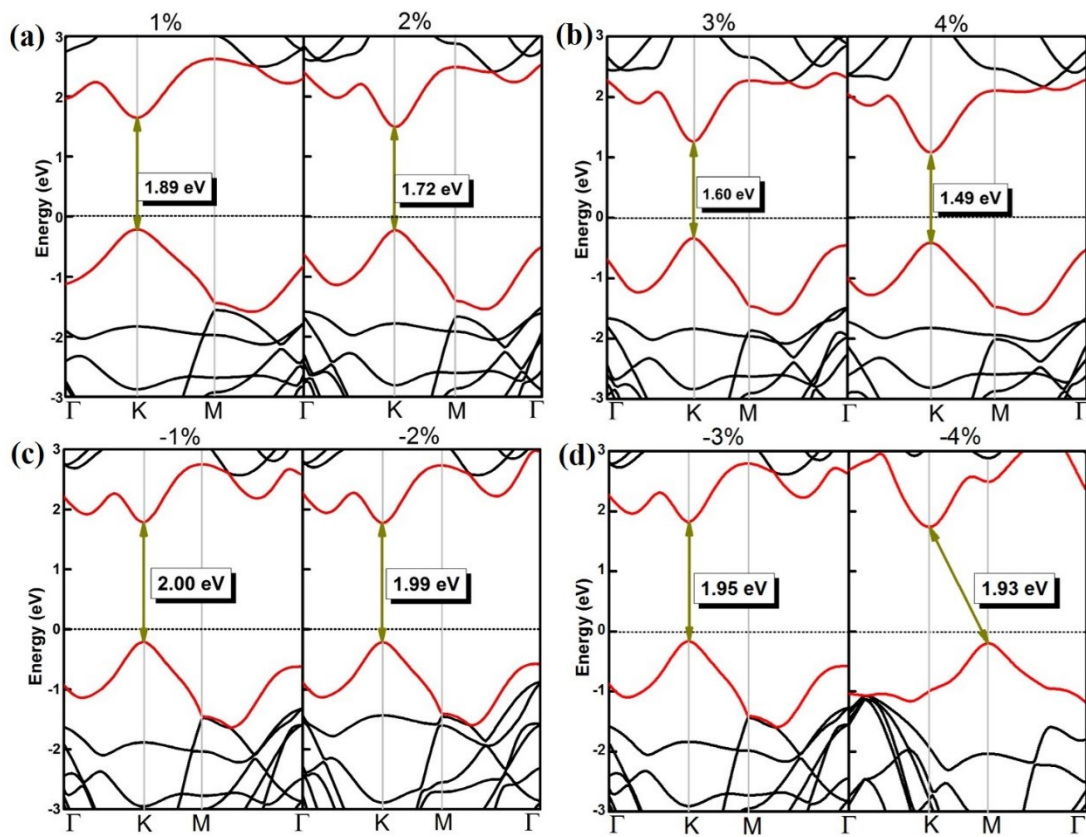


Fig. S5 Band gaps of ZnO/WSe₂ heterostructure under both biaxial strain of 1% to -4% at the HSE06 level.

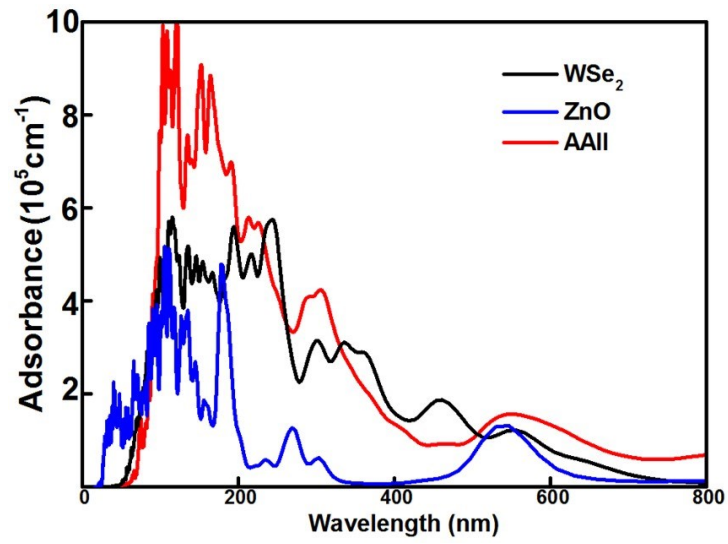


Fig.S6 Adsorption coefficient of monolayer WSe₂, ZnO, and their heterostructures at the HSE06 with SOC level.