Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

DFT investigation of the electronic and optical properties of hexagonal MX_2/ZrXO (M= W, Mo and X = S, Se) van der Waals heterostructures for photovoltaic solar cell application Study

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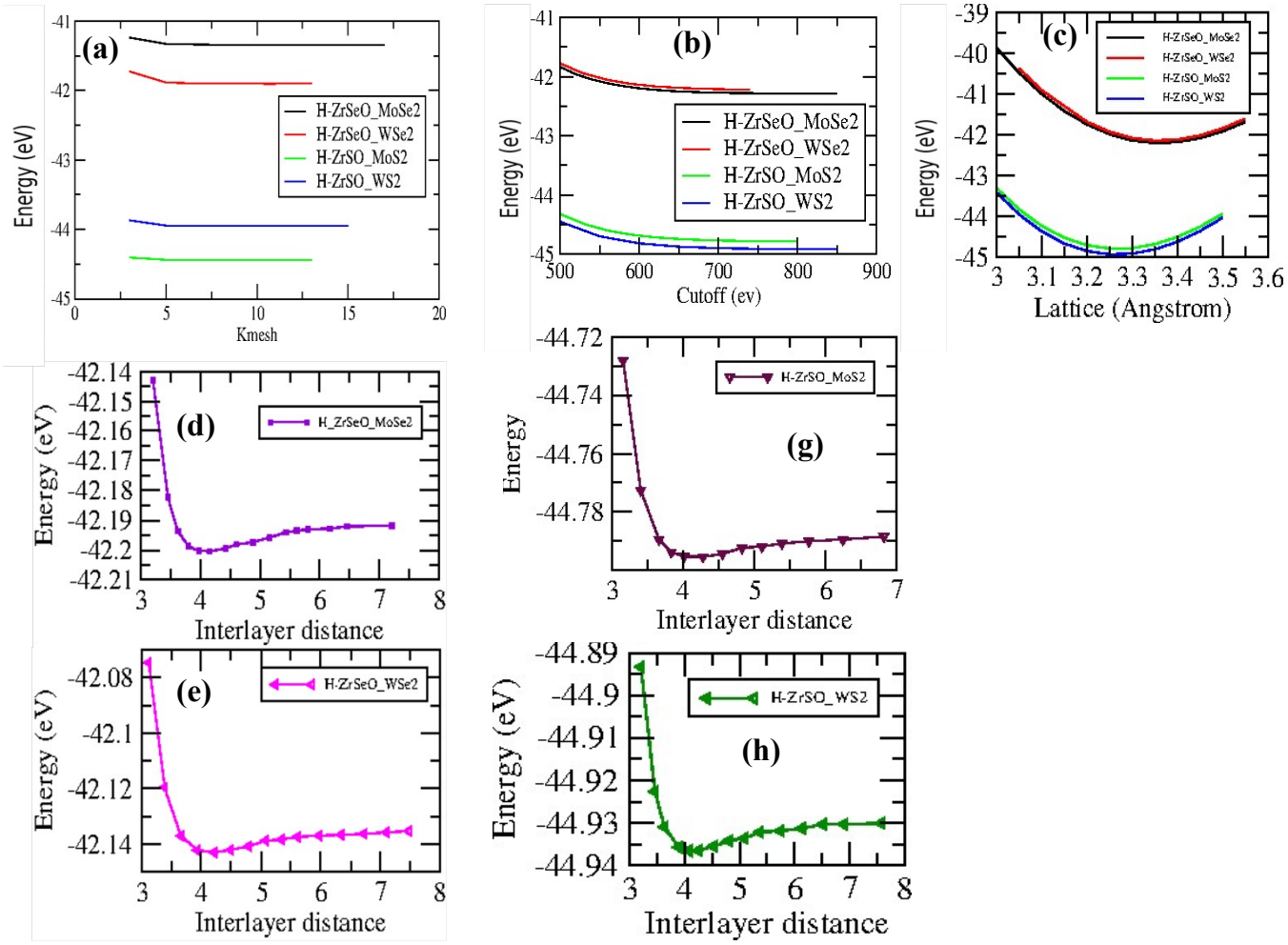

Figure S1: Convergence and geometrical optimization results of the heterostructures (a) k-mesh, (b) Cutoff Energy, (c) Lattice parameter, (d-h) Interlayer Distance, for the material's MoSe2/ZrSeO, WSe2/ZrSeO, MoS2/ZrSO, and WS2/ZrSO

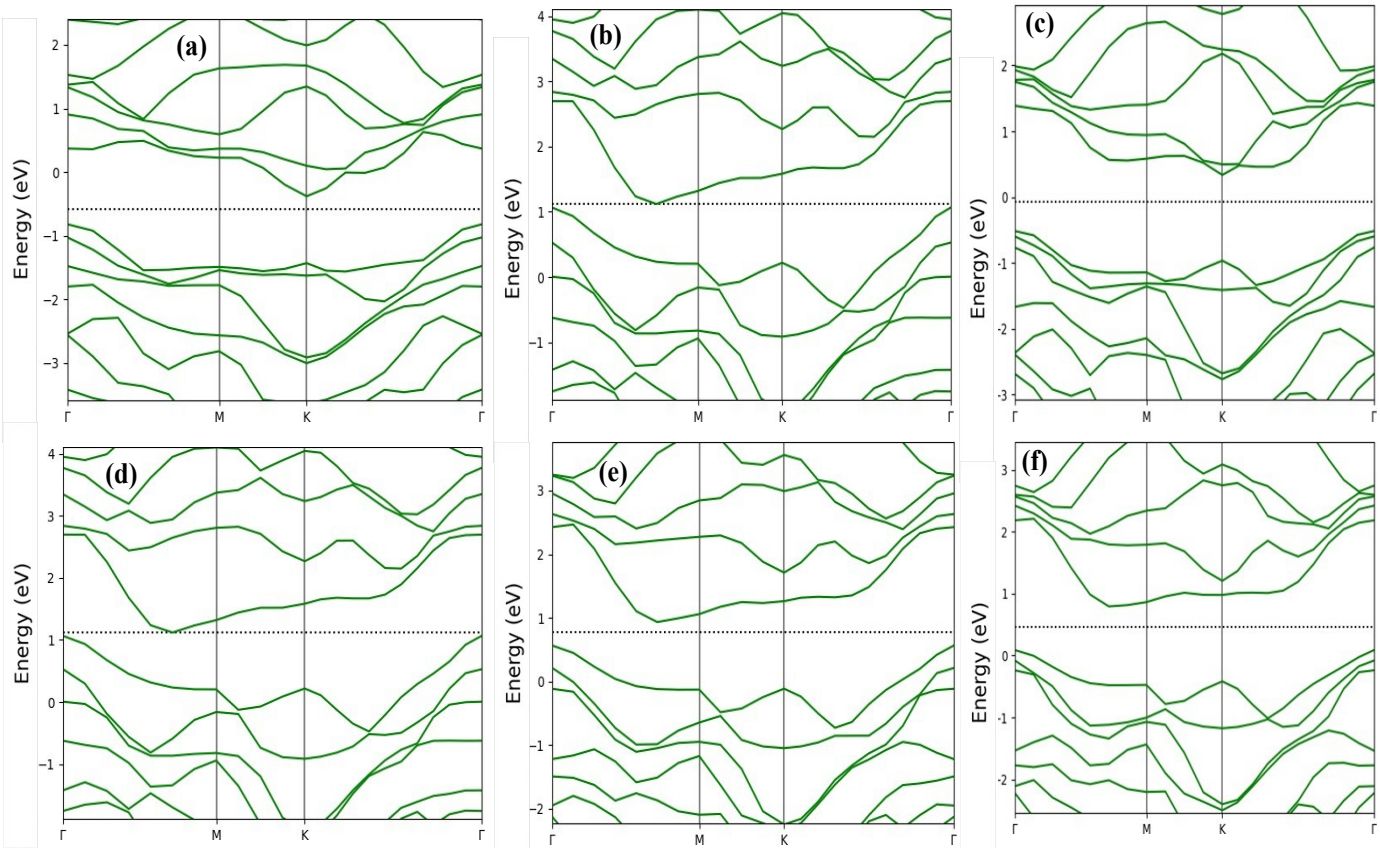

Figure S2: Band structure of the Strain effect on the band gap of the heterostructure materials (a-c) tensile strain applied with the value of (+6, +4 and +2) and (d-f) compressive strain with the value of (-6, -4, and -2) respectively

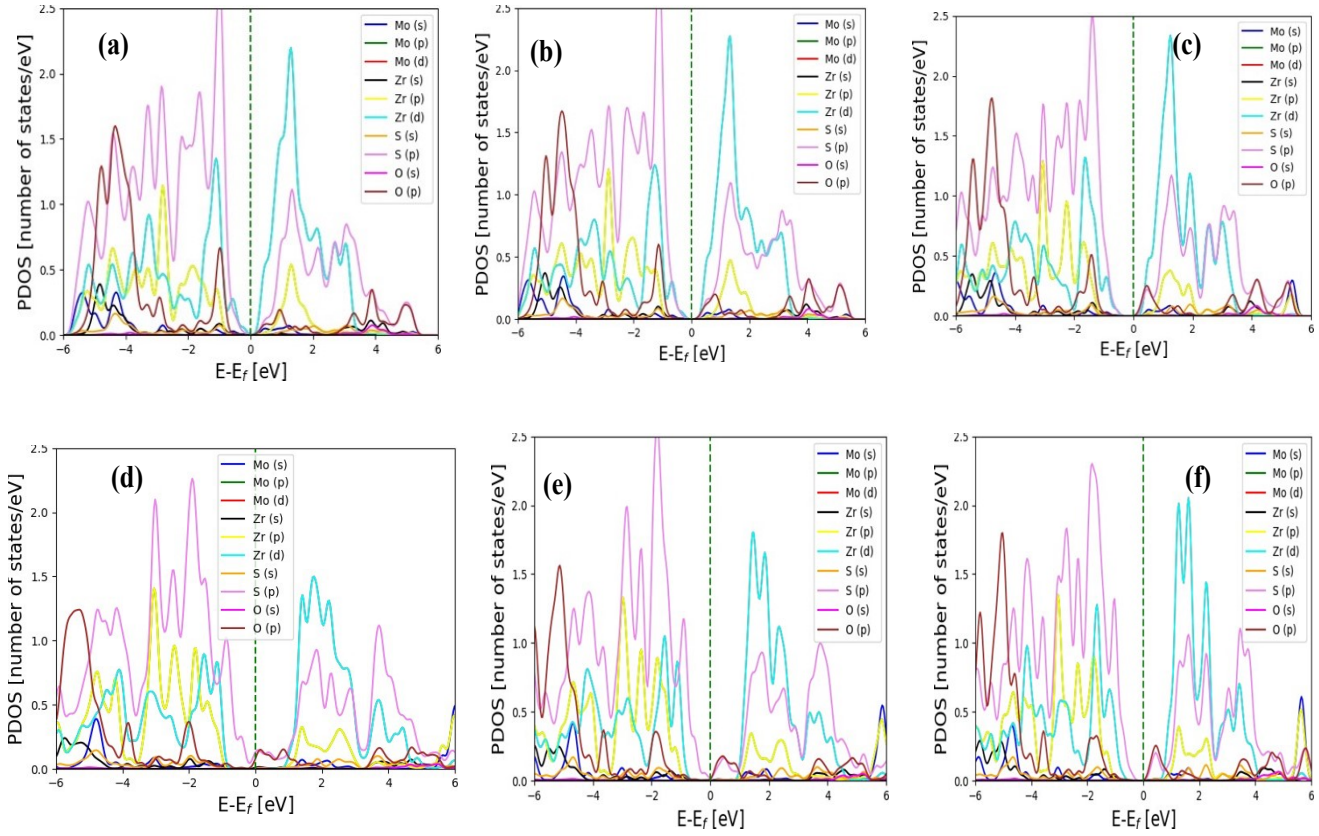

Figure S3: Project density of state for the strain effect on the band gap of the heterostructure materials (a-c) tensile strain applied with the value of (+6, +4 and +2) and (d-f) compressive strain with the value of (-6, -4, and -2) respectively

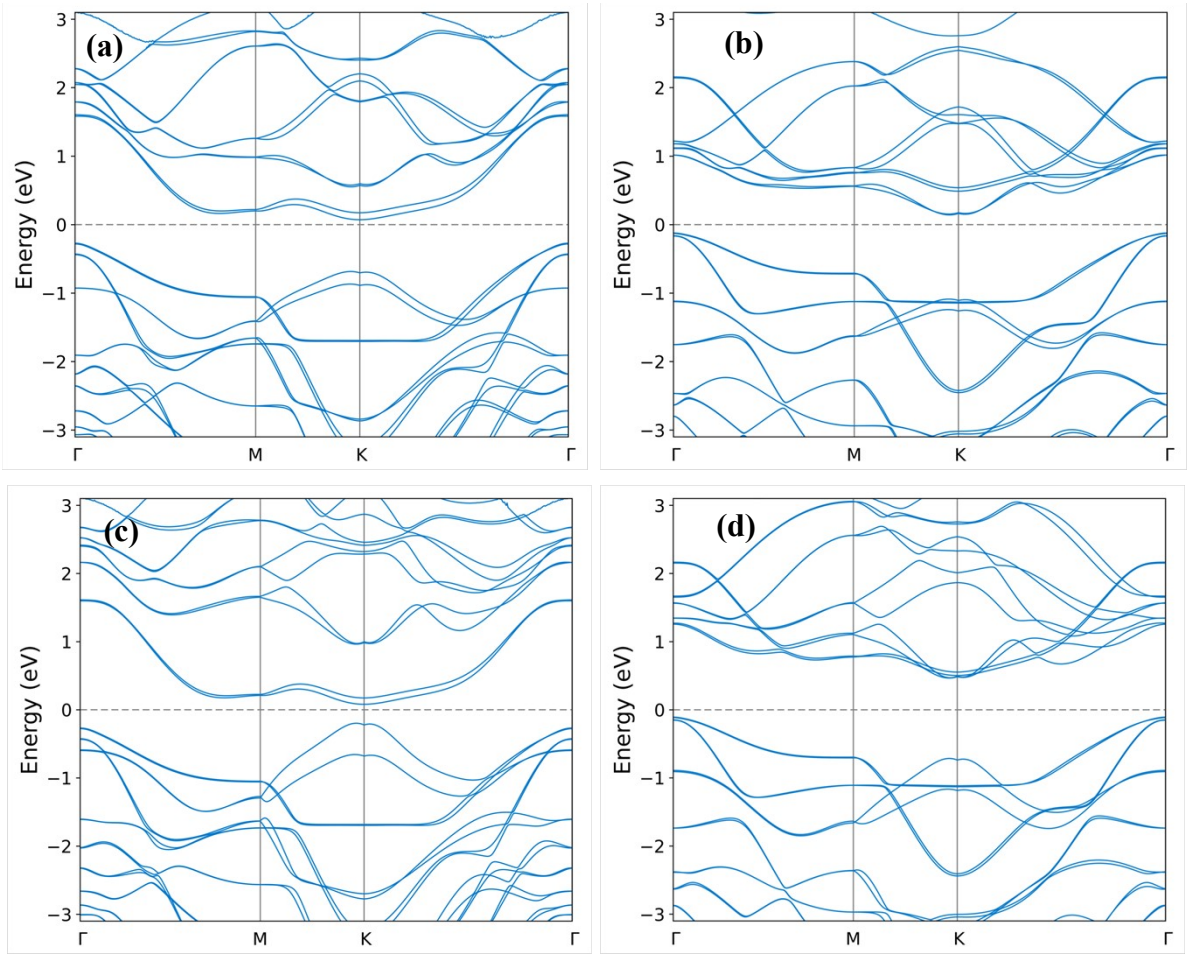

Figure S4: Band structures of (a) MoSe2/ZrSeO, (b) MoS2/ZrSO, (c) WSe2/ZrSeO, and (d) WS2/ZrSO vdW heterostructures using spin orbital coupling (SOC) effect, respectively.