Supporting Information

Interfacial aspect of ZnTe/In2Te3 heterostructures as an efficient catalyst for hydrogen evolution reaction

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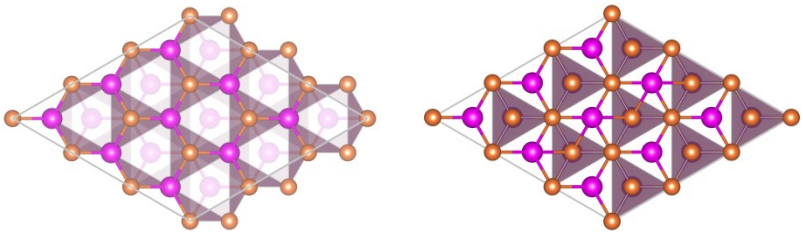

Figure S1 Top views of In_2Te_3 monolayer from the (a) *z* and (b) -*z* directions, respectively.

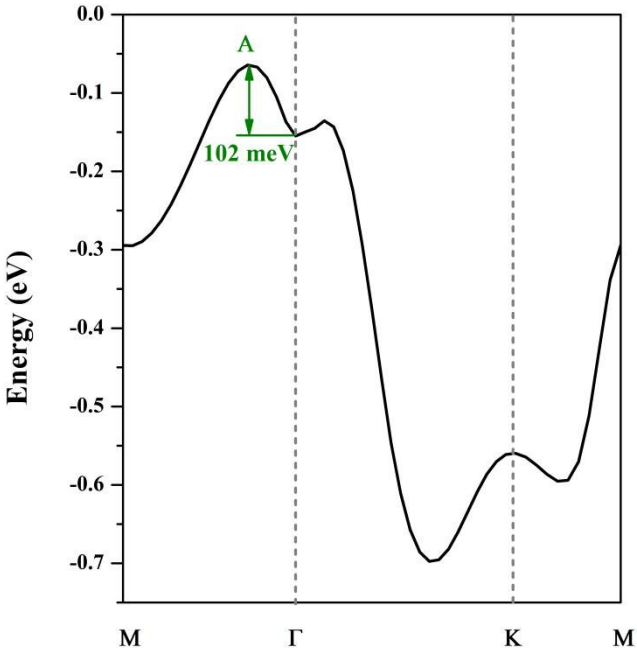

Figure S2 The enlarged band of the VBM based on HSE06 level for In_2Te_3 monolayer. The fermi level is set to 0 eV.

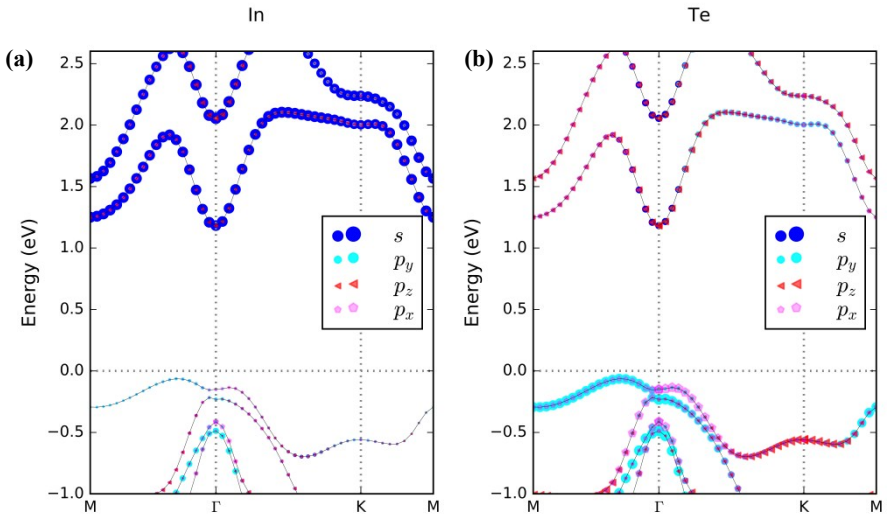

Figure S3 Main projections of the band structures and the corresponding average projections weight of (a) In atoms and (b) Te atoms for In_2Te_3 monolayer.

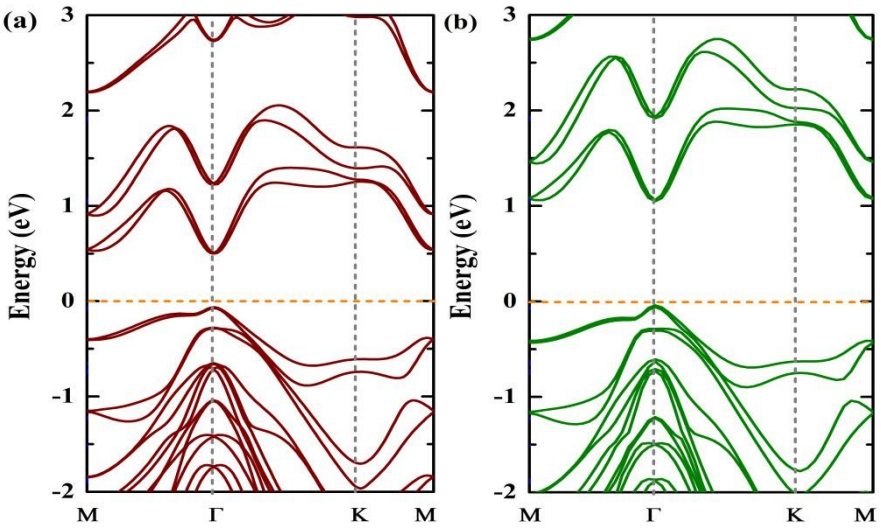

Figure S4 Calculated the band structures of In_2Te_3 monolayer by using (a) PBE+SOC and (b) HSE+SOC functionals, respectively. The dotted lines indicate the position of the Fermi level.

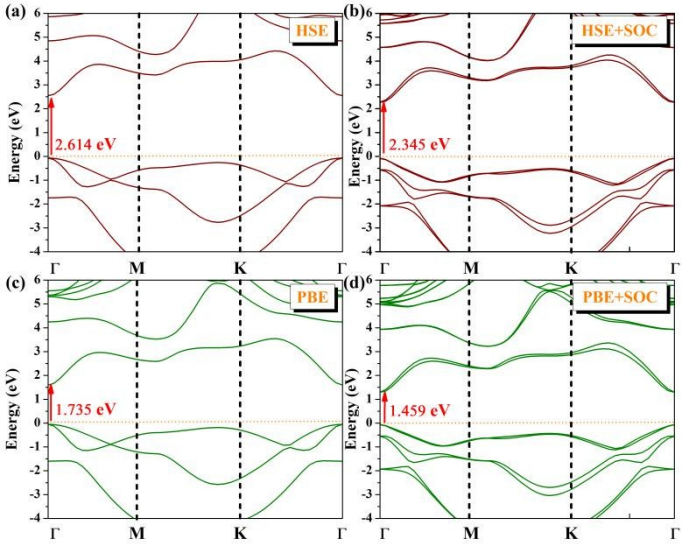

Figure S5 Calculated the band structure of 2D ZnTe monolayer by using (a) HSE, (b) HSE+SOC, (c) PBE and (d) PBE+SOC functionals, respectively. The dotted lines indicate the position of the Fermi level.

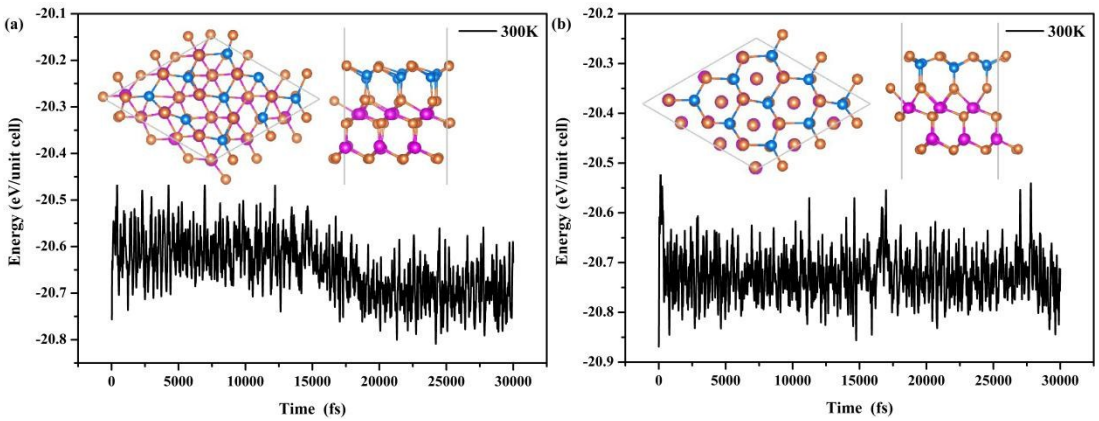

Figure S6 Variations of the total energies of (a) A-ZnTe/In_2Te_3 and (b) B-ZnTe/In_2Te_3 heterostuctures at 300 K during the time of 3 ps from AIMD simulation, respectively. Insets in (a) and (b) show the snapshots of the equilibrium structure from top and side views of the corresponding systems at 300K, respectively.

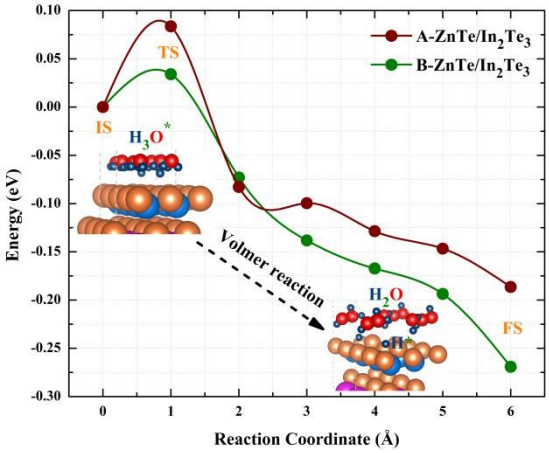

Figure S7 Minimum energy pathways of the Volmer reaction on the surface of (a) A-ZnTe/In_2Te_3 and (b) B-ZnTe/In_2Te_3 heterostuctures, respectively. The initial states contain one solvated proton and the final states the solvated proton has sdsorbed on to the top Te site as θ = 25% coverage system. Insets show side views of the initial and final state structures.

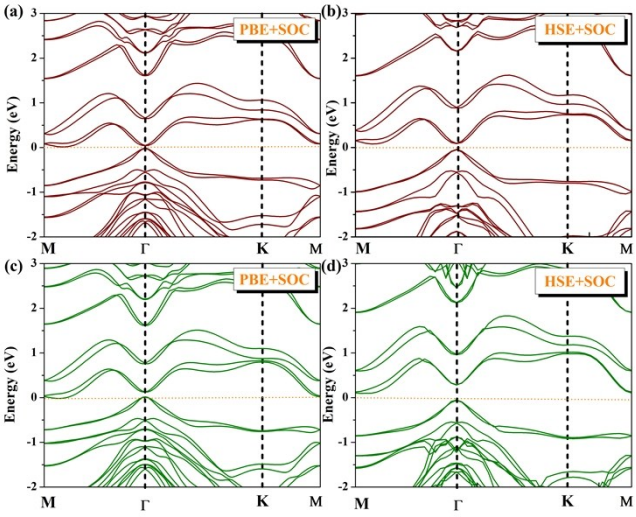

Figure S8 Calculated the band structures of ZnTe/In_2Te_3 heterostructures by using PBE+SOC and HSE+SOC functionals with (a-b) A and (c-d) B stacking orders, respectively. The dotted lines indicate the position of the Fermi level.

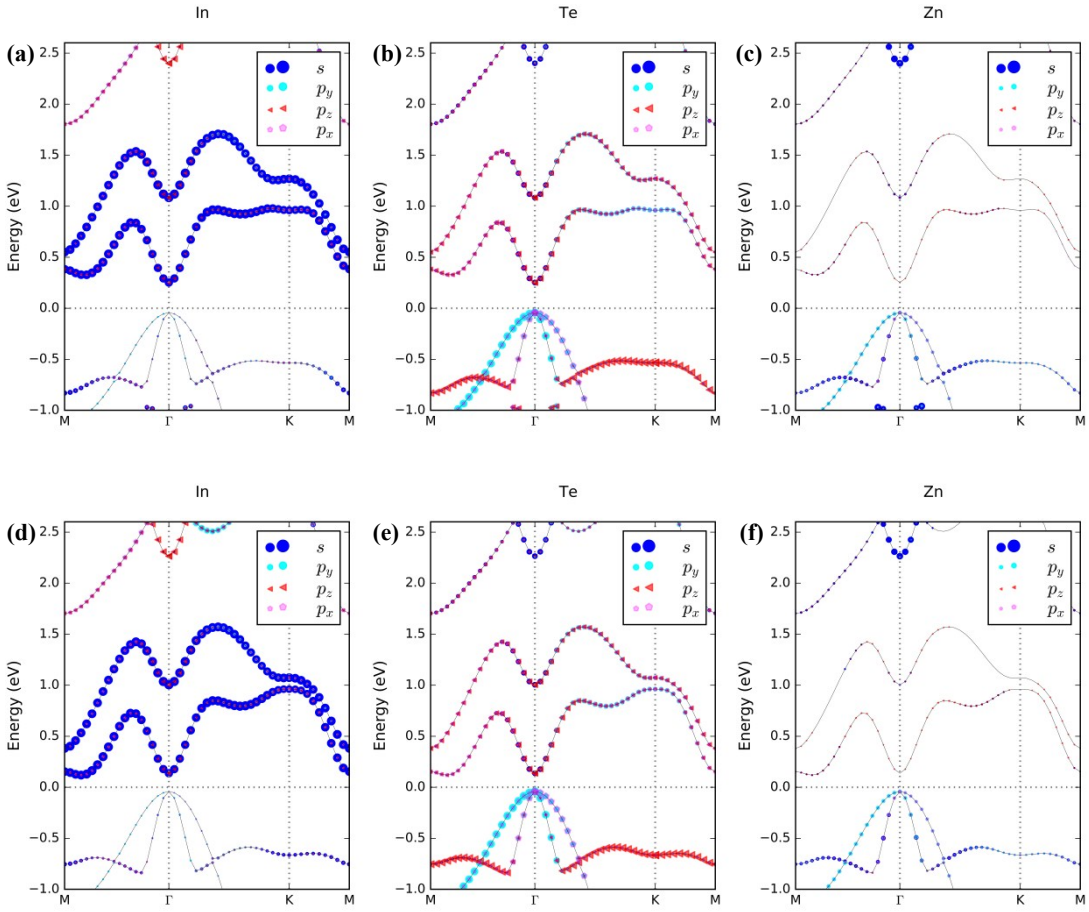

Figure S9 Main projections of the band structures and the corresponding average projections weight of (a), (d) In atoms, (b), (e) Te atoms and (c), (f) Zn atoms for A-ZnTe/In_2Te_3 (upper) and B-ZnTe/In_2Te_3 (dow) heterostructures.