Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Electronic properties of in-plane CdS/ZnSe heterostructure: Type-II band alignment for water splitting

Hongchao Yang, Jinjin Li, Lin Yu, Baibiao Huang, Yandong Ma*, and Ying Dai*

School of Physics, State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, People's Republic of China

*Corresponding author: yandong.ma@sdu.edu.cn (Y.M.); daiy60@sina.com (Y.D.)

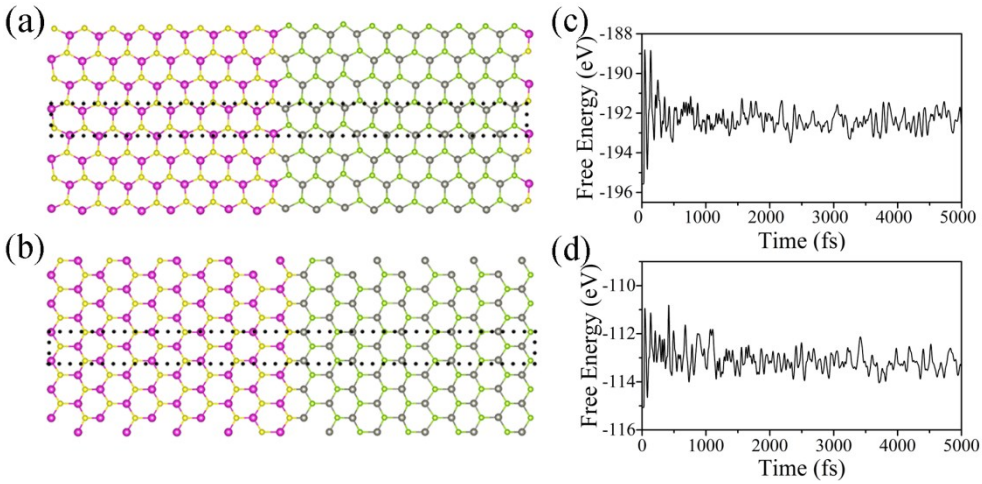

Fig. S1. Top views of the snapshots taken from the end of the AIMD simulations at the temperature of 500 K for (a) a-CdS/ZnSe and (b) z-CdS/ZnSe. The variation of the free energies for (a) a-CdS/ZnSe and (b) z-CdS/ZnSe in the AIMD simulations at 500 K during the timescale of 5 ps.

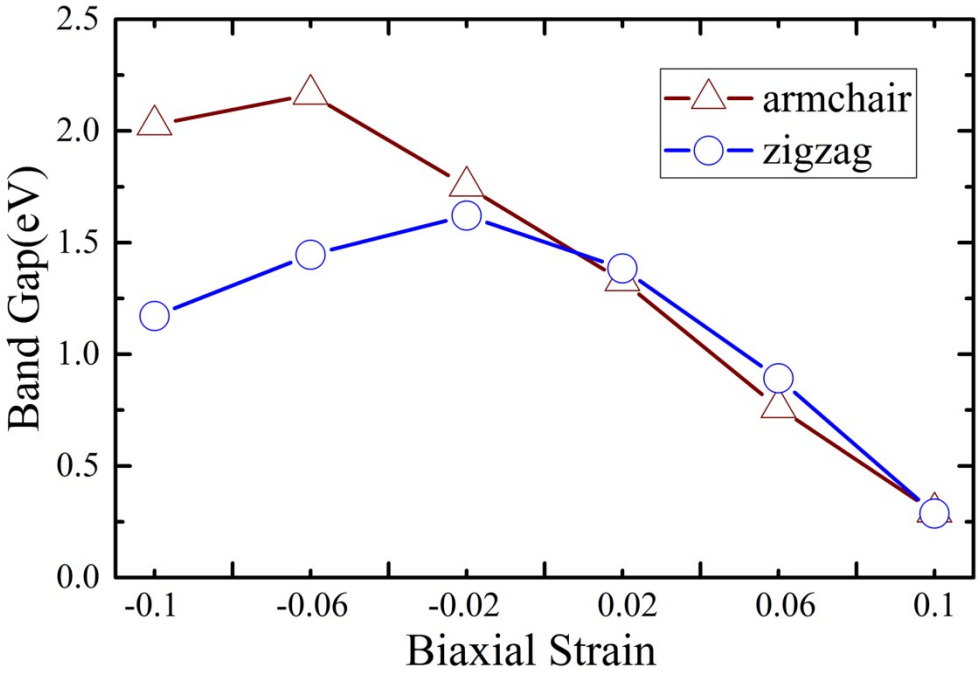

Fig. S2. The varization of band gaps of a-CdS/ZnSe and z-CdS/ZnSe as a function of biaxial strain. Blue and wine lines represent linear fitting of zigzag and armchair configurations, respectively.

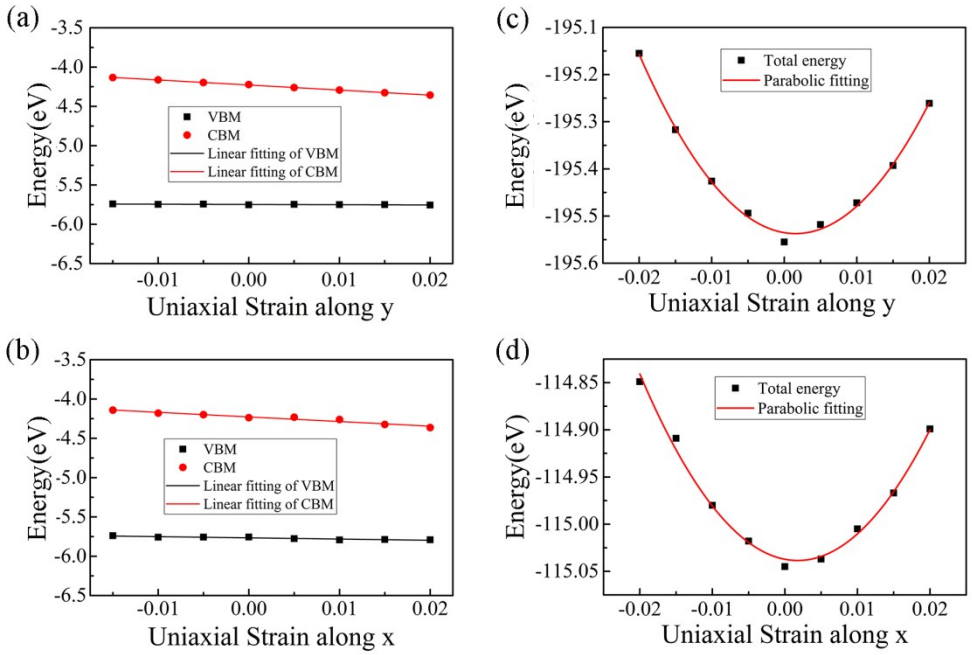

Fig. S3. Band edge positions and total energy as a function of the uniaxial strain for (a, c) a-

CdS/ZnSe and (b, d) z-CdS/ZnSe.

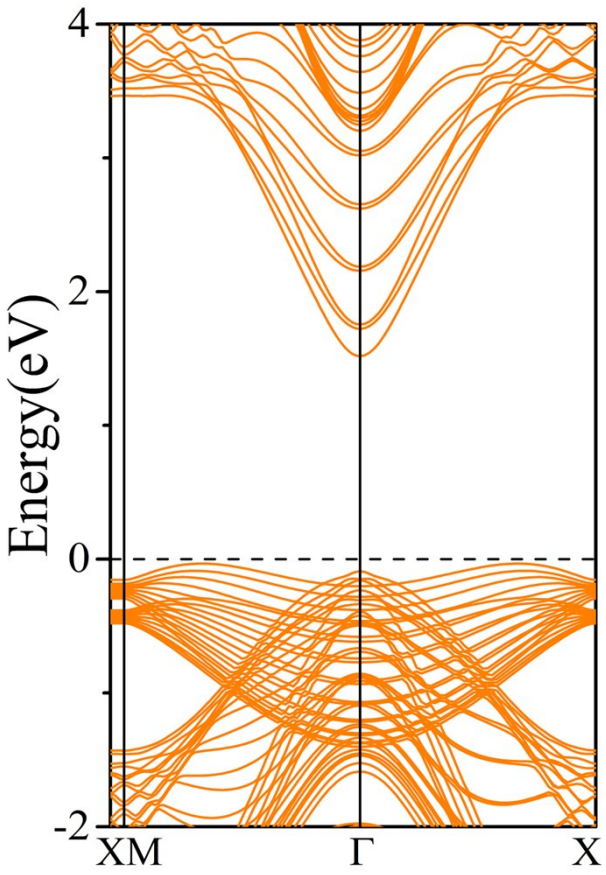

Fig. S4. Band structure of zigzag configuration with more stringent parameters (e.g. energy 10^-6 eV, forces 0.01 eV/A, doubled k-point grid), the results are almost the same with the results in the manuscript.

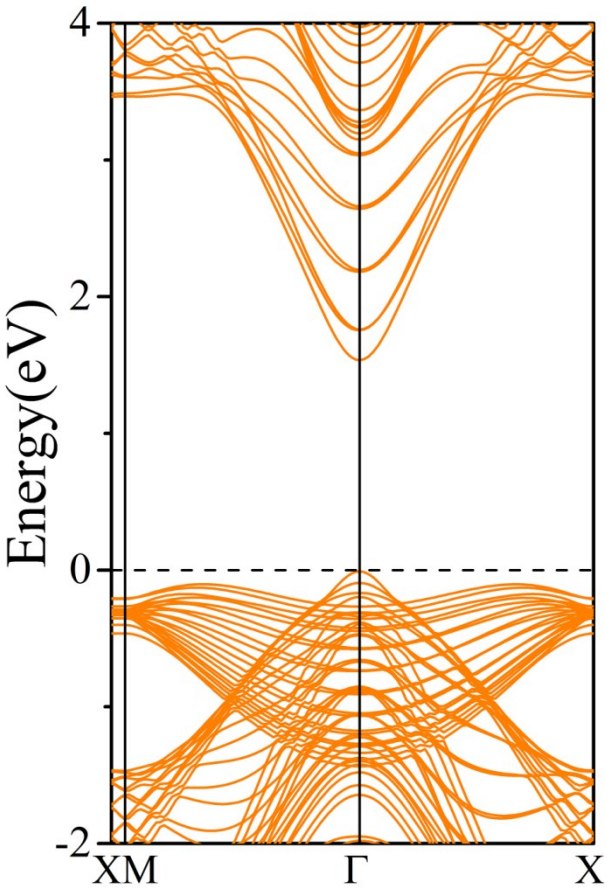

Fig. S5. Band structure of Cd-Se bonds at the edge for zigzag configuration. The value of bandgap at PBE level is 1.54 eV which is equal to the interface jointed by Zn-S bonds configuration. It's have a direct bandgap for both VBM and CBM are all located at Γ point. For these two structures, the binding energy are -4.879 eV and -4.883 eV, respectively.