Supplementary Information

First-Principles Investigation on the Electronic Structures of $CdSe_xS_{1-x}$ and Simulation of CdTe Solar Cell with $CdSe_xS_{1-x}$ Window Layer by SCAPS

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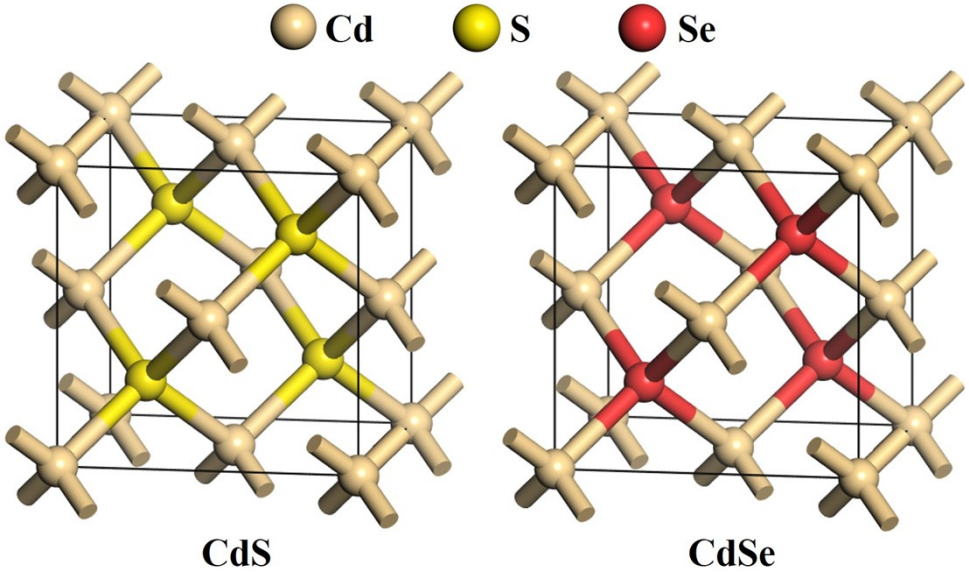
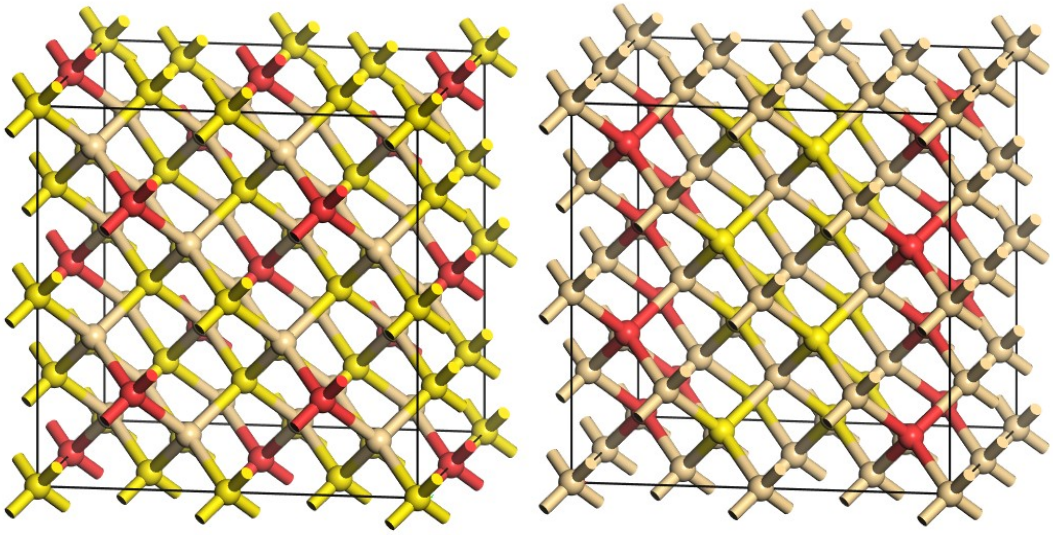
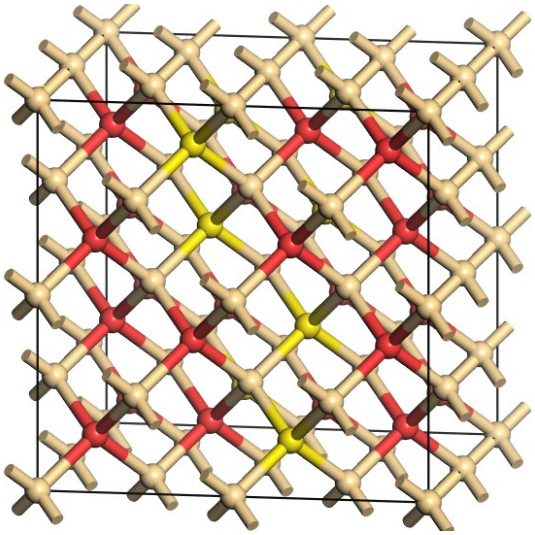


Fig.S1 Crystal structure of cubic zinc-blende CdS and CdSe

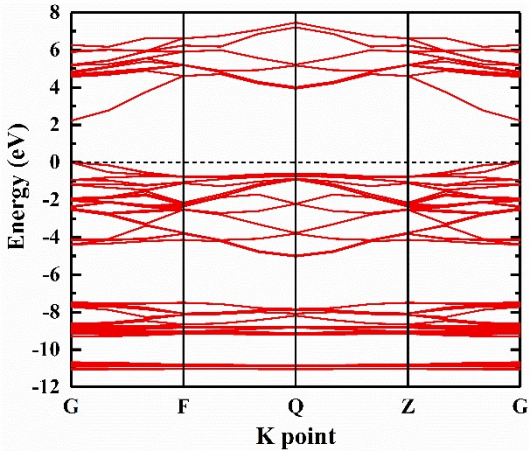


(a) x = 0.25 **(b) x = 0.5**

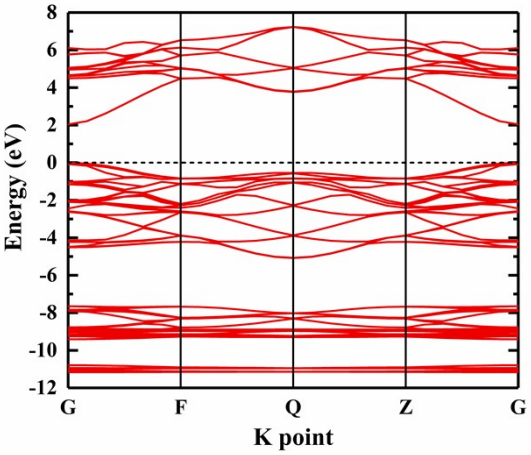


(c) x = 0.75

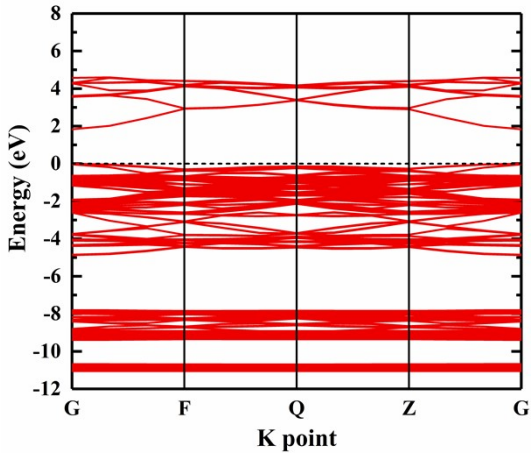
Fig.S2 Crystal structure of cubic zinc-blende $CdSe_xS_{1-x}$ supercell



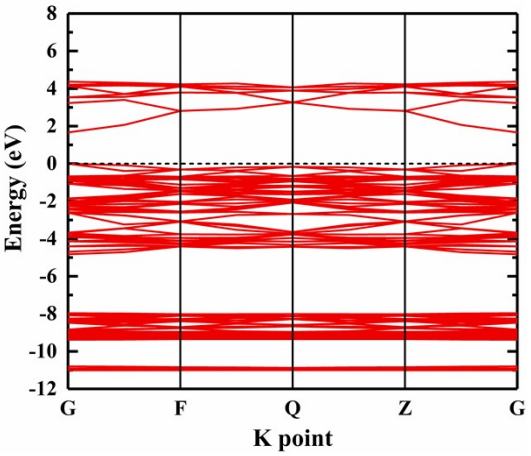
(a) x = 0.25



(b) x = 0.50



(a) x = 0.75



(b) x = 1.00 (CdSe)

Fig.S3 Band structure of cubic zinc-blende $CdSe_xS_{1-x}$ ($0.25 \leq x \leq 1.00$)