

1. (b)

Figure S1: Crystal structure of (a) stannite and (b) kesterite CZTS [1].

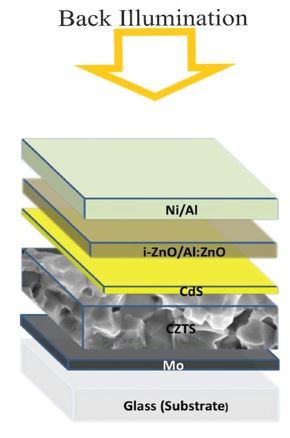
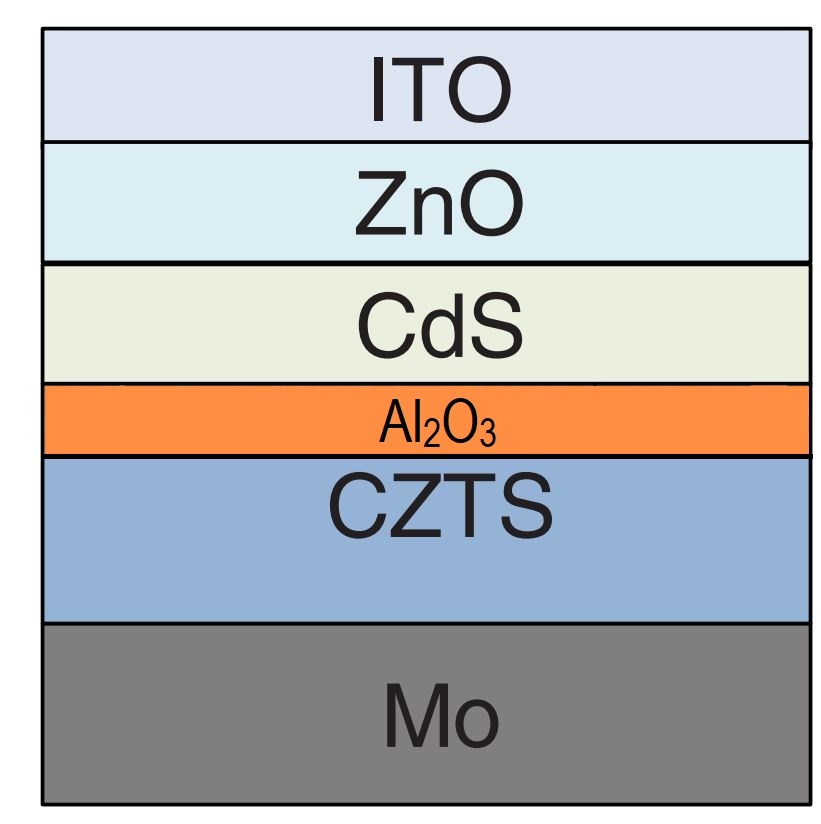
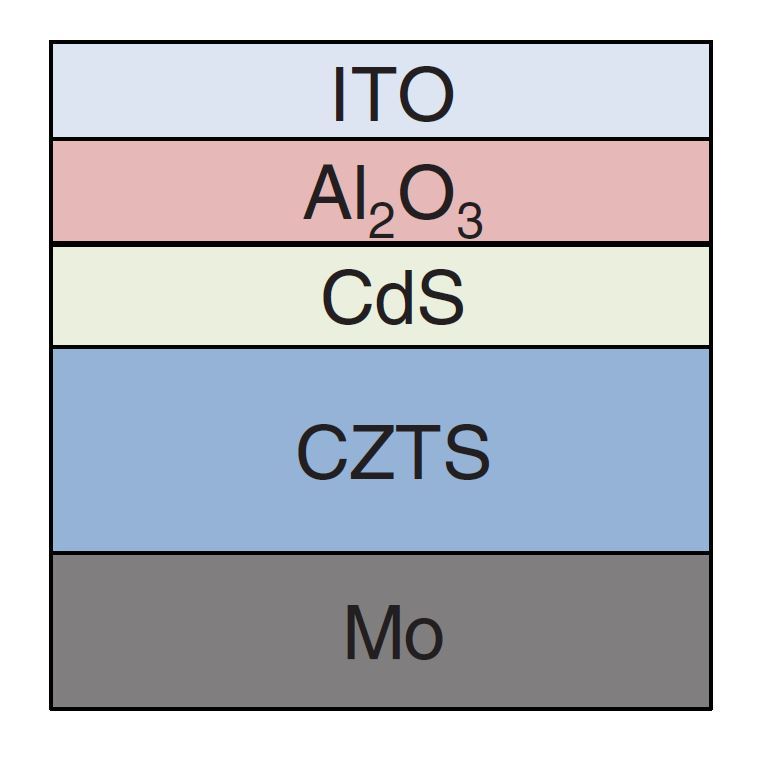


Figure S2: Typical device structure for CZTS solar cells (adapted from [2]).



1. (b)

Figure S3: Schematic of device structures with Al2O3 on the top of (a) Absorber layer (b) n-type CdS layer (adapted from [3]).

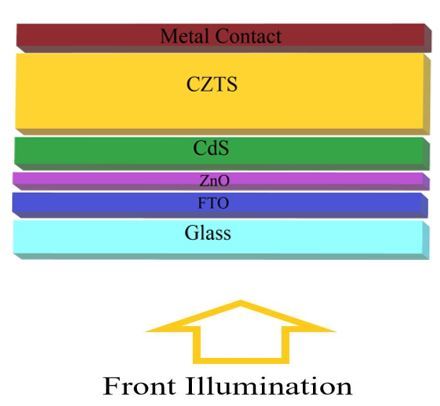


Figure S4: Schematic of CZTS device structures with FTO coated Substrate

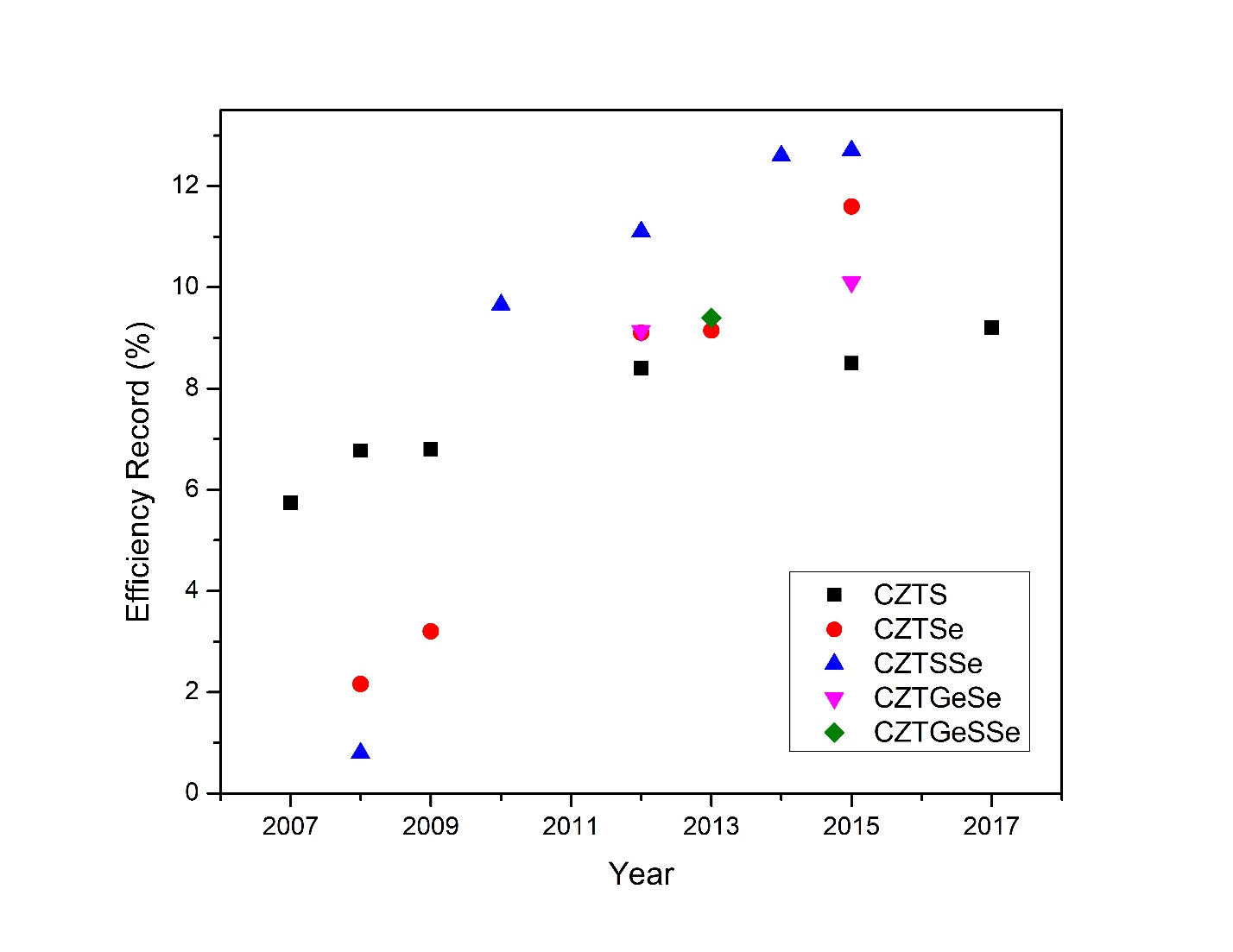


Figure S5: Improvement of conversion efficiency on CZTS-based thin-film solar cells ([4]–[23])

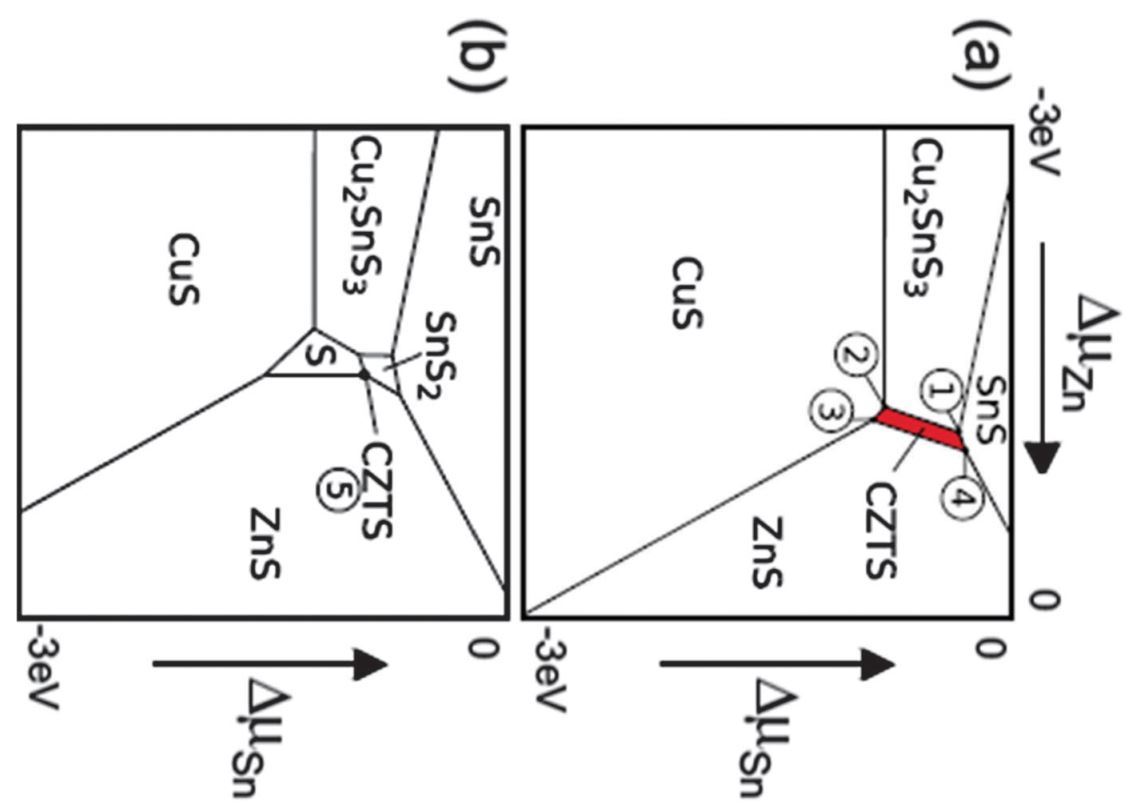


Figure S6: Chemical potential based stability diagram for tin and zinc under (a) copper-rich and (b) copper-poor conditions. Δµ is the chemical potential for the standard element. (adapted from [2]).

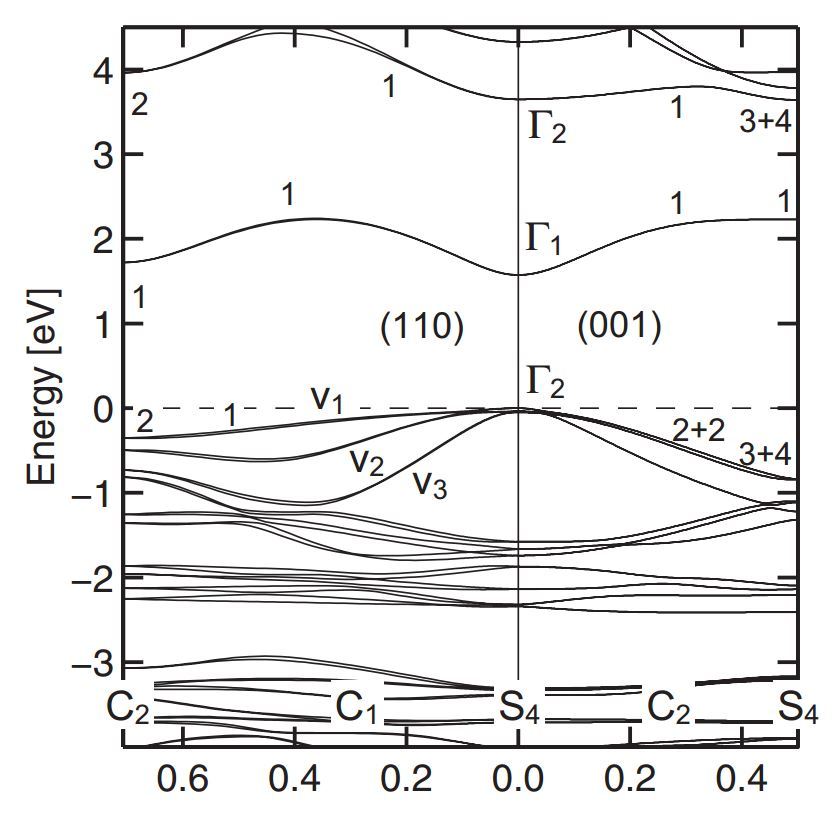


Figure S7: Electronic band structure of kesterite CZTS along with the two symmetry directions (110) and (001) (adapted from [24]).

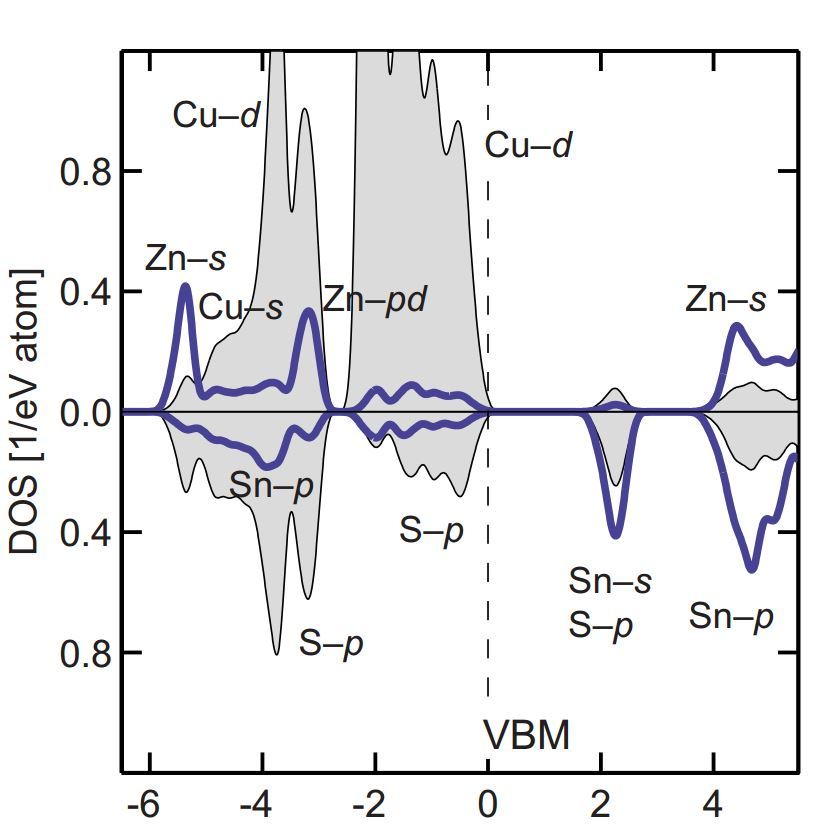


Figure S8: Atomic resolved DOS of CZTS, presented with a 0.1 eV Lorentzian broadening. The gray area in the upper panels represents the DOS of Cu atoms, and the thick blue line represents Zn atoms. In the lower panels, the gray area represents S, and the thick blue line represents Sn atoms (adapted from [25]).

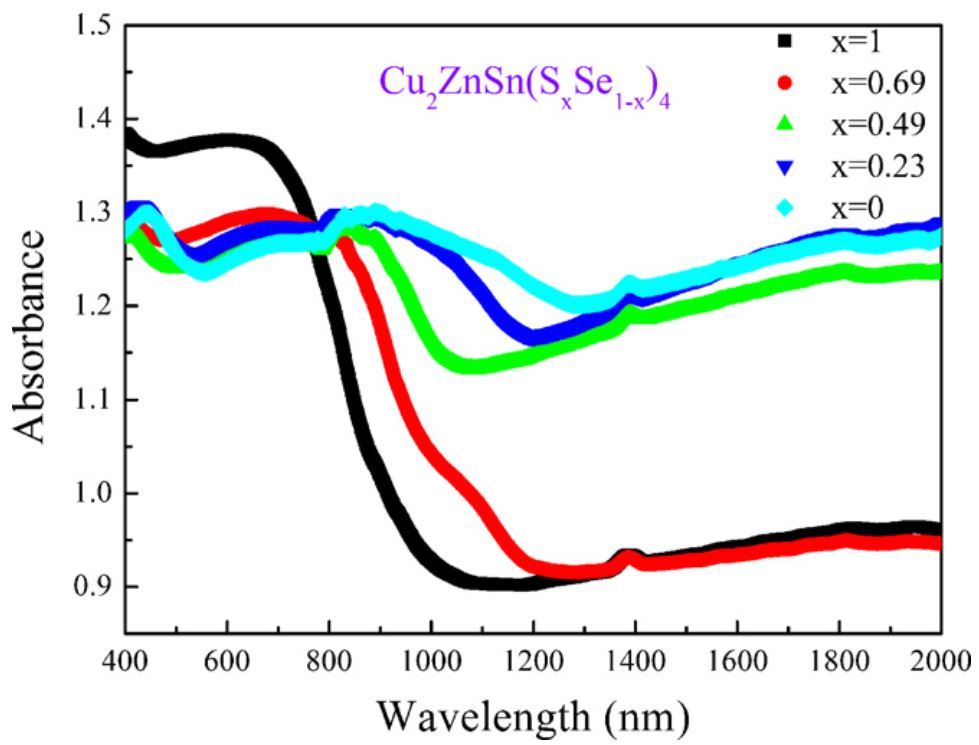
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Figure S9: Absorption spectra of Cu2ZnSn(SxSe1−x)4 powders (adapted from [26]).

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