Supplementary Information

Band alignment engineering and performance prediction of Cu_2ZnSnS_4/Ag_2ZnSnS_4-based solar cells using first-principles calculations and SCAPS-1D device simulations

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Table S1 The enhanced performance outcomes of solar cells.

	V_{OC}(V)	J_{SC}(mA/cm^2)	FF(%)	PCE(%)
ZnO/CdSe/AZTS/CZTSe/Mo	1.08	25.93	84.30	23.60
ZnO/ZnSe/AZTS/CZTSe/Mo	1.07	25.31	83.78	22.67
ZnO/CdSe/CZTS/CZTSe/Mo	0.78	35.10	82.71	22.54
ZnO/ZnSe/CZTS/CZTSe/Mo	0.78	35.70	82.20	22.75

Table S2 The combination of χ corresponding to the maximum performance parameters across different device architectures. (The left side represents the χ potential of the BSF layer, while the right side corresponds to the χ potential of the buffer layer; both are measured in electron volts (eV).)

	AZTS/CdSe	AZTS/ZnSe	CZTS/CdSe	CZTS/ZnSe
V_{OC}	4.1/4.4	4.1/4.2	4.2/4.1	4.2/3.9
J_{SC}	3.7/4.4	3.7/4.2	3.8/4.8	4.1/4.3
FF	4.2/4.3	4.2/4.2	3.9/4.3	3.9/4.3
PCE	4.2/4.3	4.2/4.1	4.0/4.3	4.0/4.3

Table S3 Absorption layer thickness corresponding to the maximum values of various performance parameters in different device architectures (The unit is nm.)

	AZTS/CdSe	AZTS/ZnSe	CZTS/CdSe	CZTS/ZnSe
V_{OC}	1500	1500	400	400
J_{SC}	1500	1500	1500	1500
FF	900	600	400	400
PCE	1300	1400	500	600