Supporting Information

Interfacial electronic and defect engineering coupling of S-scheme $CsSnBr_3/SnS_x$(x = 1, 2) heterostructures with carrier dynamics for solar cells

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Supporting Figures

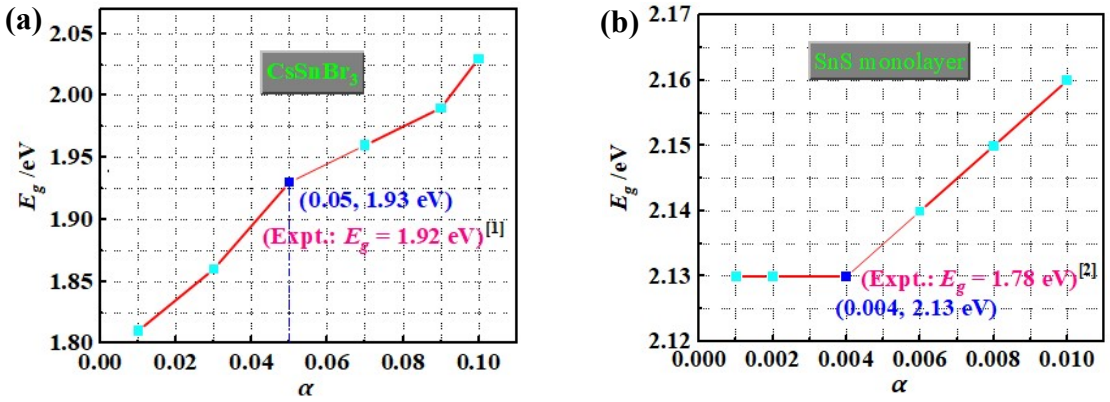


Fig. S1. The calculated band gap concerning different α parameters: (a) $CsSnBr_3$ and (b) SnS monolayer.

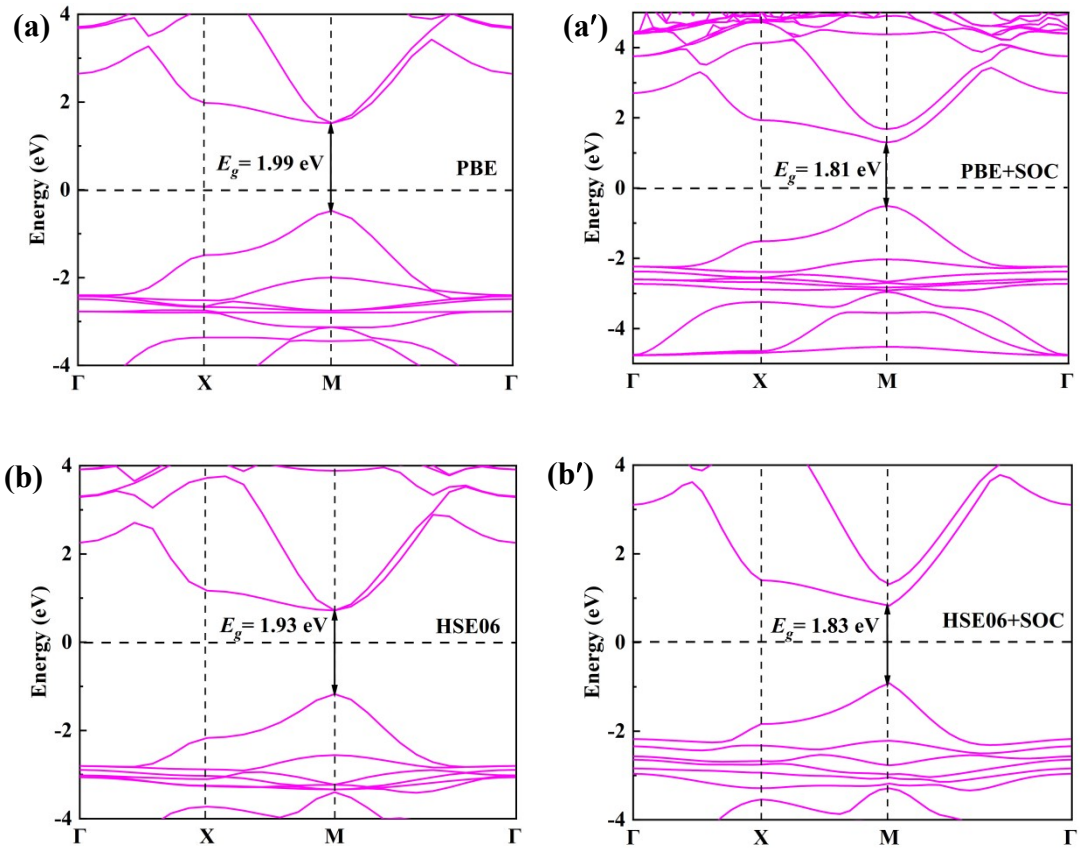


Fig. S2. Calculated band structures of the $CsSnBr_3$ bulk using (a) GGA-PBE, (b) GGA-PBE + SOC, (c) HSE06 functional and (d) HSE06 functional + SOC.

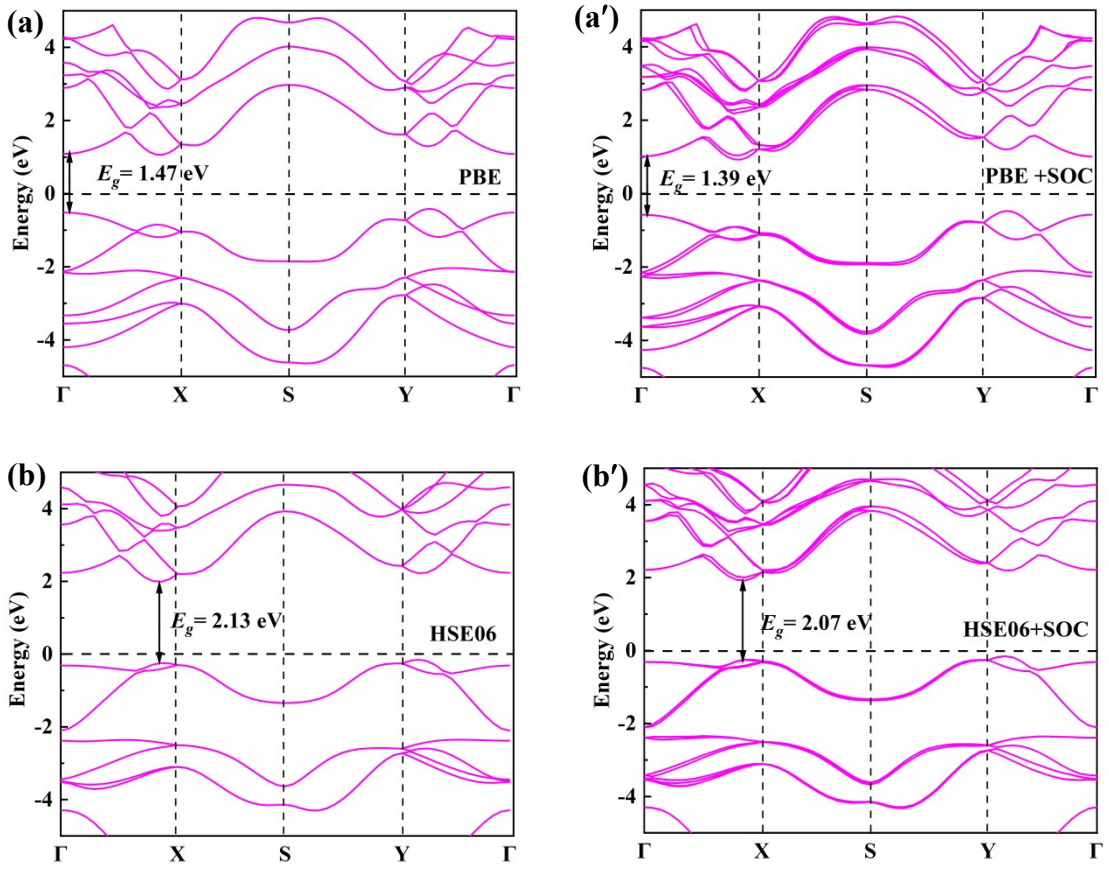


Fig. S3. Calculated band structures of the SnS monolayer using (a) GGA-PBE, (b) GGA-PBE + SOC, (c) HSE06 functional and (d) HSE06 functional + SOC.

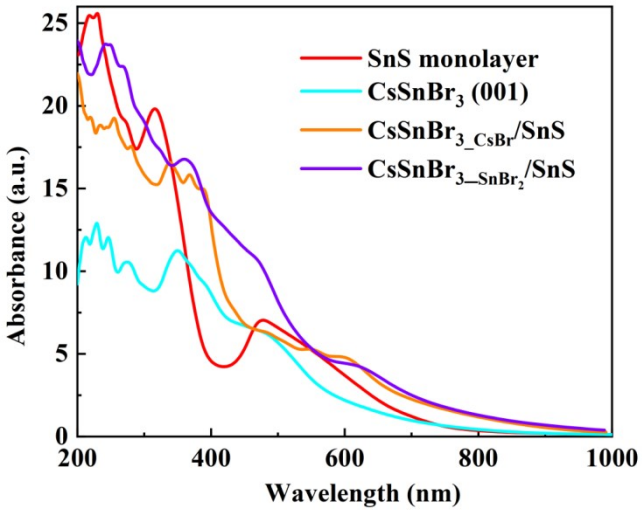


Fig. S4. Calculated optical absorption of SnS monolayer, $CsSnBr_3$ (001), $CsSnBr_3$/SnS heterostructure (with CsBr terminal) and $CsSnBr_3$/SnS heterostructure (with $SnBr_2$ terminal).

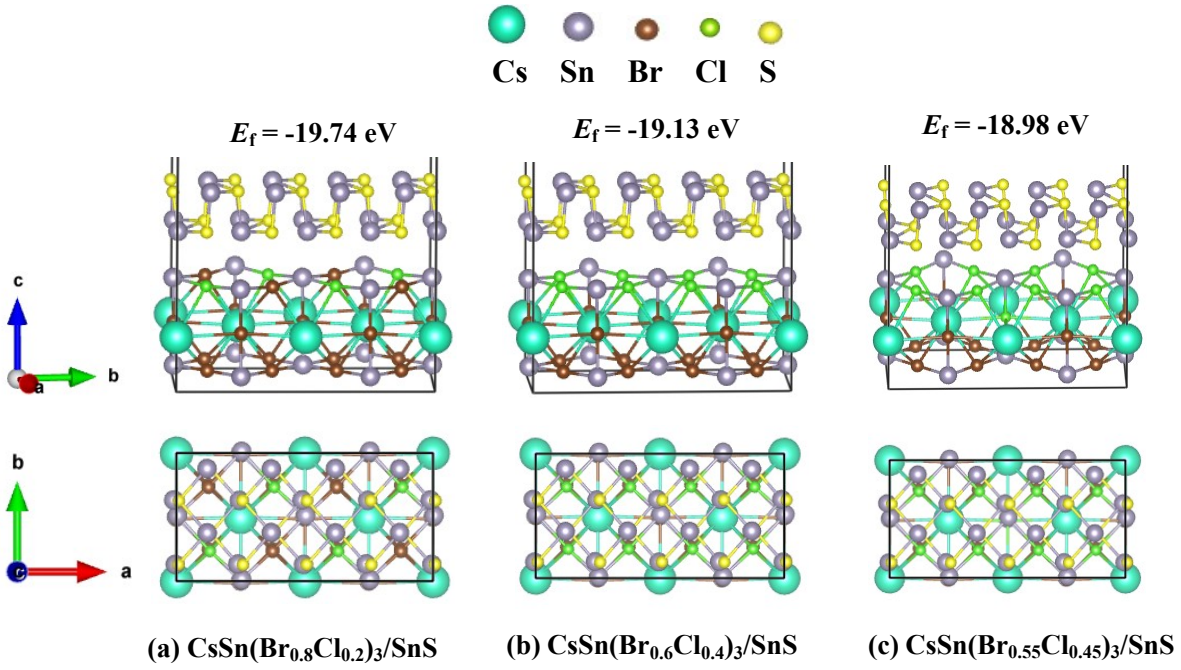


Fig. S5. Optimized crystal structure: top view and side view of the (a) $CsSn(Br_{0.8}Cl_{0.2})_3/SnS$, (b) $CsSn(Br_{0.6}Cl_{0.4})_3/SnS$, (c) $CsSn(Br_{0.55}Cl_{0.45})_3/SnS$ heterostructure, (cyan, gray, brown, green, and yellow represent the Cs, Sn, Br, Cl, and S atoms).

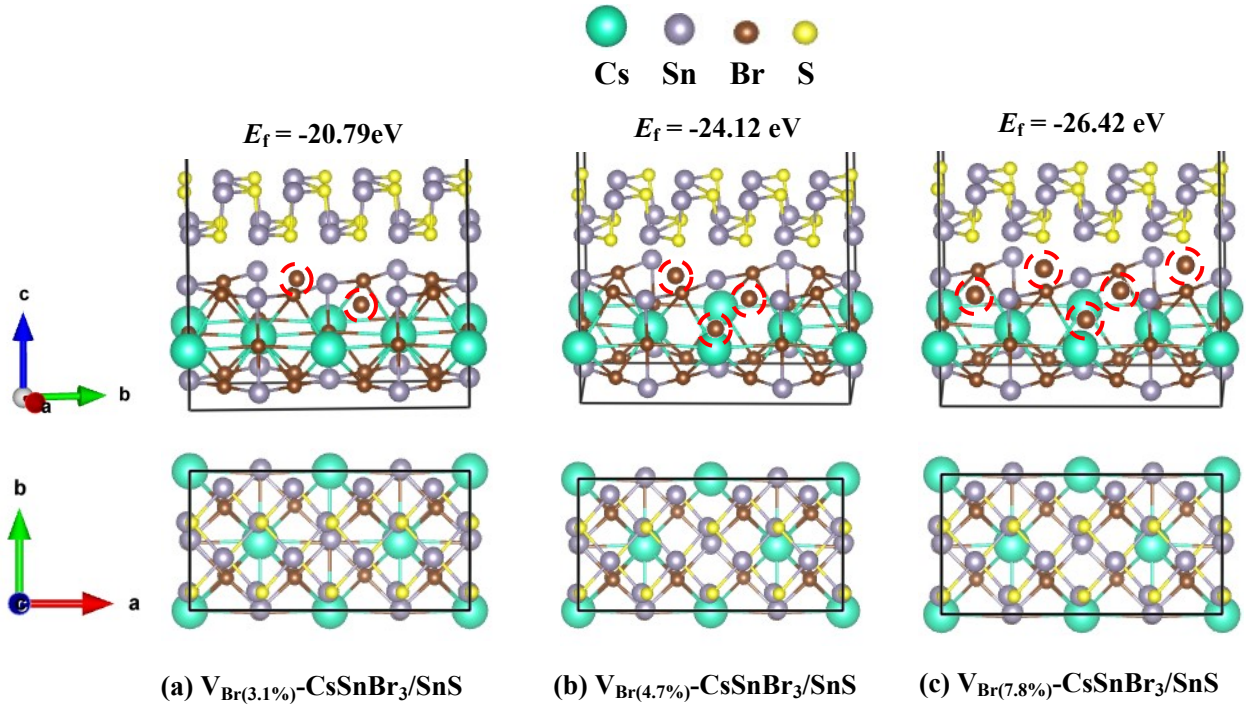


Fig. S6. Optimized crystal structure: top view and side view of the (a) $V_{Br(3.1\%)}$-$CsSnBr_3$/SnS, (b) $V_{Br(4.7\%)}$-$CsSnBr_3$/SnS, (c) $V_{Br(7.8\%)}$-$CsSnBr_3$/SnS heterostructure, (cyan, gray, brown, and yellow represent the Cs, Sn, Br, and S atoms).

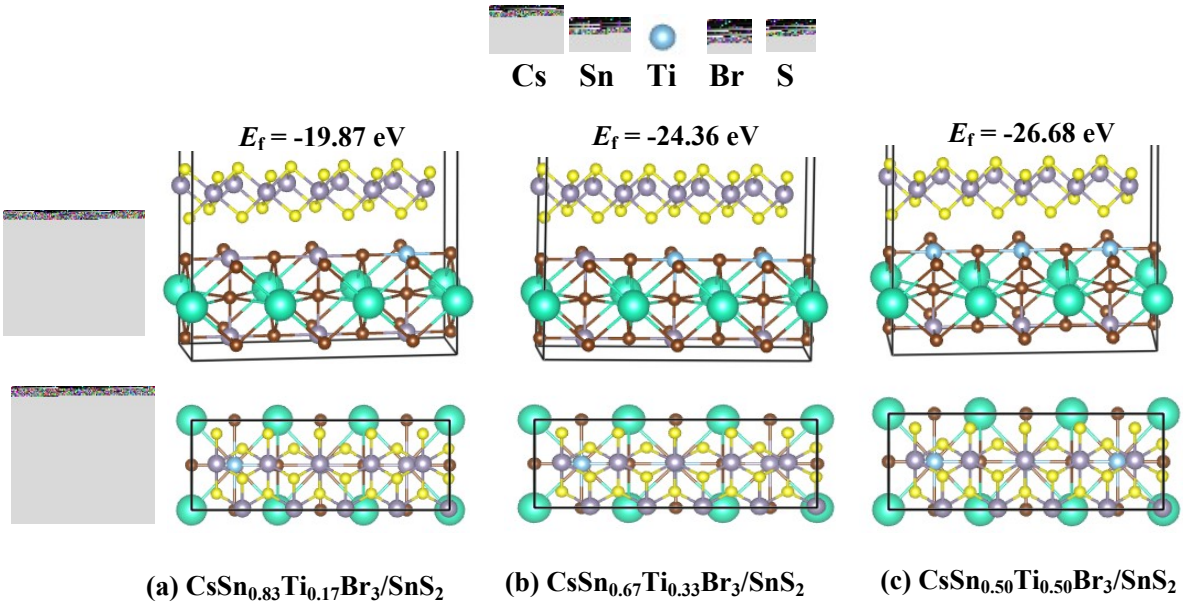


Fig. S7. Optimized crystal structure: top view and side view of the (a) $CsSn_{0.83}Ti_{0.17}Br_3/SnS_2$, (b) $CsSn_{0.67}Ti_{0.33}Br_3/SnS_2$, (c) $CsSn_{0.50}Ti_{0.50}Br_3/SnS_2$ heterostructure, (cyan, gray, sky blue, brown, and yellow represent the Cs, Sn, Ti, Br, and S atoms).

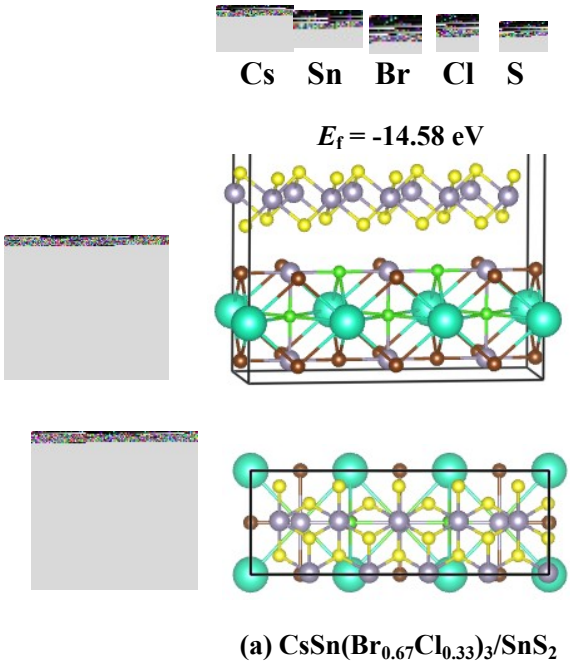


Fig. S8. Optimized crystal structure: top view and side view of (a) $CsSn(Br_{0.67}Cl_{0.33})_3/SnS_2$ heterostructure, (cyan, gray, brown, green and yellow represent the Cs, Sn, Br, Cl and S atoms).

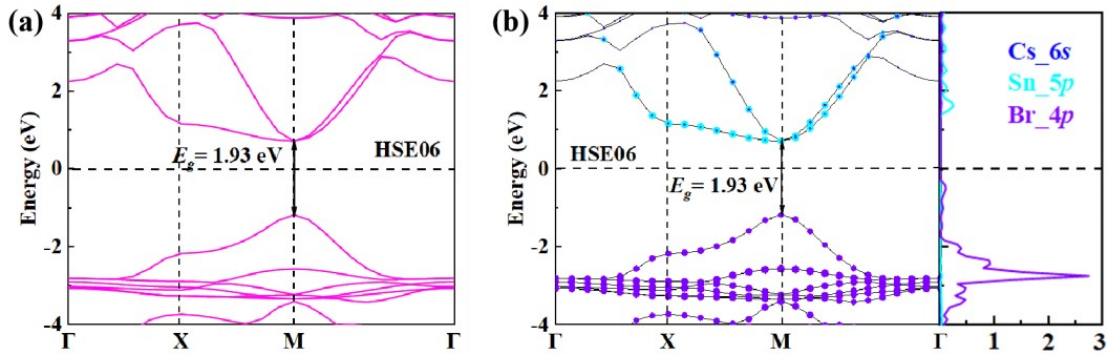


Fig. S9 Calculated: (a) band structure, (b) Projected band structure and PDOS based on HSE06 functional of the $CsSnBr_3$ bulk. The Fermi level is set to 0 eV by a horizontal black dashed line.

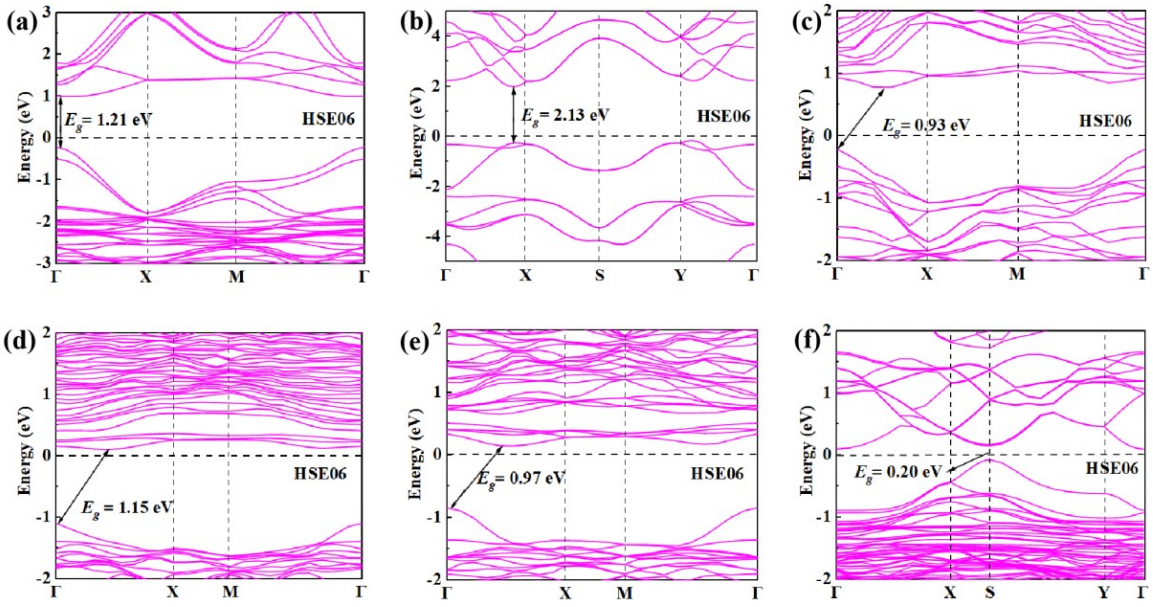
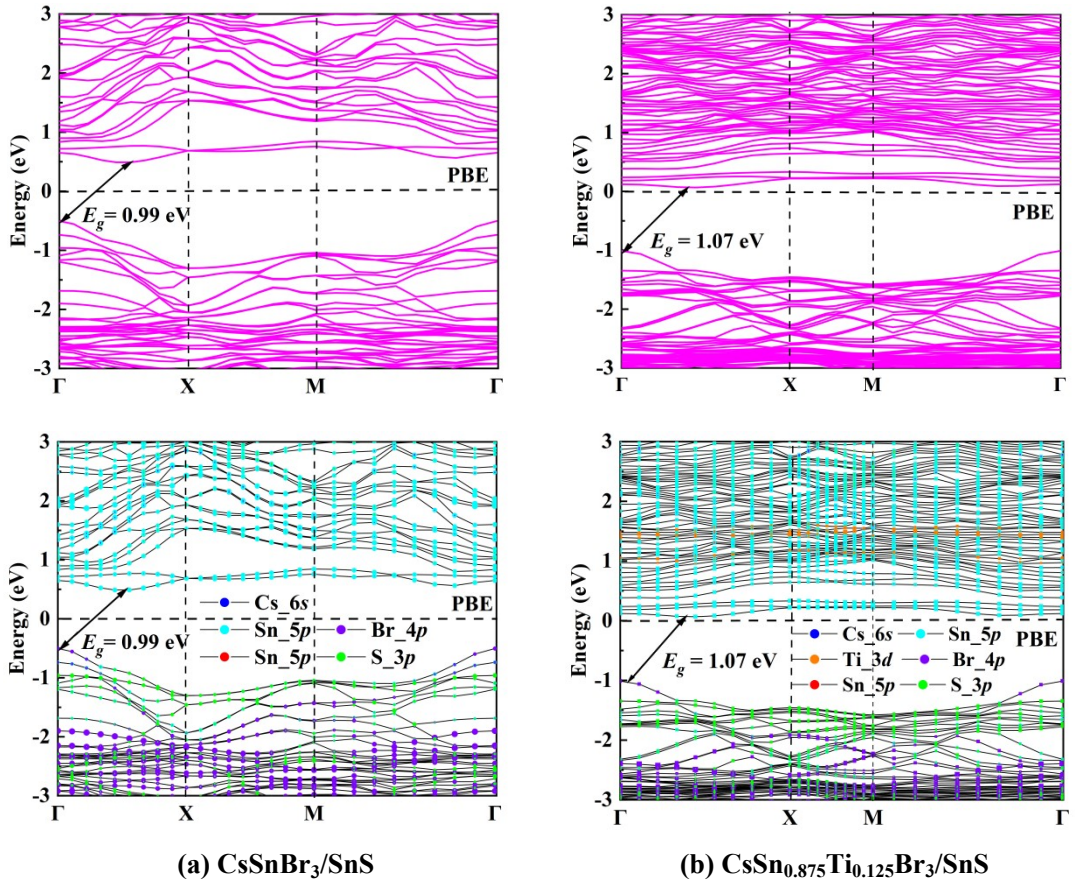
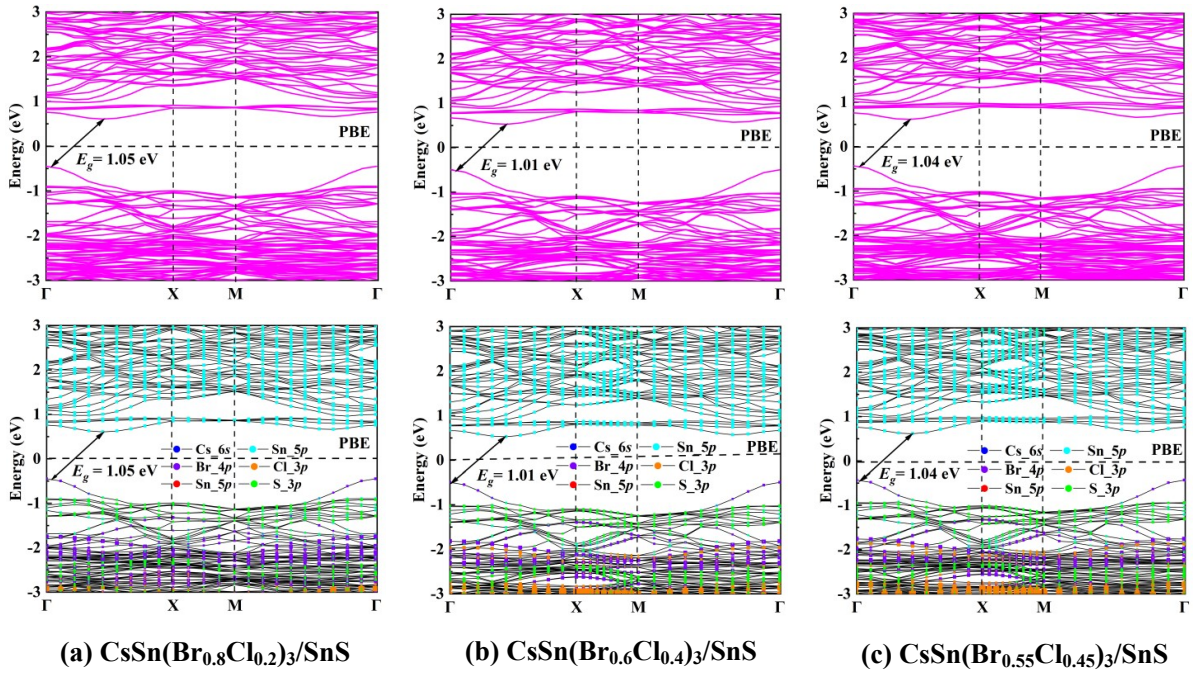


Fig. S10 Calculated band structure: (a) $CsSnBr_3$ (001), (b) SnS monolayer, (c) $CsSnBr_3$/SnS, (d) $CsSn_{0.875}Ti_{0.125}Br_3$/SnS, (e) $V_{Br(6.3\%)}$-$CsSnBr_3$/SnS, and (f) $CsSn(Br_{0.87}Cl_{0.13})_3/SnS_2$ heterostructure. The Fermi level is set to 0 eV by a horizontal black dashed line.



(a) $CsSnBr_3$/SnS **(b) $CsSn_{0.875}Ti_{0.125}Br_3$/SnS**

Fig. S11 Calculated band structure and Projected band structure: (a) $CsSnBr_3$/SnS, (b) $CsSn_{0.875}Ti_{0.125}Br_3$/SnS heterostructure with GGA-PBE. The Fermi level is set to 0 eV by a horizontal black dashed line.



(a) $CsSn(Br_{0.8}Cl_{0.2})_3/SnS$ **(b) $CsSn(Br_{0.6}Cl_{0.4})_3/SnS$** **(c) $CsSn(Br_{0.55}Cl_{0.45})_3/SnS$**

Fig. S12 Calculated band structure and Projected band structure: (a) $CsSn(Br_{0.8}Cl_{0.2})_3/SnS$, (b) $CsSn(Br_{0.6}Cl_{0.4})_3/SnS$, (c) $CsSn(Br_{0.55}Cl_{0.45})_3/SnS$ heterostructure with GGA-PBE. The Fermi level is set to 0 eV by a horizontal black dashed line.

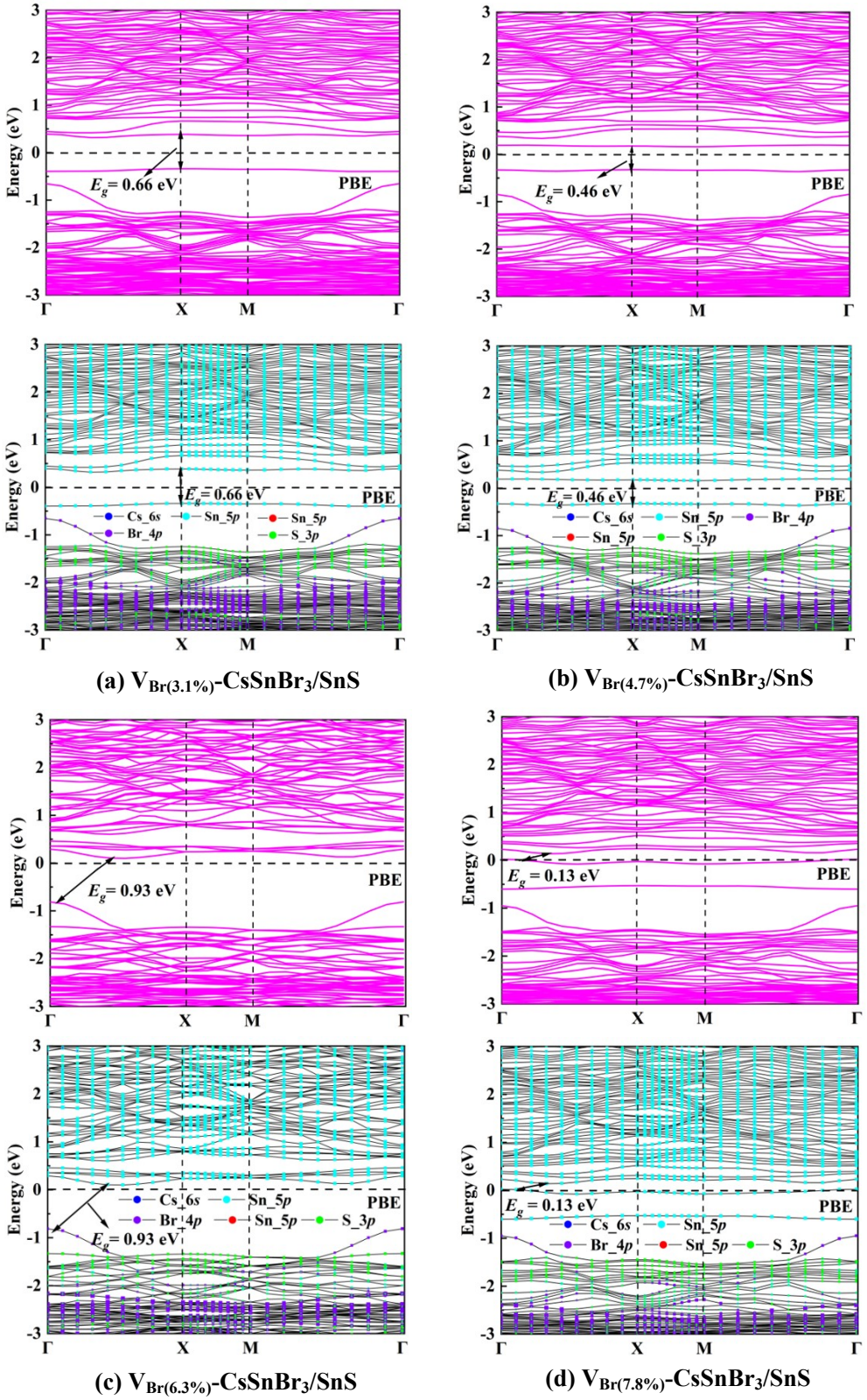


Fig. S13 Calculated band structure and Projected band structure: (a) $V_{Br(3.1\%)}$-$CsSnBr_3$/SnS, (b) $V_{Br(4.7\%)}$-$CsSnBr_3$/SnS, (c) $V_{Br(6.3\%)}$-$CsSnBr_3$/SnS, (d) $V_{Br(7.8\%)}$-$CsSnBr_3$/SnS heterostructure with GGA-PBE. The Fermi level is set to 0 eV by a horizontal black dashed line.

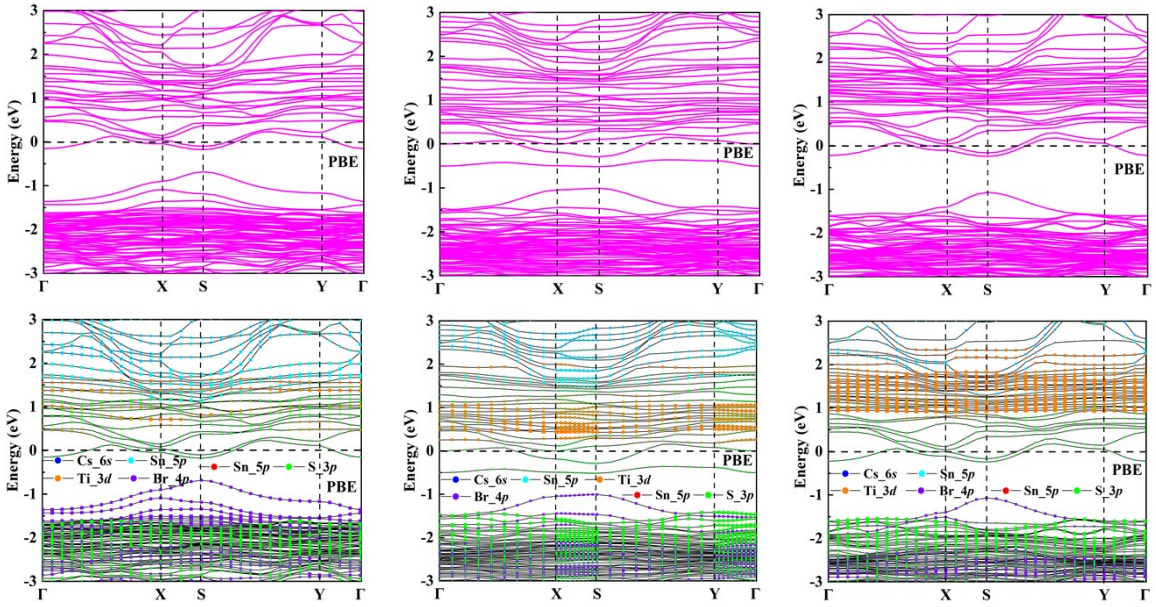


Fig. S14 Calculated band structure and Projected band structure: (a) $CsSn_{0.83}Ti_{0.17}Br_3/SnS_2$, (b) $CsSn_{0.67}Ti_{0.33}Br_3/SnS_2$, (c) $CsSn_{0.50}Ti_{0.50}Br_3/SnS_2$ heterostructure with GGA-PBE. The Fermi level is set to 0 eV by a horizontal black dashed line.

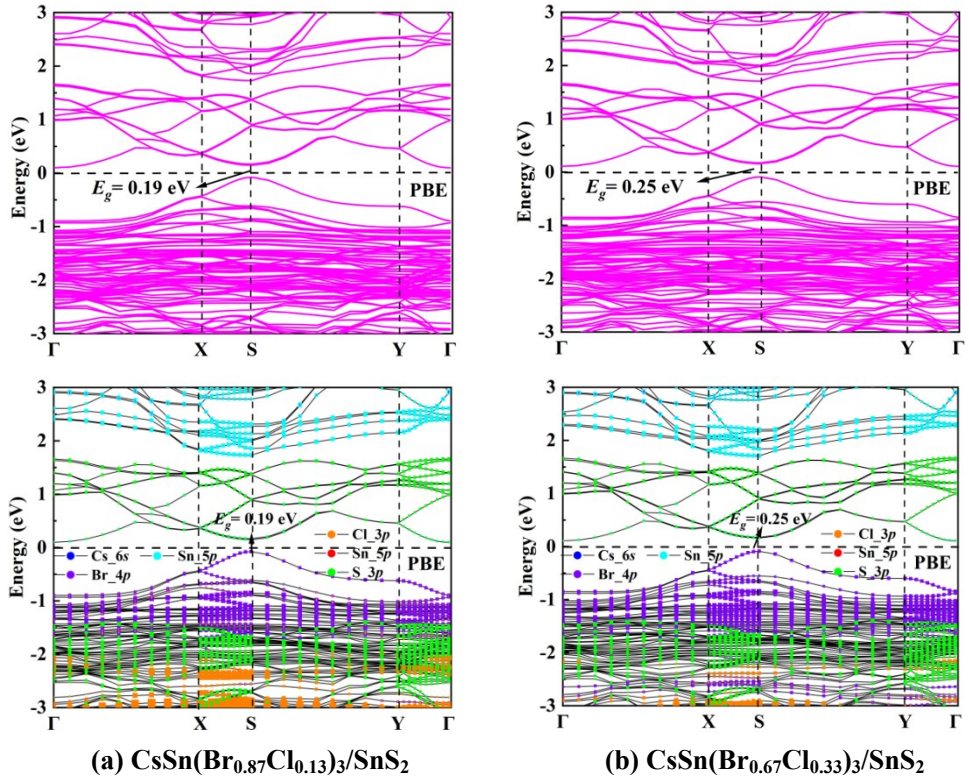


Fig. S15 Calculated band structure and Projected band structure: (a) $CsSn(Br_{0.87}Cl_{0.13})_3/SnS_2$, (b) $CsSn(Br_{0.67}Cl_{0.33})_3/SnS_2$ heterostructure with GGA-PBE. The Fermi level is set to 0 eV by a horizontal black dashed line.

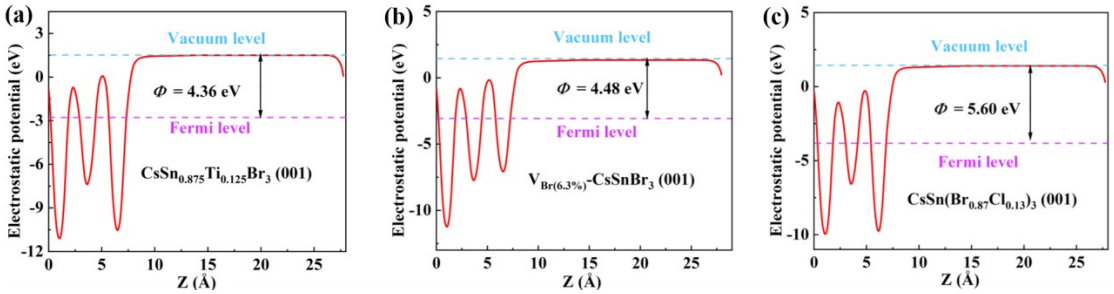


Fig. S16 Work function of (a) $CsSn_{0.875}Ti_{0.125}Br_3$ (001) surface, (b) $V_{Br(6.3\%)}$-$CsSnBr_3$ (001) surface, and (c) $CsSn(Br_{0.87}Cl_{0.13})_3$ (001) surface.

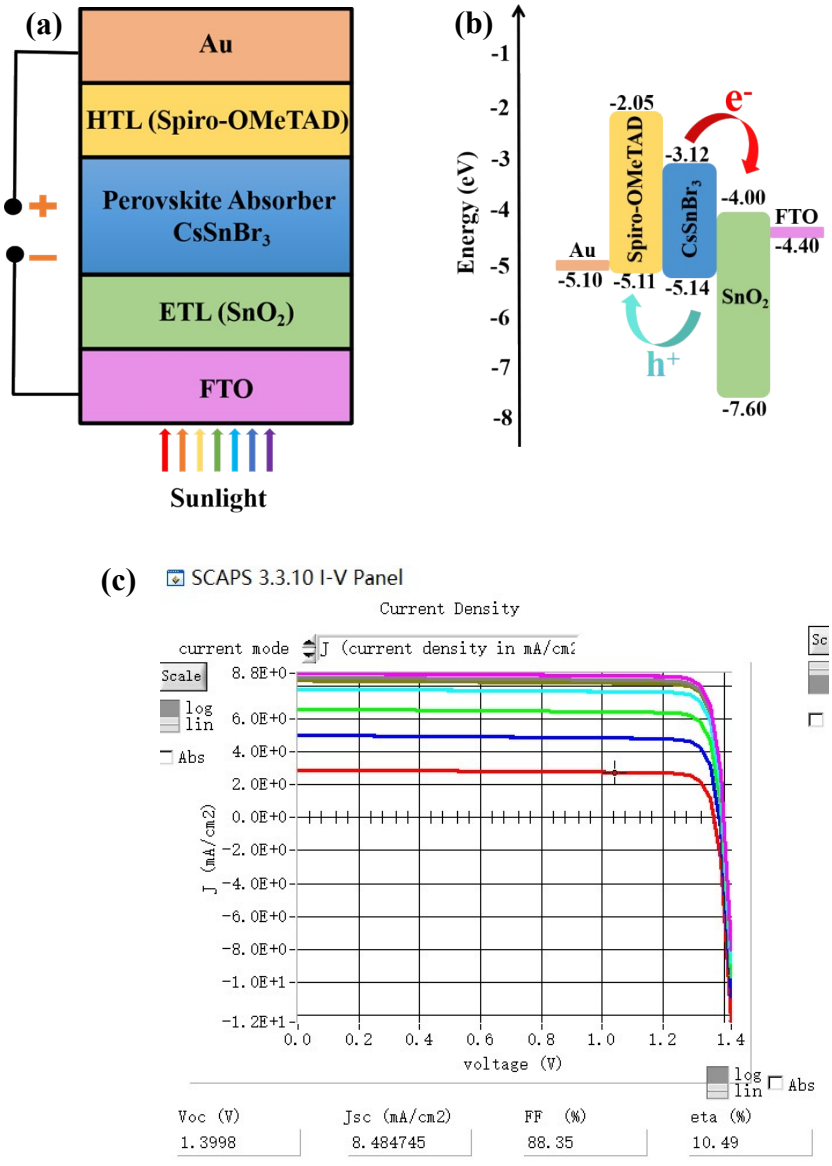


Fig. S17 Device structure of the (a) $CsSnBr_3$ perovskite solar cell, (b) Energy level diagram of the $CsSnBr_3$ perovskite device (FTO/SnO_2/$CsSnBr_3$/Spiro-OMeTAD/Au), and (c) Simulated results (V_{oc}, J_{sc}, FF, and PCE).

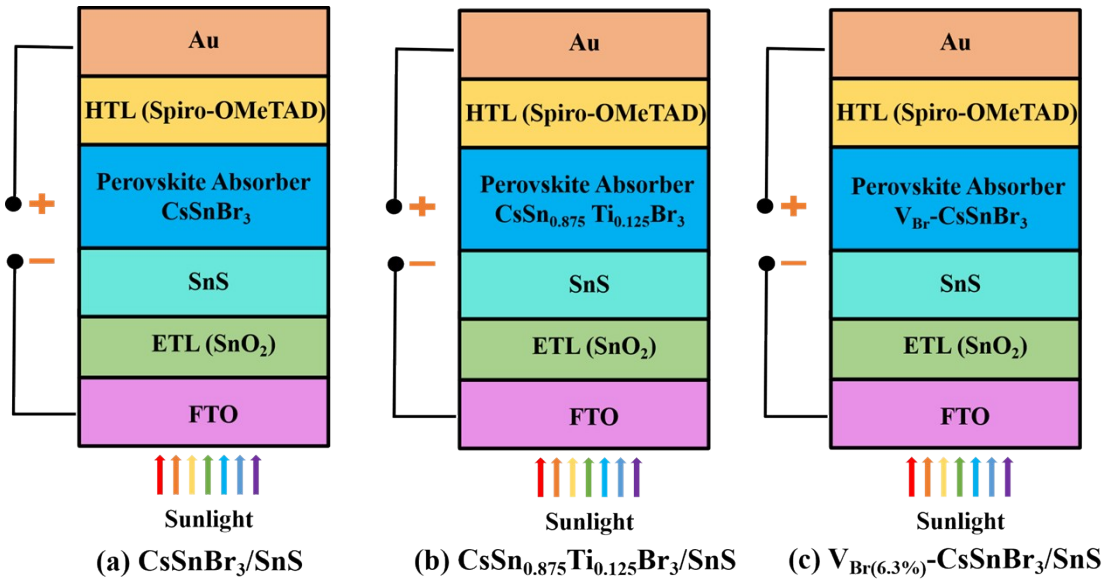


Fig. S18 Solar cells device structure of the (a) $CsSnBr_3/SnS$, (b) $CsSn_{0.875}Ti_{0.125}Br_3/SnS$, and (c) $V_{Br(6.3\%)}$-$CsSnBr_3/SnS$ heterostructure.

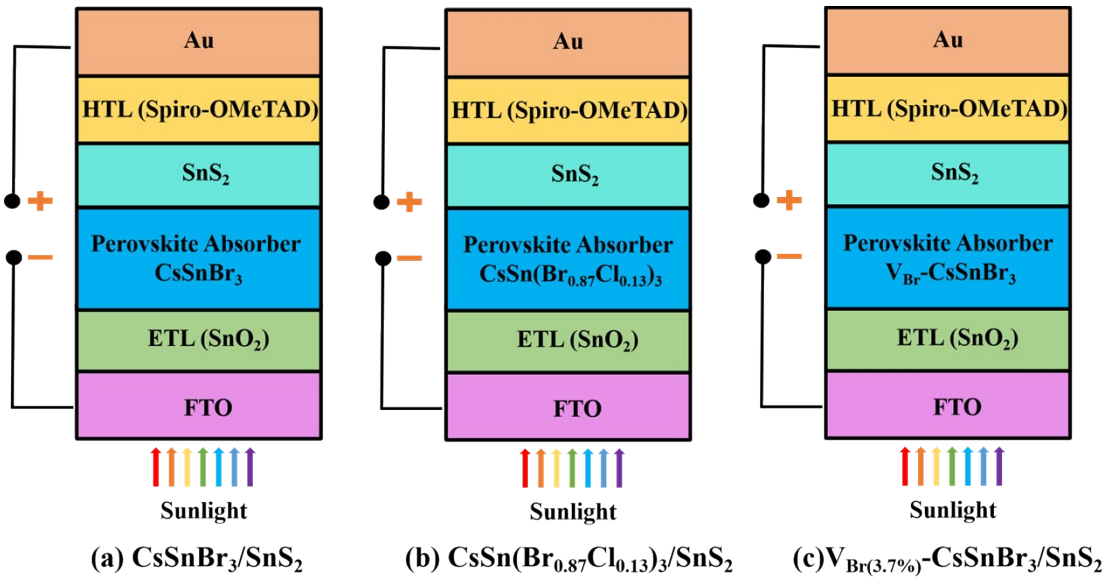


Fig. S19 Solar cells device structure of the (a) $CsSnBr_3/SnS_2$, (b) $CsSn(Br_{0.87}Cl_{0.13})_3/SnS_2$, and (c) $V_{Br(3.7\%)}$-$CsSnBr_3/SnS_2$ heterostructure.

Table S1. Input parameters of the Electron transfer layer, Hole transfer layer, and FTO.

Parameters	SnO_2 [3]	Spiro-OMeTAD[4]	FTO [5]
Thickness (nm)	100	200	100
E_g (eV)	3.50	3.00	3.50
Electron Affinity, χ (eV)	4.00	2.45	4.00
Relative permitivity, ε_r	9.00	3.00	9.00
Effective CB density of states, Nc (cm^{-3})	2.2×10^{18}	2.2×10^{18}	2.0×10^{18}
Effective VB density of states, Nv (cm^{-3})	2.2×10^{18}	1.9×10^{19}	1.8×10^{19}
Electron mobility, μ_n (cm^2/Vs)	20	100	20
Hole mobility, μ_p (cm^2/Vs)	10	100	10
Electron Thermal Velocity (cm/s)	1.0×10^{17}	1.0×10^{17}	1.0×10^{17}
Hole Thermal Velocity (cm/s)	1.0×10^{17}	1.0×10^{17}	1.0×10^{17}
Donor concentration, N_D (cm^{-3})	1.0×10^{17}	0	1.0×10^{15}
Acceptor concentration, N_A (cm^{-3})	0	2.0×10^{19}	0
Defect density, N_t ($1/cm^3$)	1.0×10^{15}	1.0×10^{15}	1.0×10^{15}

Table S2. Input parameters of the $CsSnBr_3$ absorber layer, SnS absorber layer, and SnS_2 absorber layer.

Parameters	$CsSnBr_3$[6]	SnS [7]	SnS_2[8]
Thickness (nm)	470	400	400
E_g (eV)	0.20-1.15	2.13	2.13
Electron Affinity, χ (eV)	4.07	4.20	4.24
Relative permitivity, ε_r	5.90	13.00	10.00
Effective CB density of states, Nc (cm^{-3})	1.0×10^{19}	1.18×10^{18}	2.2×10^{18}
Effective VB density of states, Nv (cm^{-3})	1.0×10^{19}	4.76×10^{18}	1.8×10^{19}
Electron mobility, μ_n (cm^2/Vs)	2	30	500
Hole mobility, μ_p (cm^2/Vs)	2	9.4	500
Electron Thermal Velocity (cm/s)	1.0×10^{17}	1.0×10^{17}	1.0×10^{17}
Hole Thermal Velocity (cm/s)	1.0×10^{17}	1.0×10^{17}	1.0×10^{17}
Donor concentration, N_D (cm^{-3})	0	1.0×10^{17}	1.0×10^{17}
Acceptor concentration, N_A (cm^{-3})	1.0×10^{15}	0	0
Defect density, N_t ($1/cm^3$)	1.0×10^{15}	1.0×10^{15}	1.0×10^{15}

$CsSnBr_3$ CIF

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$CsSnBr_3$/SnS heterostructure CIF

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S31	S	0.62854	0.49053	0.37840	0.01267	Uiso	1.00
S32	S	0.63032	0.24215	0.37947	0.01267	Uiso	1.00
Sn33	Sn	0.00000	0.75000	0.03038	0.01267	Uiso	1.00
Sn34	Sn	0.50000	0.50000	0.03038	0.01267	Uiso	1.00
Sn35	Sn	0.01385	0.74550	0.20385	0.01267	Uiso	1.00
Sn36	Sn	0.51385	0.99550	0.20385	0.01267	Uiso	1.00
Sn37	Sn	0.13015	0.50459	0.30019	0.01267	Uiso	1.00
Sn38	Sn	0.13370	0.76059	0.30081	0.01267	Uiso	1.00
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Sn41	Sn	0.37938	0.63041	0.38810	0.01267	Uiso	1.00
Sn42	Sn	0.37663	0.88034	0.38846	0.01267	Uiso	1.00
Sn43	Sn	0.87663	0.63034	0.38846	0.01267	Uiso	1.00
Sn44	Sn	0.87938	0.88041	0.38810	0.01267	Uiso	1.00
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Br47	Br	0.25000	0.87500	0.03038	0.01267	Uiso	1.00
Br48	Br	0.75000	0.62500	0.03038	0.01267	Uiso	1.00
Br49	Br	0.23408	0.62518	0.19553	0.01267	Uiso	1.00
Br50	Br	0.73408	0.87518	0.19553	0.01267	Uiso	1.00
Br51	Br	0.23349	0.86877	0.19671	0.01267	Uiso	1.00
Br52	Br	0.73349	0.61877	0.19671	0.01267	Uiso	1.00
Br53	Br	0.98456	0.74925	0.11493	0.01267	Uiso	1.00
Br54	Br	0.48456	0.99925	0.11493	0.01267	Uiso	1.00
Cs55	Cs	0.99761	0.99938	0.10840	0.01267	Uiso	1.00
Cs56	Cs	0.49761	0.74938	0.10840	0.01267	Uiso	1.00

S57	S	0.38234	0.61817	0.30984	0.01267	Uiso	1.00
S58	S	0.37640	0.86626	0.31004	0.01267	Uiso	1.00
S59	S	0.87640	0.61626	0.31004	0.01267	Uiso	1.00
S60	S	0.88234	0.86817	0.30984	0.01267	Uiso	1.00
S61	S	0.13032	0.99215	0.37947	0.01267	Uiso	1.00
S62	S	0.12855	0.74053	0.37840	0.01267	Uiso	1.00
S63	S	0.62854	0.99053	0.37840	0.01267	Uiso	1.00
S64	S	0.63032	0.74215	0.37947	0.01267	Uiso	1.00

$CsSnBr_3/SnS_2$ heterostructure CIF

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_audit_creation_method 'Materials Studio'
_symmetry_space_group_name_H-M 'P1'
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_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy

Cs1	Cs	0.00000	0.00000	0.12115	0.01267	Uiso	1.00
Cs2	Cs	0.00000	0.33333	0.12115	0.01267	Uiso	1.00
Cs3	Cs	0.00000	0.66667	0.12115	0.01267	Uiso	1.00
Sn4	Sn	0.50000	0.16667	0.03305	0.01267	Uiso	1.00
Sn5	Sn	0.50000	0.50000	0.03305	0.01267	Uiso	1.00
Sn6	Sn	0.50000	0.83333	0.03305	0.01267	Uiso	1.00
Sn7	Sn	0.50000	0.16667	0.20925	0.01267	Uiso	1.00
Sn8	Sn	0.50000	0.50000	0.20925	0.01267	Uiso	1.00

Sn9	Sn	0.50000	0.83333	0.20925	0.01267	Uiso	1.00
Br10	Br	0.00000	0.16667	0.03305	0.01267	Uiso	1.00
Br11	Br	0.00000	0.50000	0.03305	0.01267	Uiso	1.00
Br12	Br	0.00000	0.83333	0.03305	0.01267	Uiso	1.00
Br13	Br	0.00000	0.16667	0.20925	0.01267	Uiso	1.00
Br14	Br	0.00000	0.50000	0.20925	0.01267	Uiso	1.00
Br15	Br	0.00000	0.83333	0.20925	0.01267	Uiso	1.00
Br16	Br	0.50000	0.00000	0.03305	0.01267	Uiso	1.00
Br17	Br	0.50000	0.33333	0.03305	0.01267	Uiso	1.00
Br18	Br	0.50000	0.66667	0.03305	0.01267	Uiso	1.00
Br19	Br	0.50000	0.00000	0.20925	0.01267	Uiso	1.00
Br20	Br	0.50000	0.33333	0.20925	0.01267	Uiso	1.00
Br21	Br	0.50000	0.66667	0.20925	0.01267	Uiso	1.00
Br22	Br	0.50000	0.16667	0.12115	0.01267	Uiso	1.00
Br23	Br	0.50000	0.50000	0.12115	0.01267	Uiso	1.00
Br24	Br	0.50000	0.83333	0.12115	0.01267	Uiso	1.00
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S26	S	0.18351	0.10362	0.30855	0.02660	Uiso	1.00
S27	S	0.68351	0.20362	0.30855	0.02660	Uiso	1.00
S28	S	0.18351	0.30362	0.30855	0.02660	Uiso	1.00
S29	S	0.68351	0.40362	0.30855	0.02660	Uiso	1.00
S30	S	0.18351	0.50362	0.30855	0.02660	Uiso	1.00
S31	S	0.68351	0.60362	0.30855	0.02660	Uiso	1.00
S32	S	0.18351	0.70362	0.30855	0.02660	Uiso	1.00
S33	S	0.68351	0.80362	0.30855	0.02660	Uiso	1.00
S34	S	0.18351	0.90362	0.30855	0.02660	Uiso	1.00
Sn35	Sn	0.01684	0.00362	0.35745	0.02406	Uiso	1.00
Sn36	Sn	0.51684	0.10362	0.35745	0.02406	Uiso	1.00
Sn37	Sn	0.01684	0.20362	0.35745	0.02406	Uiso	1.00
Sn38	Sn	0.51684	0.30362	0.35745	0.02406	Uiso	1.00
Sn39	Sn	0.01684	0.40362	0.35745	0.02406	Uiso	1.00
Sn40	Sn	0.51684	0.50362	0.35745	0.02406	Uiso	1.00
Sn41	Sn	0.01684	0.60362	0.35745	0.02406	Uiso	1.00
Sn42	Sn	0.51684	0.70362	0.35745	0.02406	Uiso	1.00
Sn43	Sn	0.01684	0.80362	0.35745	0.02406	Uiso	1.00
Sn44	Sn	0.51684	0.90362	0.35745	0.02406	Uiso	1.00
S45	S	0.35017	0.00362	0.40634	0.02660	Uiso	1.00
S46	S	0.85017	0.10362	0.40634	0.02660	Uiso	1.00
S47	S	0.35017	0.20362	0.40634	0.02660	Uiso	1.00
S48	S	0.85017	0.30362	0.40634	0.02660	Uiso	1.00
S49	S	0.35017	0.40362	0.40634	0.02660	Uiso	1.00
S50	S	0.85017	0.50362	0.40634	0.02660	Uiso	1.00
S51	S	0.35017	0.60362	0.40634	0.02660	Uiso	1.00
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S53	S	0.35017	0.80362	0.40634	0.02660	Uiso	1.00
S54	S	0.85017	0.90362	0.40634	0.02660	Uiso	1.00

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