Supporting Information

Probing High-Efficiency $Cs_{0.05}(FA_{0.77}MA_{0.23})_{0.95}Pb(I_{0.77}Br_{0.23})_3$ -Based Perovskite Solar Cells through first principles computations and SCAPS-1D Simulation

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Table S1. Simulation parameters for different ETL materials of the PSC device

Parameters	ITO	C_{60} [1]	SnO_2 [1]	ZnO [1]	IGZO [1]	PCBM [1]
Thickness d (μm)	0.5	0.1	0.1	0.1	0.1	0.1
Band gap E_g (eV)	3.5	1.7	3.6	3.3	3.05	2.08
Electron Affinity χ (eV)	4.1	3.9	4	4	4.16	3.95
Relative Permittivity ε_r	9	4.2	9	9	10	4
Effective Density of States (CB) N_C ($1/m^3$)	2.2×10^{18}	1×10^{19}	2×10^{18}	3×10^{18}	5×10^{18}	1.8×10^{18}
Effective Density of States (VB) N_V ($1/m^3$)	3.8×10^{18}	5×10^{20}	1×10^{19}	2×10^{19}	5×10^{18}	2×10^{18}
Electron Mobility μ_n (cm^2/Vs)	20	8.0×10^{-2}	100	100	15	0.2
Hole Mobility μ_p (cm^2/Vs)	10	3.5×10^{-3}	25	25	0.1	0.2
Acceptor Density N_A ($1/cm^3$)	0	0	0	0	0	0
Donor Density N_D ($1/cm^3$)	1×10^{21}	1×10^{18}	1×10^{17}	1×10^{17}	1×10^{17}	1×10^{18}
Defect Density N_t	1×10^{17}	1×10^{14}	1×10^{14}	1×10^{14}	1×10^{14}	1×10^{14}

Table S2. Simulation parameters for different HTL materials and absorber layer of the PSC device.

Parameters	V_2O_5[1]	Cu_2O [1]	CuSCN [1]	CBTS [2]	$CuSbS_2$ [3]	$Cs_{0.05}(FA_{0.77}MA_{0.23})_{0.95}Pb(I_{0.77}Br_{0.23})_3$ [4]
Thickness d (μm)	0.1	0.1	0.1	0.6	0.3	0.2
Band gap E_g (eV)	2.4	2.17	3.6	1.9	1.5	1.68
Electron Affinity χ (eV)	4.6	3.20	1.9	3.6	4.5	4.5
Relative Permittivity ε_r	10	7.11	8.5	5.4	10	10
Effective Density of States (CB) N_C ($1/m^3$)	1×10^{19}	1.8×10^{18}	2.2×10^{18}	2.2×10^{18}	8×10^{19}	2.2×10^{18}
Effective Density of States (VB) N_V ($1/m^3$)	5×10^{20}	2.2×10^{18}	1.8×10^{19}	2.2×10^{18}	8×10^{19}	1.8×10^{19}
Electron Mobility μ_n(cm^2/Vs)	3.2×10^{2}	80	100	30	49	6
Hole Mobility μ_p(cm^2/Vs)	4.0×10^{1}	80	25	10	49	24
Acceptor Density N_A($1/cm^3$)	1×10^{18}	1×10^{18}	1×10^{18}	2×10^{16}	1×10^{17}	1×10^{15}
Donor Density N_D ($1/cm^3$)	0	0	0	0	0	0
Defect Density N_t	1×10^{14}	1×10^{14}	1×10^{14}	2×10^{14}	1×10^{14}	1×10^{14}

Table S3. Summarizing the absorption coefficient values used for each layer in the simulation.

Material	Layer type	Absorption coefficient (cm^{-1})
ITO	Transparent contact	10^4
PCBM	Electron transport layer (ETL)	10^4
$Cs_{0.05}(FA_{0.77}MA_{0.23})_{0.95}Pb(I_{0.77}Br_{0.23})_3$	Absorbent layer	10^5
$CuSbS_2$	Hole Transport Layer (HTL)	10^5

Table S4. Electrical properties of interface.

Parameters and units	PCBM /mixed perovskite	Mixed perovskite/$CuSbS_2$
Defect type	Neutral	Neutral
Total density	10^{10}	10^{10}
Energetic distribution	Single	Single
Energy level with respect to reference (eV)	0.6	0.6

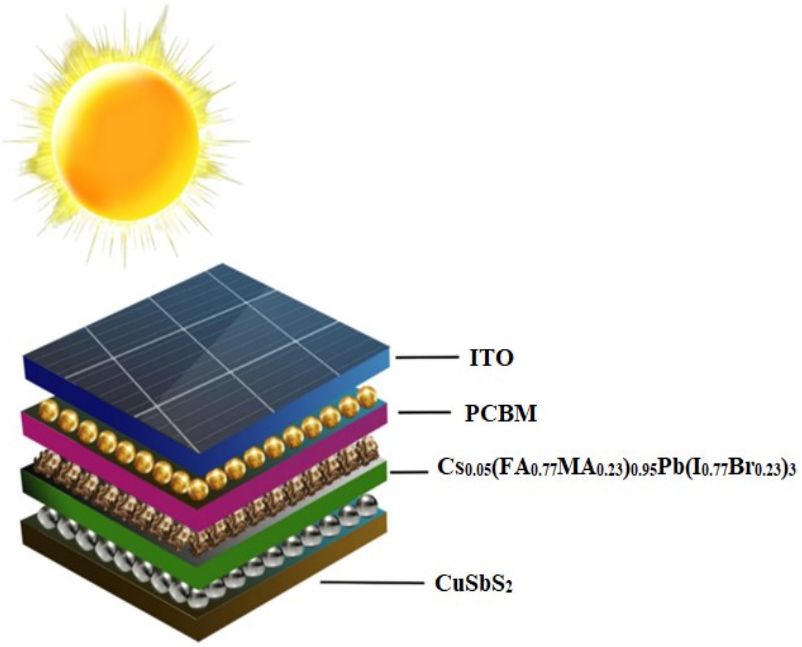


Fig. S1. Schematic representation of perovskite solar cell.

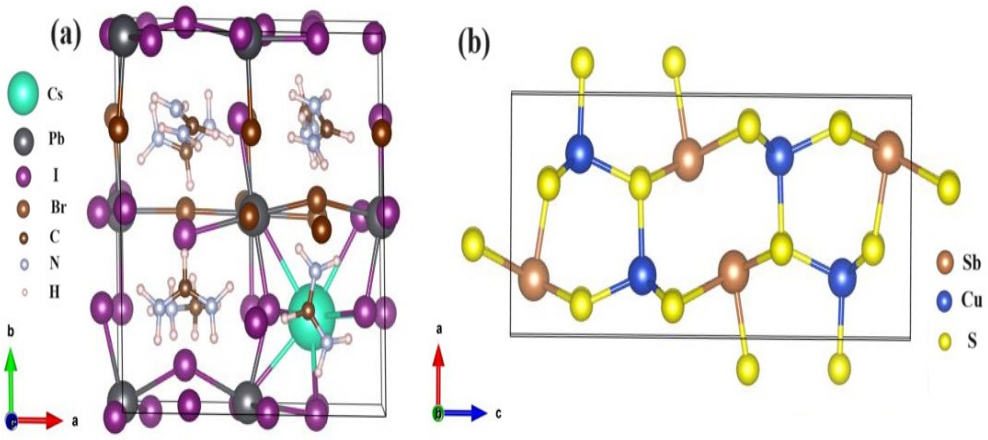
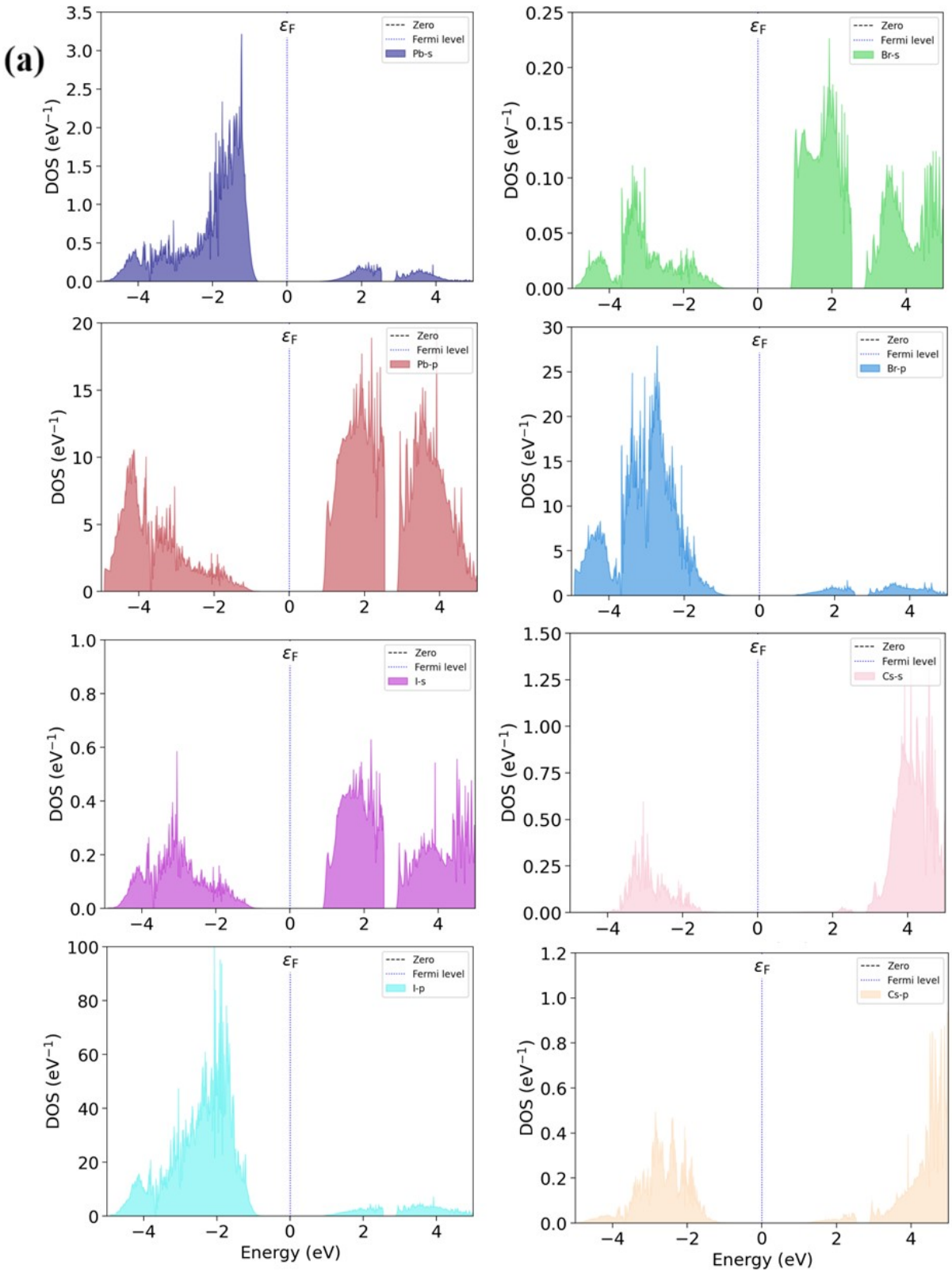


Fig. S2. Schematic structure representation of (a) supercell $(Cs_{0.14}(FA_{0.85}MA_{0.14})_{0.88}Pb(I_{0.83}Br_{0.17})_3$ and (b) $CuSbS_2$.


(a)
Zero
Fermi level
Pb-s
Br-s
Pb-p
Br-p
I-s
Cs-s
I-p
Cs-p
ε_F
DOS (eV^{-1})
Energy (eV)

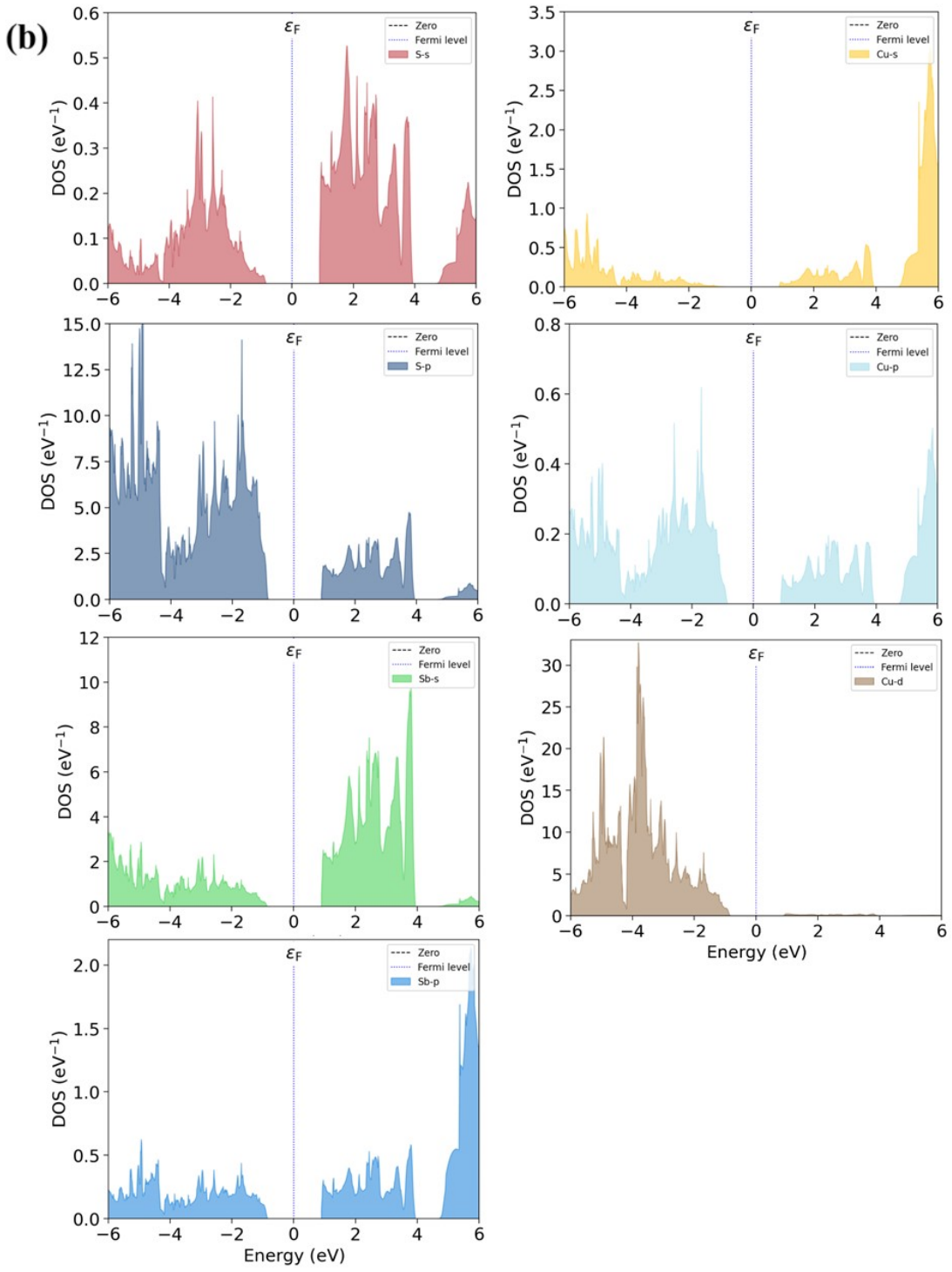


Fig. S3. Partial density of the states of (a) $Cs_{0.14}(FA_{0.85}MA_{0.14})_{0.88}Pb(I_{0.83}Br_{0.17})_3$ and (b) $CuSbS_2$ in the equilibrium geometry. The Fermi level was positioned along the dashed black line.

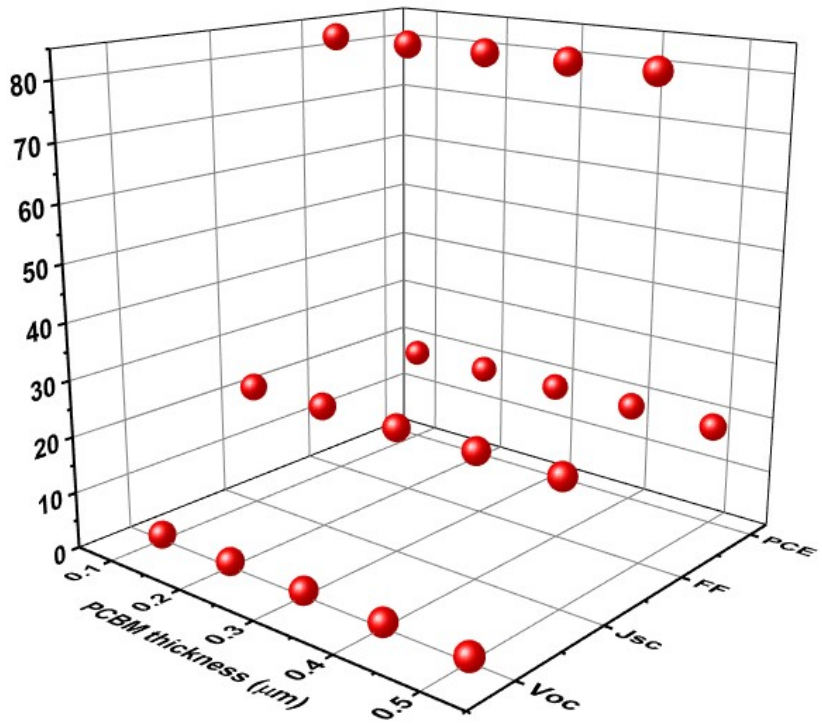


Fig. S4. Influence of PCBM ETL thickness in V_{OC}, J_{SC}, FF and PCE.

References

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