

Supporting Information for

Inorganic Lead-Free B- γ -CsSnI₃ Perovskite Solar Cells Using Diverse

Electron-Transporting Materials: A Simulation Study

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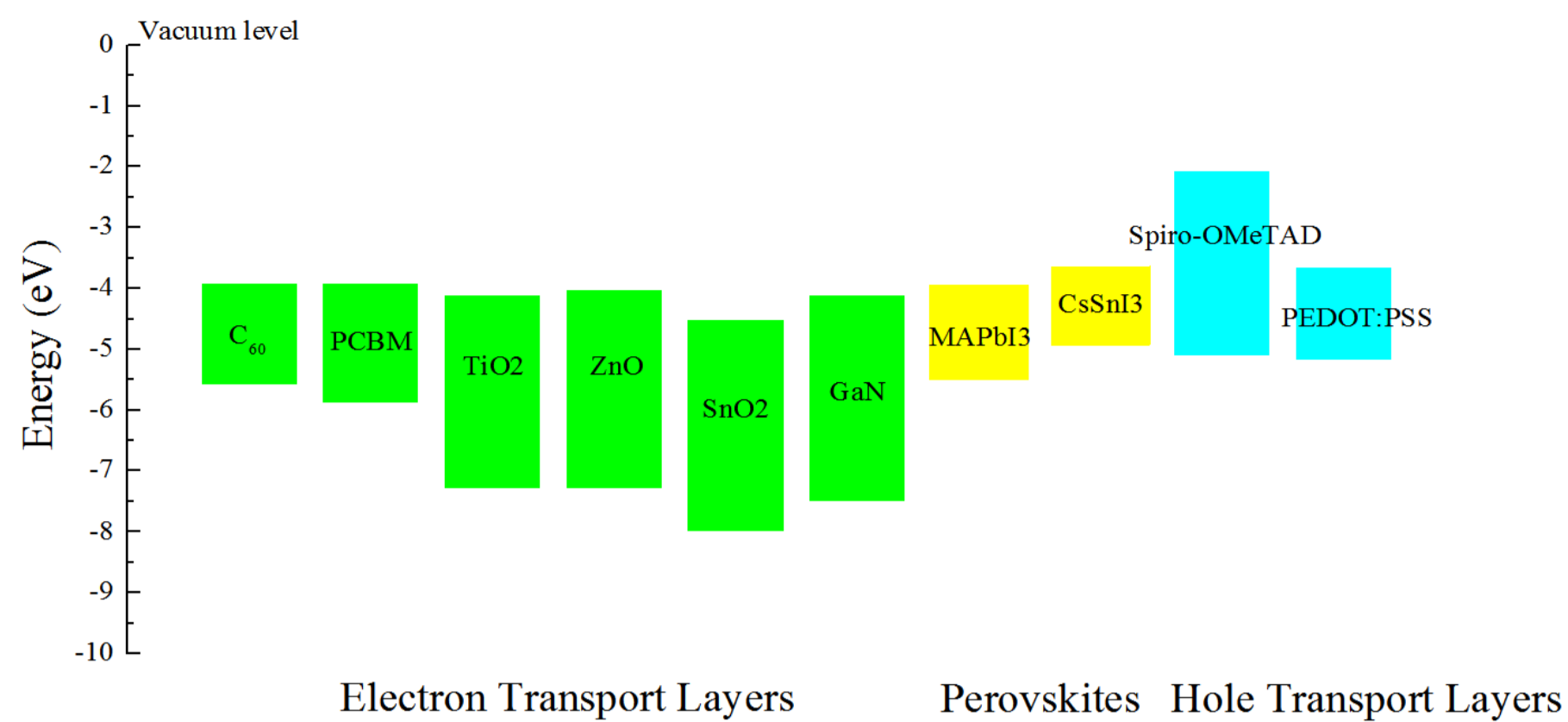
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Table S1. Material parameters used in the simulation

Parameters	CsSnI ₃	TiO ₂	ZnO	SnO ₂	GaN	C ₆₀	PCBM	Spiro-OMeTAD	PEDOT:PSS
Band gap E _g (eV)	1.3 [1]	3.2 [1]	3.3 [13]	3.5 [18]	3.4 [21]	1.7 [28]	2 [33]	3.06 [36]	1.55 [34]
Electron affinity χ (eV)	3.62 [1]	4.1 [7]	4 [13]	4.5 [18]	4.1 [22]	3.9 [29]	3.9 [33]	2.05 [36]	3.63 [34]
Dielectric constant ε	48.2 [2]	55 [8]	8.656 [14]	9 [18]	9.5 [23]	4.25 [28]	4 [33]	3 [37]	3 [40]
Electron/hole mobility (cm ² /V/s)	50/400 [3, 4]	0.006/0.006 [9]	100/25 [14]	100/25 [18]	Caughy-Thomas approximation (doping concentration dependent) [24]	1.6/1.6 [28]	0.01/0.01 [33]	2.00E-04/2.00E-4 [37]	9.00E-03/9.00E-3 [40]
Effective density of states in the conduction band N _C (cm ⁻³)	1.57E+19 [5]	1.00E+21 [9]	2.20E+18 [15]	2.20E+18 [18]	2.30E+18 [23]	1.44E+21 [30]	1.00E+21 [33]	1.00E+19 [38]	1.00E+19 [40]
Effective density of states in the valence band N _V (cm ⁻³)	1.47E+18 [5]	2.00E+20 [9]	1.80E+19 [15]	1.80E+19 [18]	4.60E+19 [23]	1.44E+21 [30]	2.00E+20 [33]	1.00E+19 [38]	1.00E+19 [40]
Minority lifetime	6.6 ns [3]	15 ms [10]	1 ns [16]	2.27 ns [19]	0.1 ns (for electrons) [25], 6.5 ns (for holes) [26]	1 μs [31]	1 μs [34]	0.1 μs [38]	1 μs [34]
Surface recombination velocities (cm/s)	2000 [3]	12 [11]	13 [11]	265 [11]	50000 [27]	4600 (assumed to be the same as PCBM)	4600 [11]	3100 [11]	4900 [11]
Absorption coefficient (1/cm ⁻¹)	[6]	[12]	[17]	[20]	[21]	[32]	[35]	[39]	[41]
Initial donor concentration (cm ⁻³)	0	5E+19	1E+18	1E+18	1E+18	5E+17	5E+17	0	0
Optimal donor concentration (cm ⁻³)	0	1E+21	1E+18	1E+18	1E+18	5E+18	5E+18	0	0
Initial acceptor concentration (cm ⁻³)	5E+17 [3]	0	0	0	0	0	0	3E+17	1E+20
Initial thickness (nm)	variable	25	25	25	25	30	30	400	40
Optimal thickness (nm)	100~200								

Figure S1. Energy band alignment of all contact materials and CsSnI₃ adopted in this study



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