

Supplementary materials

High-Efficiency Electron Transport Layer-Free Perovskite/GeTe Tandem Solar Cell: Numerical Simulation

Mostafa M. Salah ^{1,2,*}, Abdelhalim Zekry ², Mohamed Abouelatta ², Ahmed Shaker ², Mohamed Mousa ¹, Fathy Z. Amer ³, Roaa I. Mubarak ³ and Ahmed Saeed ¹

¹ Electrical Engineering Department, Future University in Egypt, Cairo 11835, Egypt; mohamed.mossa@fue.edu.eg (M.M.); asaeed@fue.edu.eg (A.S.)

² Faculty of Engineering, Ain Shams University, Cairo 11535, Egypt; aaazekry@hotmail.com (A.Z.); m.abouelatta@eng.asu.edu.eg (M.A.); ahmed.shaker@eng.asu.edu.eg (A.S.)

³ Electronics & Communication Engineering Department, Faculty of Engineering, Helwan University, Cairo 11795, Egypt; fathy_amer@h-eng.helwan.edu.eg (F.Z.A.); roaa_ibrahim@h-eng.helwan.edu.eg (R.I.M.)

* Correspondence: mostafa.abdulkhaled@fue.edu.eg

Table S1. Physical parameters of the incident, transmitted spectrum definitions, and their units.

Symbol	Definition	Unit
$S(\lambda)$	The power density of the light spectrum transmitted from the top sub-cell to the bottom sub-cell	W/m ²
$S_o(\lambda)$	The incident spectrum is AM 1.5	
x	The layer number	
n	The total number of layers of the sub-cell	
α	The absorption coefficient	cm ⁻¹
d	The thickness of each layer	cm
A_α	A pre-factor of 10 ⁵	cm ⁻¹ .eV ^{-1/2}
h	The Plancks constant	eV.sec
ν	The spectrum frequency	Hz
E_g	The energy gap of the material	eV

Table S2. Materials parameters of the top sub-cell used in SCAPS-1D simulator.

Parameters	TCO	MAPbI _{3-x} Cl _x	Cu ₂ O	ZnOS
Thickness (nm)	500	500	100	50
E_g (eV)	3.5 [45]	1.55 [31]	2.1 [58]	2.83 [59]
Electron affinity (eV)	4 [31]	3.9 [31]	3.2 [58]	3.6 [30]
Relative permittivity	9	6.5 [3]	7.11 [58]	9 [59]
Effective conduction band density N_c (cm ⁻³)			2.2 × 10 ¹⁸	
Effective valence band density N_v (cm ⁻³)			1.8 × 10 ¹⁸	
Thermal velocity of electrons $v_{th,n}$ (cm/s)			1 × 10 ⁷ [56]	
Thermal velocity of holes $v_{th,p}$ (cm/s)				
Electron mobility μ_e (cm ² V ⁻¹ s ⁻¹)	20	2 [58]	3.4	100 [25]
Hole mobility μ_p (cm ² V ⁻¹ s ⁻¹)	10	2 [58]	3.4	25 [25]
Acceptor concentration N_A (cm ⁻³)	0	0	1 × 10 ¹⁸ [56]	0

Donor concentration N_D (cm^{-3})	2×10^{19}	0	0	2×10^{18} [25]
Electrons capture cross-section (cm^2)		2×10^{-14} [56]		1×10^{-15}
Holes capture cross-section (cm^2)				
Energy level with respect to Reference (eV)			0.6 [56]	
Characteristic energy (eV)			0.1 [25]	
N_t (cm^{-3})	1×10^{15} [45]	2×10^{11} [45]	1×10^{15} [45]	1×10^{15} [45]

Table S3. Materials parameters of the top bottom-cell used in SCAPS-1D simulator.

Parameters	GeTe	CdS	ZnO
Thickness (nm)	2000	50	50
E_g (eV)	0.8 [60]	2.45 [61]	3.30 [61,62]
Electron affinity (eV)	4.8 [57]	4.4 [57]	4.6 [57]
Relative permittivity	36 [60]	10 [46]	9 [46]
χ (eV)	4.8	4.4	4.6
N_c (cm^{-3})	10^{16}	2.2×10^{18}	2.2×10^{18}
μ_e ($\text{cm}^{-2} \text{V}^{-1} \text{s}^{-1}$)		100	
N_D (cm^{-3})	0	10^{20}	10^{20}
N_v (cm^{-3})	10^{17}	1.8×10^{19}	1.8×10^{19}
μ_p ($\text{cm}^{-2} \text{V}^{-1} \text{s}^{-1}$)	20	25	25
N_A (cm^{-3})	2×10^{16}	0	0

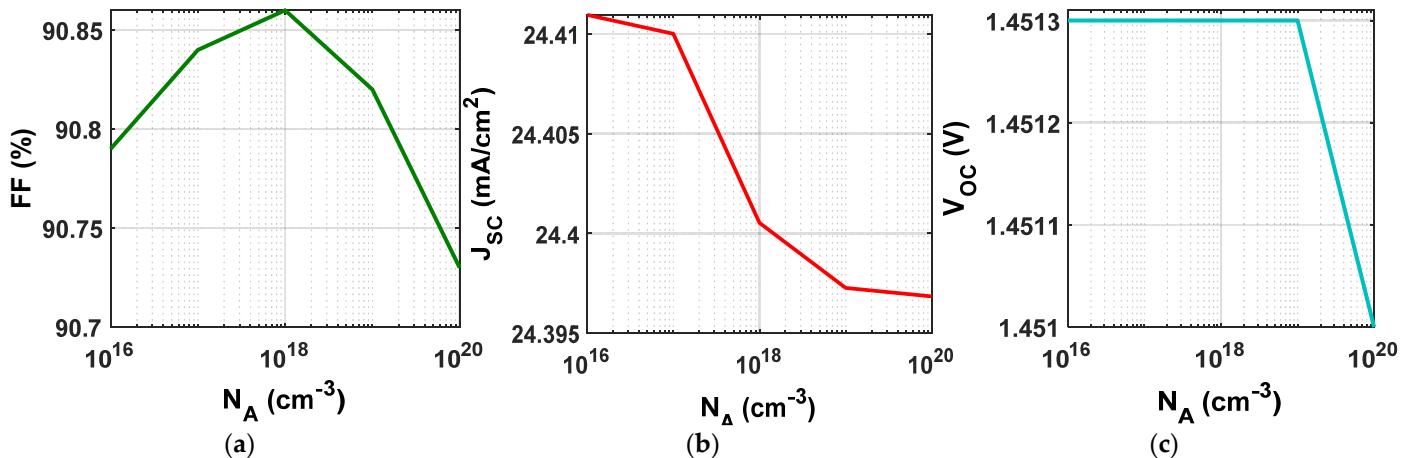


Figure S1. Performance metrics variations of the simulated PSC depending on the N_A Cu₂O: (a) FF, (b) J_{sc} , and (c) V_{oc} .

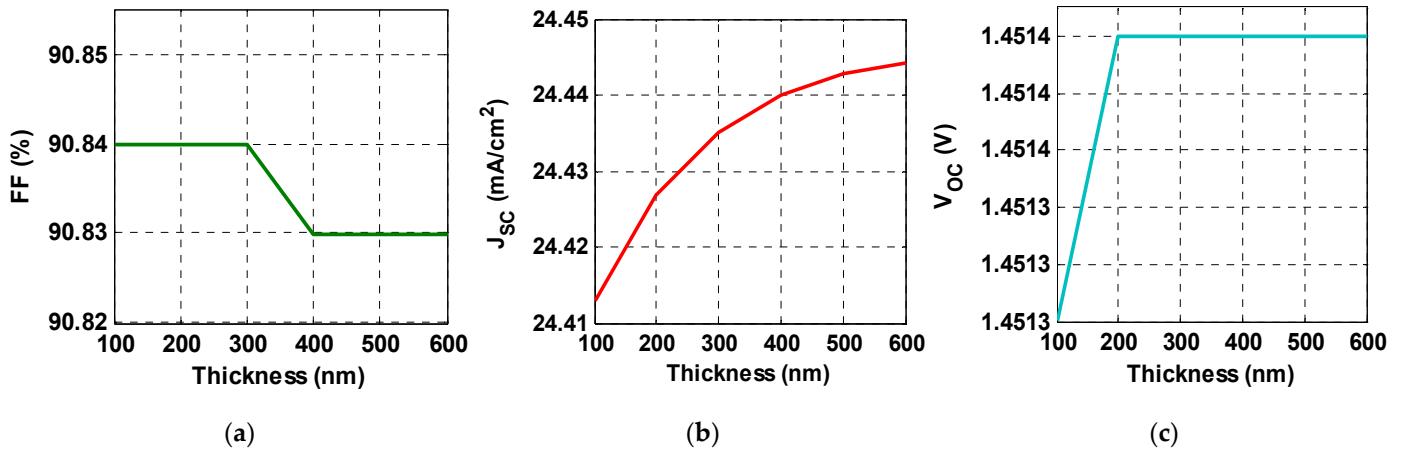


Figure S2. Performance metrics variations of the simulated PSC depending on the thickness of HTM: (a) FF, (b) J_{sc} , and (c) V_{oc} .

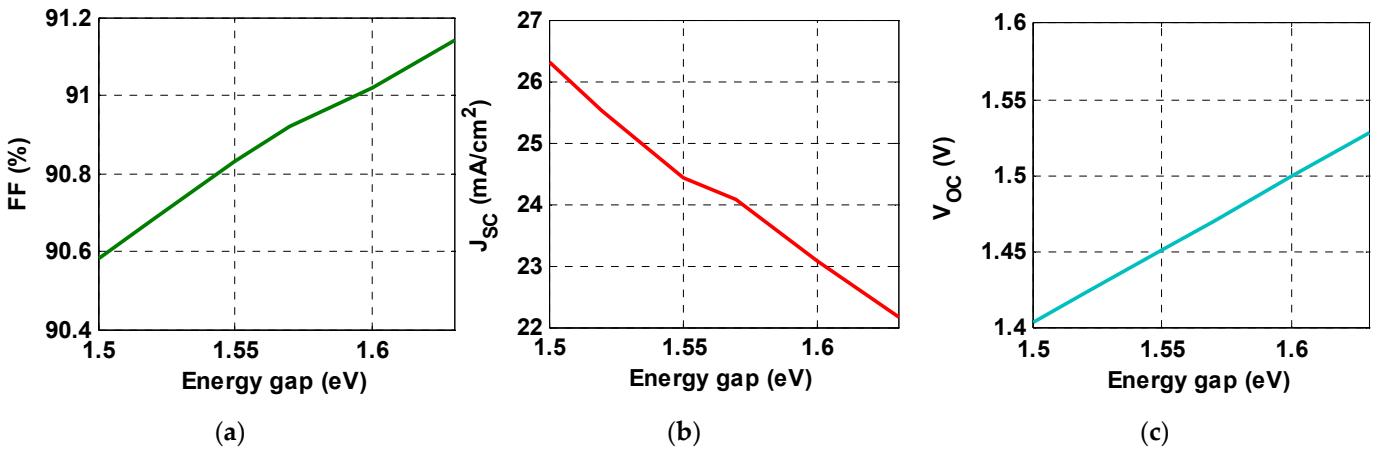


Figure S3. Performance metrics variations of the simulated PSC depending on the E_g of the absorber layer: (a) FF, (b) J_{sc} , and (c) V_{oc} .

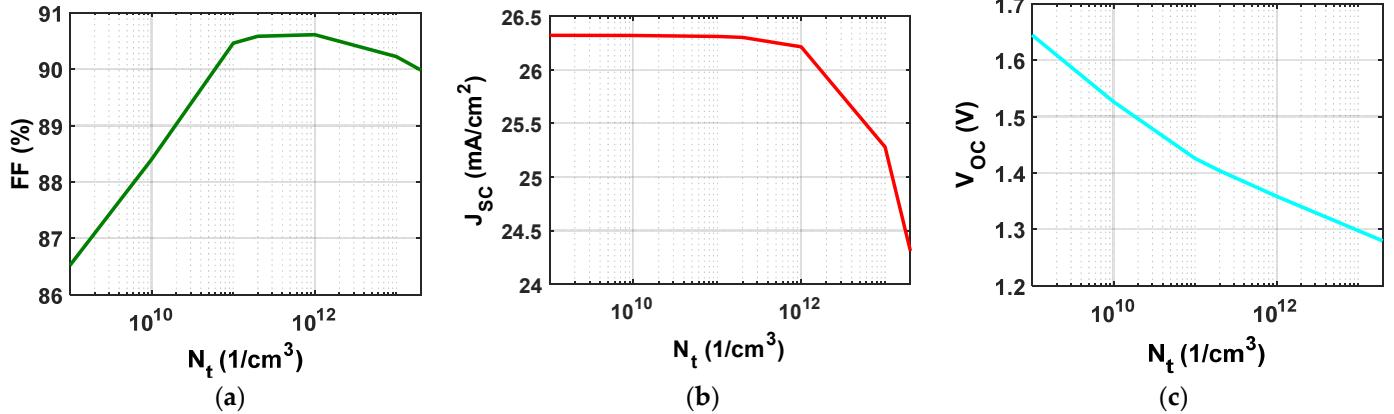


Figure S4. Performance metrics variations of the simulated PSC depending on the N_t of the absorber layer: (a) FF, (b) J_{sc} , and (c) V_{oc} .