Supporting Information

Design and Optimization of all-thin-film CdSe/Si Tandem Solar Cells Using SCAPS-1D Simulation

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Supplementary Note S1

Main physical modeling equations utilized in SCAPS-1D in steady state.

Semiconductor Equation	Equation Formula	Description
Poisson	$\frac{d^2\Psi}{dx^2} = \frac{q}{\varepsilon}(n - p + N_A^- - N_D^+ + n_t - p_t)$	These are the main equations utilized in numerical solution in SCAPS-1D, where they are solved self consistently until convergence occurs.
Continuity	$\frac{1}{q}\frac{dJ_n}{dx} = U_n - G(x)$ $\frac{1}{q}\frac{dJ_p}{dx} = G(x) - U_p$	
Bulk SRH	$R_{RSH,bulk} = \frac{(np - n_i^2)}{\tau_p(n + n_1) + \tau_n(p + p_1)}$	The bulk SRH recombination is characterized by bulk minority lifetimes (τ_n and τ_p).
Interface SRH	$R_{RSH,int} = \frac{(n_{if}p_{if} - n_i^2)}{\frac{p_{if} + p_1}{S_n} + \frac{n_{if} + n_1}{S_p}}$	The interface SRH recombination is characterized by interface recombination velocities (S_n and S_p).
Transport	$J_n = qn\mu_n E + qD_n\frac{dn}{dx}$ $J_p = qp\mu_p E - qD_p\frac{dp}{dx}$	Transport equations are utilized to calculate current densities of electrons and holes based on the drift-diffusion model.

Where U is the recombination rate; includes radiative, Auger, deep traps, and impact ionization, recombination through deep traps in E_g is modeled by the Shockley Read Hall (SRH) theory, and $G(x)$ is the rate of solar-induced carrier generation. x represents the distance below the exposed semiconductor surface, J_p and J_n are the hole and electron current densities, respectively. q is the electron charge, ε is the permittivity, and ψ is the Electrostatic potential. N_A^- and N_D^+ are the acceptor and donor ionized concentrations, respectively. p_t, n_t, p, and n are the trapped hole, electron concentrations, hole and *e*lectron densities, respectively.

Supplementary Note S2

The light spectrum transmitted from the top sub-cells to the bottom sub-cells is given by,

$$S(\lambda) = S_o(\lambda).\prod_{i=1}^{N} e^{-\alpha_i d_i} \quad \text{(S1)}$$

$S(\lambda)$ is termed as the filtered spectrum. The incident spectrum for single-junction cells and top sub-cells in the multi-junction cells is air mass (AM 1.5), $S_o(\lambda)$. α_i corresponds to the absorption coefficient for the ith layer, and *N* is the number of layers in the top sub-cell.

Table S1. Simulation parameters of the bulk defects within CdSe layer.

Defect type	Single Donor	Single Donor
Capture cross sections (cm^2)	4.73×10^{-13}	3.39×10^{-13}
Energetic distribution	Gaussian	Gaussian
Energy level below CBM (eV)	0.506	0.257
Defect Density (cm^{-3})	8.18×10^{14}	2.84×10^{14}

Table S2. PV parameters of the CdSe cell under various optimization steps.

Parameters	Defects optimization	Work function optimization	Series resistance optimization
J_{SC} (mA/cm^2)	19.35	19.36	19.36
V_{OC} (V)	1.082	1.127	1.127
FF (%)	74.86	75.42	80.72
PCE (%)	15.68	16.47	17.62

Table S3. Voltage losses and open-circuit voltage parameters for the CdSe solar cell under initial and fully optimized conditions.

CdSe Cell	V_{OC}^{rad} (V)	V_{OC} (V)	ΔV_{OC}^{rad} (V)	$\Delta V_{OC}^{rad, below-gap}$ (V)	$\Delta V_{OC}^{non-rad}$ (V)	ΔV_{OC}^{total} (V)
Intial	1.285	0.584	0.260	0.185	0.701	1.146
Fully-optimized	1.288	1.127	0.260	0.183	0.161	0.603