

Electronic Supplementary Information:

Broadband Light Absorption in Cadmium Telluride Thin-Film Solar Cells via Composite Light-Trapping Techniques

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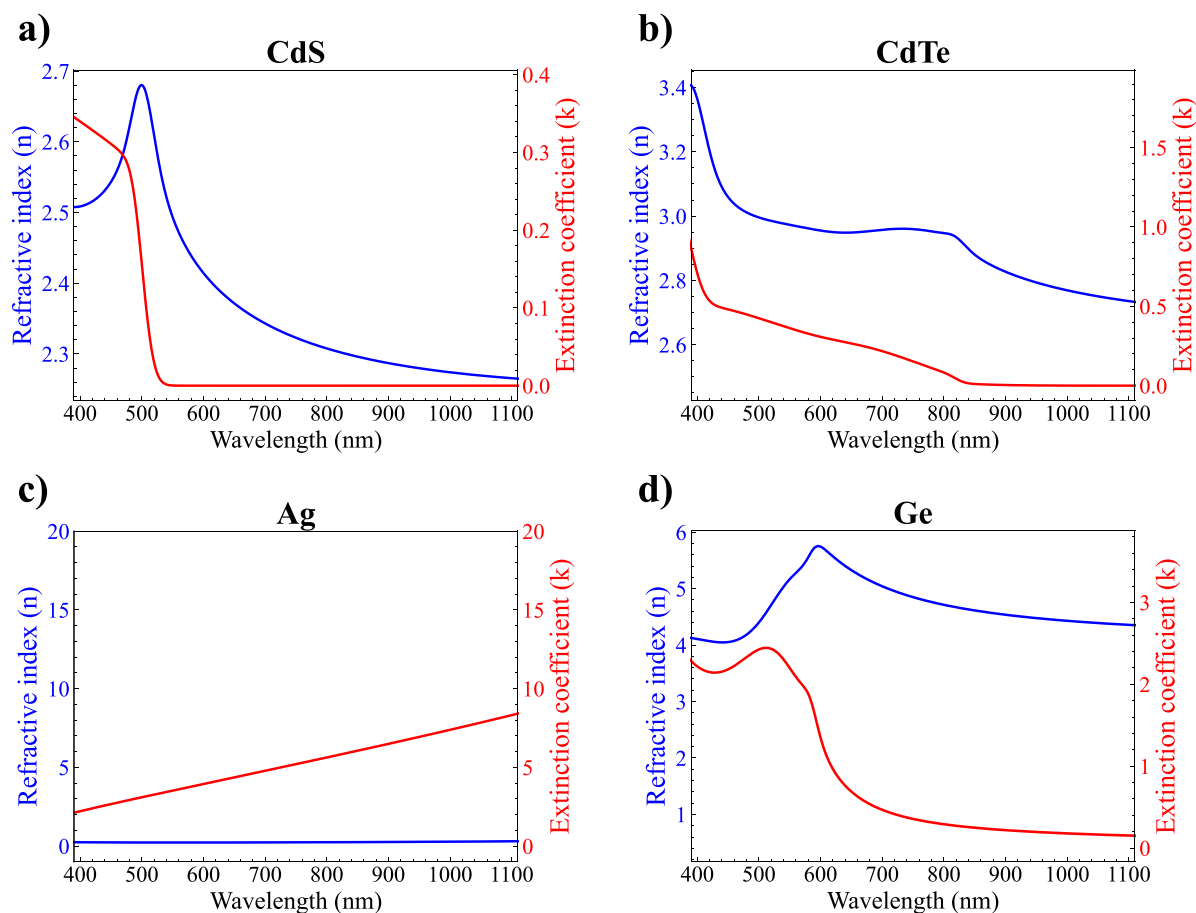


Figure S1: Refractive index (n) and extinction coefficient (k) spectra of (a) CdS, (b) CdTe, (c) Ag, and (d) Ge.

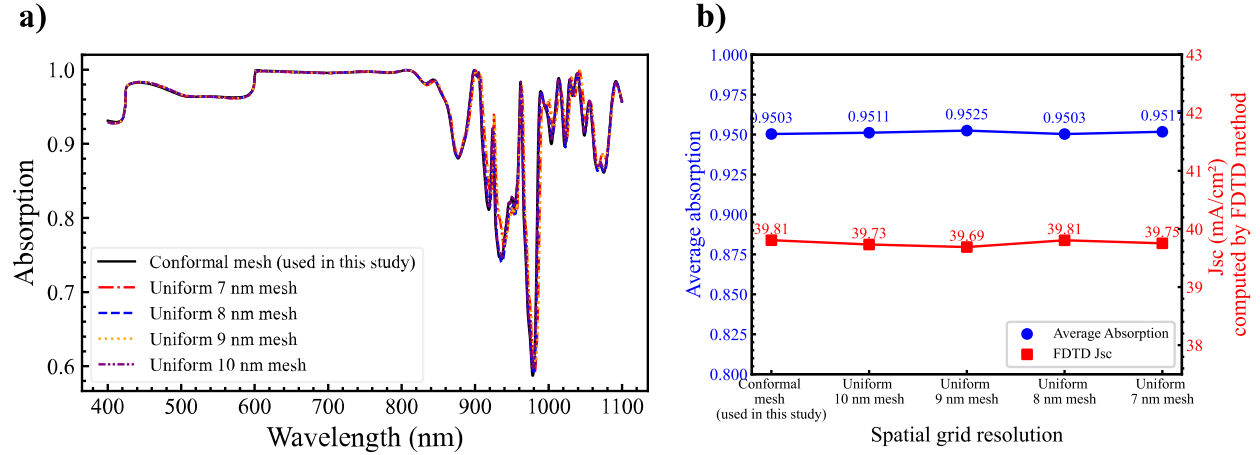


Figure S2: Mesh convergence test of the proposed structure. (a) Absorption spectra for conformal mesh and uniform mesh sizes of 7 nm, 8 nm, 9 nm, and 10 nm. (b) Average absorption and Jsc computed by the FDTD method for conformal mesh and uniform mesh sizes of 7nm, 8nm, 9nm, and 10 nm.

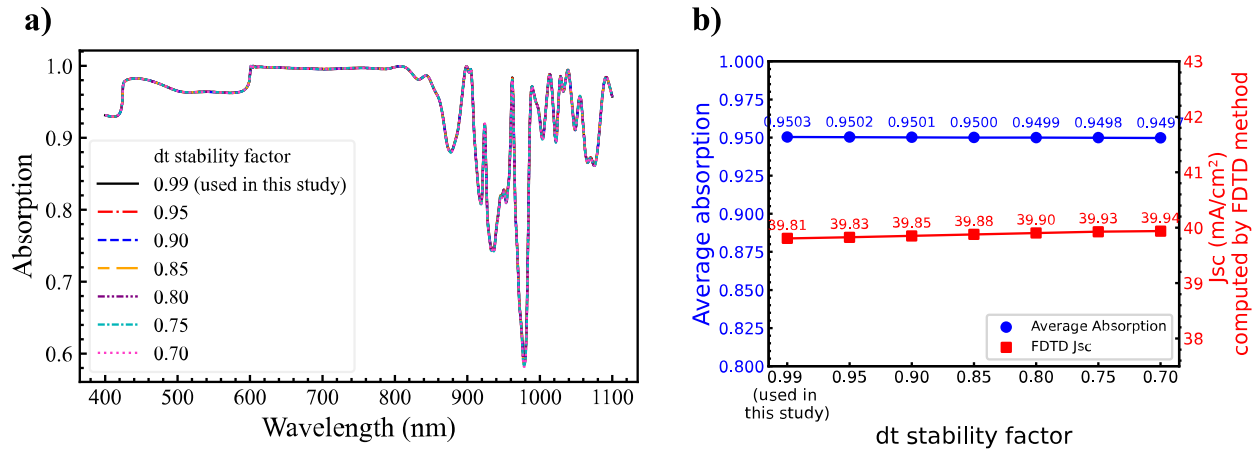


Figure S3: Time step convergence test of the proposed structure. (a) Absorption spectra for the dt stability factor of 0.99, 0.95, 0.90, 0.85, 0.80, 0.75, and 0.70. (b) Average absorption and Jsc computed by the FDTD method for the dt stability factor of 0.99, 0.95, 0.90, 0.85, 0.80, 0.75, and 0.70.

Table S1. CHARGE parameters for electrical simulations.¹⁻²

Parameters	Description	CdTe	CdS
E_g	Bandgap	1.61 eV	2.56 eV
ϵ_r	Relative permittivity	10.2	10
μ_n	Electron mobility	$1050 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$	$340 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$
μ_p	Hole mobility	$100 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$	$340 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$
m_n	Effective mass of electron	$0.11/m_e$	$0.21/m_e$
m_h	Effective mass of hole	$0.76/m_e$	$1.015/m_e$
N_a	Uniform acceptor doping concentration	$2 \times 10^{14} \text{ cm}^{-3}$	-
N_d	Uniform donor doping concentration	-	$1.1 \times 10^{18} \text{ cm}^{-3}$
τ_n	Trap-assisted (Rsrh) electron recombination lifetime	$1 \times 10^{-6} \text{ s}$	$1 \times 10^{-6} \text{ s}$
τ_p	Trap-assisted (Rsrh) hole recombination lifetime	$1 \times 10^{-6} \text{ s}$	$1 \times 10^{-6} \text{ s}$
$C_{n,\text{Auger}}$	Auger recombination of electrons at 300 K	$1 \times 10^{-34} \text{ cm}^6\text{s}^{-1}$	$1 \times 10^{-34} \text{ cm}^6\text{s}^{-1}$
$C_{p,\text{Auger}}$	Auger recombination of holes at 300 K	$1 \times 10^{-34} \text{ cm}^6\text{s}^{-1}$	$1 \times 10^{-34} \text{ cm}^6\text{s}^{-1}$
$C_{\text{Radiative}}$	Radiative recombination coefficient at 300 K	$1 \times 10^{-20} \text{ cm}^3\text{s}^{-1}$	$1 \times 10^{-20} \text{ cm}^3\text{s}^{-1}$

$*m_e$ = rest mass of electron

Table S2. Photovoltaic parameters, i.e., short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill-factor (FF), and power conversion efficiency (PCE) as a function of nanocone texture base diameter (d_{cone}) and height (h_{cone}). J_{sc} , V_{oc} , fill factor, and PCE for bare CdTe TFSCs are 24.33 mA/cm², 978 mV, 0.6455, and 15.36%, respectively.

Nanocone base diameter (nm)	Nanocone height (nm)	J_{sc} (mA/cm ²)	V_{oc} (mV)	Fill Factor	PCE (%)
300	50	25.21	929.6	0.8172	19.15
	100	26.67	925.0	0.8259	20.37
	150	28.03	925.8	0.8287	21.50
	200	28.95	926.1	0.8301	22.25
	250	29.42	926.1	0.8313	22.65
	300	29.66	925.9	0.8323	22.86
	350	29.77	925.8	0.8340	22.99
	400	29.81	925.7	0.8355	23.05

400	50	25.10	930.3	0.8156	19.04
	100	26.44	925.0	0.8242	20.16
	150	27.97	926.0	0.8268	21.41
	200	29.18	926.7	0.8282	22.39
	250	29.88	927.1	0.8292	22.97
	300	30.27	927.0	0.8307	23.31
	350	30.58	927.0	0.8317	23.58
	400	30.74	926.7	0.8341	23.76
500	50	25.12	930.4	0.8149	19.04
	100	26.40	924.9	0.8232	20.10
	150	26.43	924.5	0.8247	20.15
	200	29.31	926.8	0.8258	22.43
	250	30.47	927.6	0.8263	23.35
	300	31.14	927.9	0.8273	23.90
	350	31.71	928.4	0.8275	24.36
	400	31.85	928.2	0.8291	24.51
600	50	25.01	930.2	0.8150	18.96
	100	26.06	924.8	0.8218	19.80
	150	27.39	925.4	0.8235	20.87
	200	28.98	926.4	0.8233	22.10
	250	30.04	927.1	0.8240	22.95
	300	31.00	927.8	0.8246	23.72
	350	31.69	928.3	0.8252	24.28
	400	32.09	928.7	0.8259	24.62
700	50	25.01	930.0	0.8128	18.90
	100	25.87	925.6	0.8213	19.66
	150	26.98	925.0	0.8225	20.53
	200	28.17	925.5	0.8228	21.45
	250	29.05	926.1	0.8232	22.15
	300	29.74	926.6	0.8242	22.71
	350	30.52	927.0	0.8250	23.34
	400	31.10	927.7	0.8254	23.81
800	50	25.12	930.0	0.8126	18.99
	100	26.13	925.9	0.8200	19.84
	150	27.34	925.5	0.8205	20.76
	200	28.40	926.1	0.8205	21.58
	250	29.47	926.9	0.8207	22.42
	300	30.16	927.4	0.8216	22.98
	350	30.89	927.7	0.8227	23.58

900	400	31.21	928.0	0.8241	23.87
	50	24.89	929.9	0.8132	18.82
	100	25.43	925.5	0.8212	19.33
	150	26.28	924.7	0.8221	19.98
	200	27.10	924.6	0.8231	20.62
	250	28.13	925.2	0.8227	21.41
	300	28.88	925.9	0.8229	22.00
	350	29.89	926.8	0.8225	22.79
	400	30.62	927.5	0.8225	23.36

Table S3. Photovoltaic parameters i.e. short-circuit current density (Jsc), open-circuit voltage (Voc), fill-factor (FF), and power conversion efficiency (PCE) as a function of Ge NP diameter (d_{Ge}) and position (z_{Ge}). Jsc, Voc, fill factor, and PCE for bare CdTe TFSCs are 24.33 mA/cm², 978 mV, 0.6455, and 15.36%, respectively. Note that the Ge NP data was generated on the optimized texture structure where both the CdS-CdTe surface layers were textured as NCs with a base diameter and height of 600 nm and 400 nm, respectively.

Nanoparticle diameter (nm)	Nanoparticle position (nm)	Jsc (mA/cm ²)	Voc (mV)	Fill Factor	PCE (%)
50	500	32.15	928.8	0.8259	24.66
	600	32.10	928.7	0.8259	24.62
	700	32.12	928.7	0.8259	24.64
	800	32.14	928.7	0.8259	24.65
	900	32.13	928.7	0.8259	24.65
	1000	32.14	928.7	0.8259	24.65
	1100	32.13	928.7	0.8259	24.65
	1200	32.14	928.7	0.8258	24.65
100	500	32.28	929.0	0.8268	24.80
	600	32.07	928.8	0.8272	24.64
	700	32.22	928.9	0.8266	24.73
	800	32.21	928.9	0.8265	24.73
	900	32.19	928.8	0.8264	24.71
	1000	32.18	928.8	0.8261	24.69
	1100	32.27	928.9	0.8256	24.74
	1200	32.17	928.8	0.8256	24.67
150	500	32.77	929.8	0.8313	25.33
	600	32.45	929.4	0.8306	25.05

	700	32.55	929.4	0.8293	25.09
	800	32.39	929.2	0.8283	24.93
	900	32.56	929.3	0.8273	25.03
	1000	32.56	929.2	0.8262	25.00
	1100	32.62	929.2	0.8250	25.00
	1200	32.75	929.2	0.8232	25.05
200	500	33.53	931.0	0.8371	26.13
	600	33.82	931.1	0.8343	26.27
	700	33.67	930.9	0.8326	26.10
	800	33.26	930.2	0.8306	25.70
	900	32.69	929.5	0.8290	25.19
	1000	33.19	929.9	0.8267	25.51
	1100	33.27	929.7	0.8241	25.49
	1200	33.68	929.8	0.8188	25.64
250	500	34.47	932.2	0.8385	26.94
	600	34.49	932.0	0.8368	26.90
	700	34.40	931.8	0.8348	26.75
	800	33.67	930.8	0.8332	26.11
	900	32.94	929.8	0.8303	25.44
	1000	33.53	930.3	0.8278	25.82
	1100	34.03	930.4	0.8233	26.07
	1200	33.85	929.9	0.8180	25.75
300	500	35.38	933.2	0.8406	27.76
	600	35.02	932.7	0.8396	27.42
	700	34.51	932.0	0.8372	26.93
	800	33.64	930.9	0.8356	26.17
	900	34.01	931.1	0.8325	26.36
	1000	34.02	930.8	0.8285	26.24
	1100	34.11	930.5	0.8234	26.13
	1200	34.37	930.2	0.8154	26.07

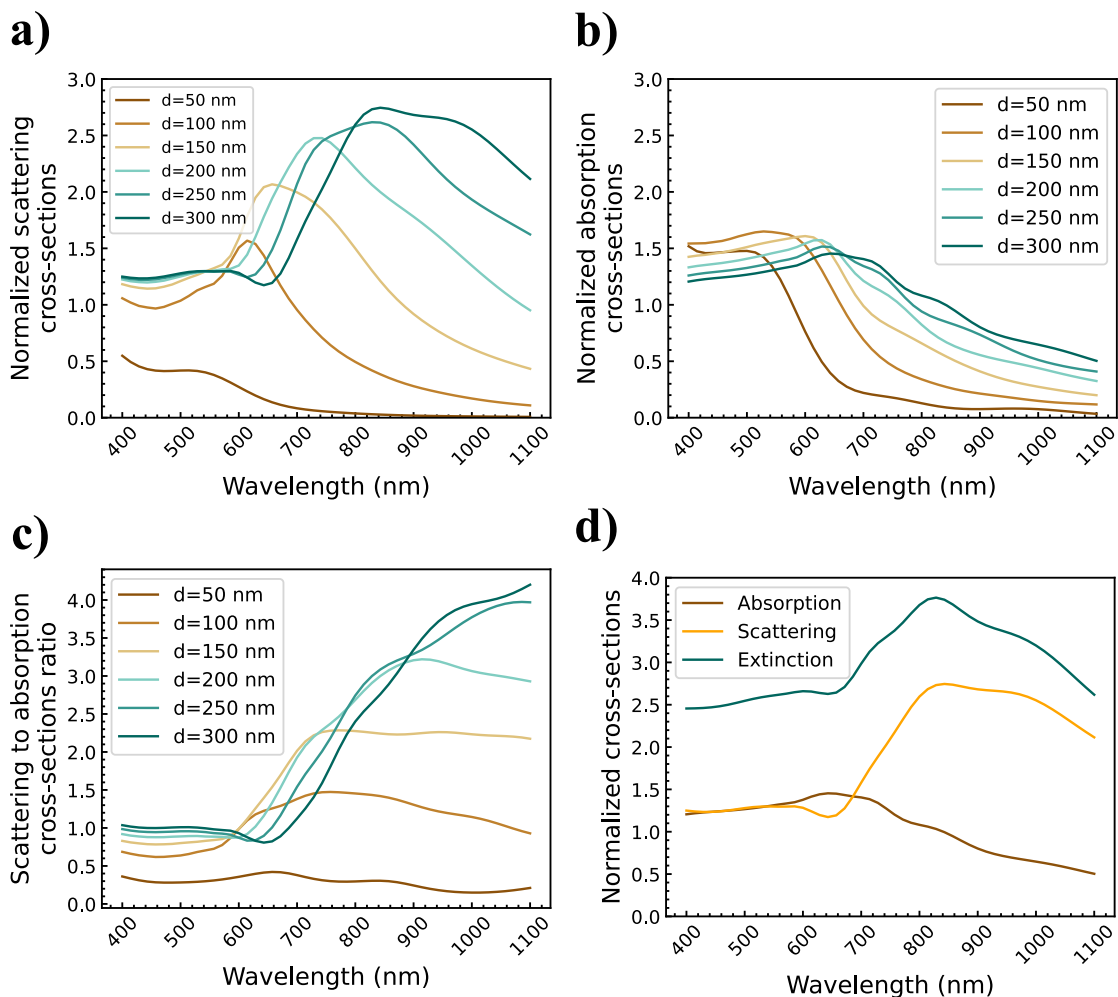


Figure S4: (a) Mie analysis for Ge NP showing (a) normalized scattering cross-sections for $d = 50, 100, 150, 200, 250, 300$ nm, (b) normalized absorption cross-sections for $d = 50, 100, 150, 200, 250, 300$ nm, (c) scattering to absorption cross-sections for $d = 50, 100, 150, 200, 250, 300$ nm, (d) normalized absorption, scattering, extinction cross-section for $d = 300$ nm.

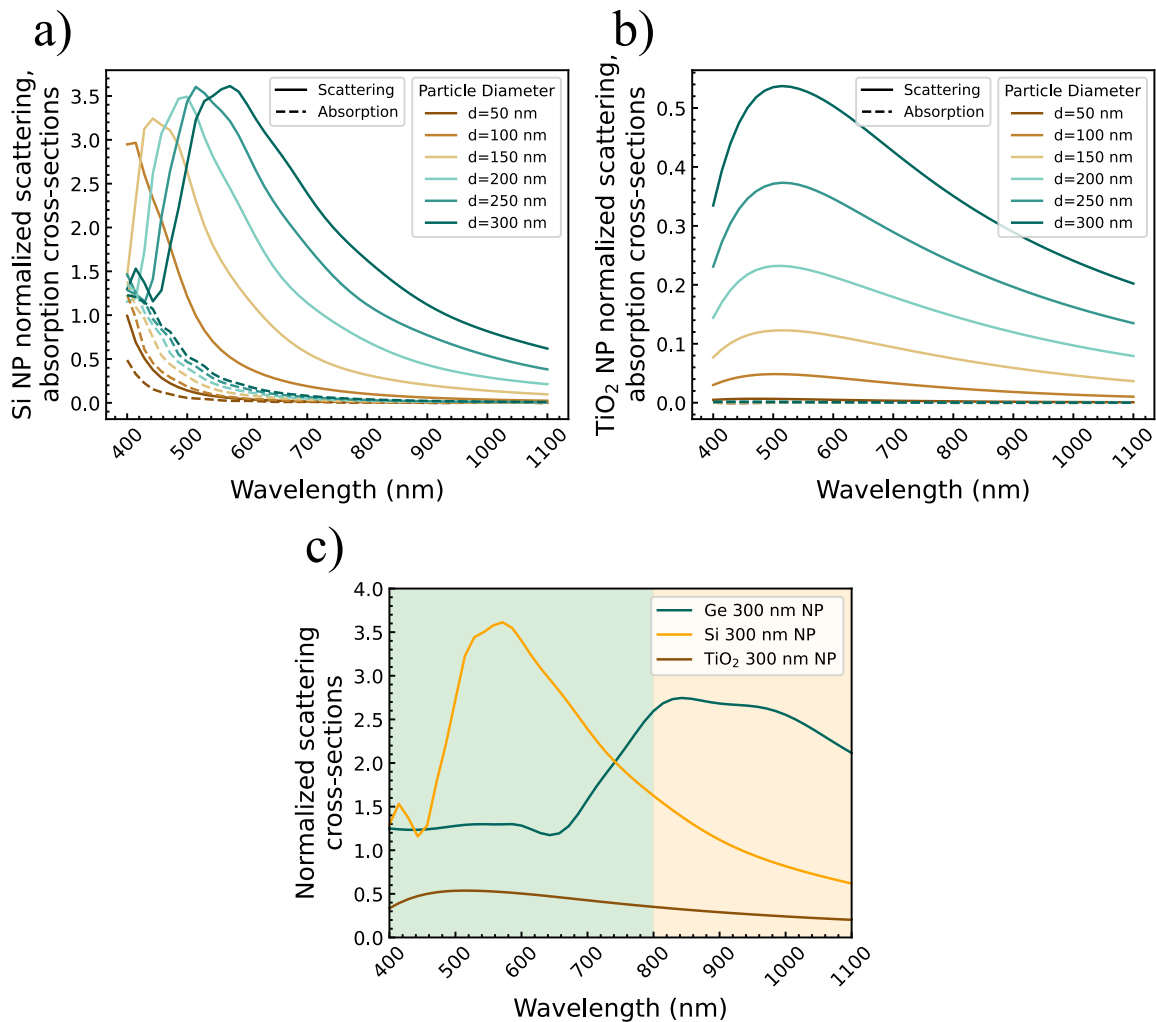


Figure S5: Mie analysis showing (a) normalized scattering, absorption cross-sections of Si NP for $d = 50, 100, 150, 200, 250, 300$ nm, (b) normalized scattering, absorption cross-sections of TiO₂ NP for $d = 50, 100, 150, 200, 250, 300$ nm, (c) normalized scattering cross-sections for optimal NPs ($d = 300$ nm) of each material i.e. Ge, Si and TiO₂.

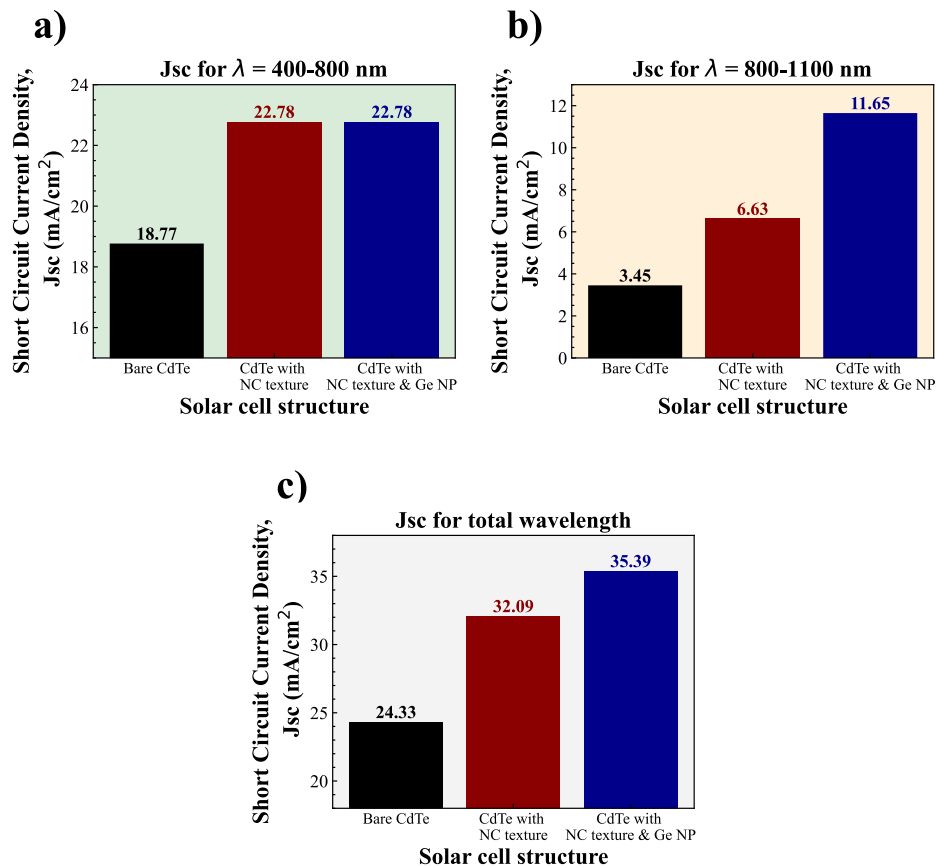


Figure S6: (a) Jsc for 400-800 nm wavelength range, (b) Jsc for 800-1100 nm wavelength range, (c) Jsc for the total wavelength range (400-1100 nm) of bare CdTe TFSCs, NC textured CdTe, and NC textured CdTe with Ge NP.

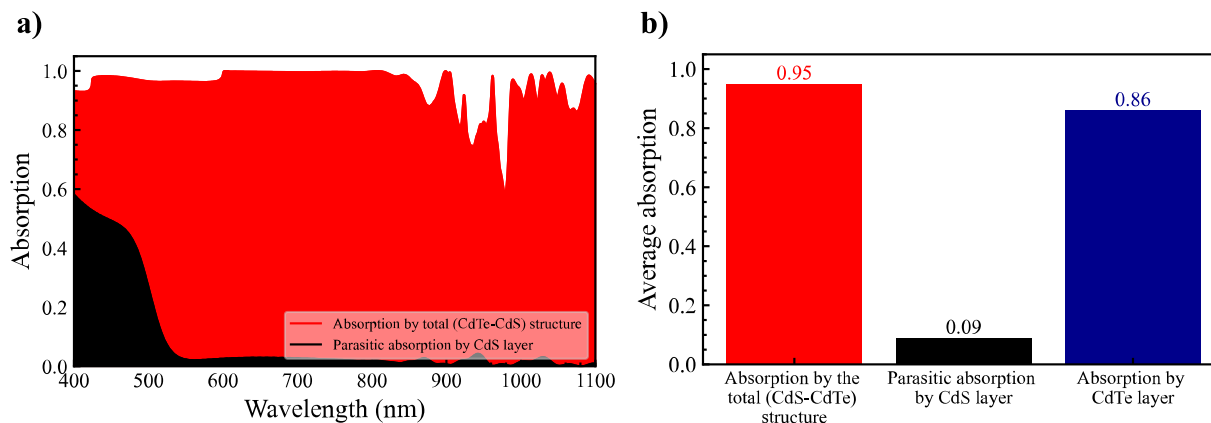


Figure S7: (a) Parasitic absorption loss by the CdS window layer compared to the absorption by the total (CdS-CdTe) structure. (b) Average absorption by the total (CdS-CdTe) structure, CdS window layer, and the CdTe absorber layer.

Table S4. Photovoltaic parameters, i.e., short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill-factor (FF), and power conversion efficiency (PCE) for the proposed structure without any recombination and series resistance, with bulk recombination, and with series resistance. Note that all the simulations in this study consider bulk recombination but not the series resistance.

Loss mechanisms in solar cells	J_{sc} (mA/cm ²)	V_{oc} (mV)	Fill factor	PCE (%)
No recombination/series resistance	35.40	933.3	0.8406	27.77
Bulk recombination (Shockley-Read-Hall, Radiative, and Auger)	35.38	933.2	0.8406	27.76
Series resistance	35.38	938.1	0.7890	26.19

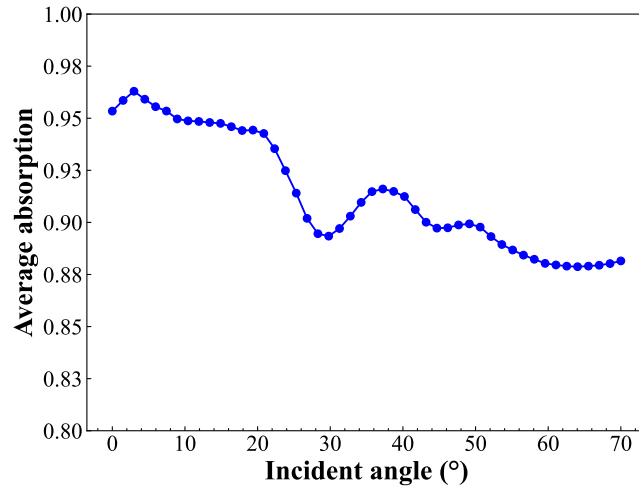


Figure S8: Average absorption of NC textured CdTe TFSC with embedded Ge NP structure as a function of incident angle variation of 0° to 70°.

References

1. R. B. Sultan, A. Al Suny, M. H. Hossain, T. Noor, and M. H. Chowdhury, Heliyon, 2024.
2. <https://optics.ansys.com/hc/en-us/articles/360034919113-Semiconductor-Material-Model-Properties>