Unlocking the Full Potential of Solar Cell Materials: Parameter Sensitivity Analysis and Optimization Using Response Surface Modelling

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Parameter	SnSe	TiO ₂ [1]	SnO ₂
Thickness (µm)	1.2	0.10	0.2
Band gap (eV)	1-1.5 [2]	2.26	3.6 [3]
Electron Affinity (eV)	4.2 [2], [4]	4.1-4.5	4.53 [3]
Valence band density of states (cm ⁻³)	1.6 x10 ¹⁸	6 x10 ¹⁷	1 x10 ¹⁹ [5]
Conduction band density of states (cm ⁻³)	1.45 x10 ¹⁸	2 x10 ¹⁷	1 x10 ¹⁹ [6]
Radiative recombination coefficient (cm ³ s ⁻¹)	2.9 x10 ⁻¹¹	1 x10 ⁻⁸	1 x10 ⁻⁸
Mobility of electron/hole (cm²/Vs)	130/56.7 [7]	100/50	5/2.5 [6]
Absorption coefficient	5 x10 ⁴ [2]	-	-
Uniform Acceptor density (cm ⁻³)	9x10 ¹⁵ - 4x10 ¹⁶	-	-
Uniform donor density (cm ⁻³)	-	1 x10 ¹⁷	1x10¹⁹ [5]

Table S1. Input parameters/variables for the device

Band gap of the TiO₂ is taken as 2.26 (which can be easily obtained after doping[8], [9].

LAYER 1		SnSe		LAYER 2		TiO2	
thickness (µm)	•	1.200]	thickness (µm)	•	0.100	
		uniform pure A	(y=0) 👻			uniform pure A	(y=0) 👻
The layer is pure A: y	r = 0, uniform	0.000		The layer is pure A: y	r = 0, uniform	0.000	
Semiconductor Property P of the pure material		pure A (y = 0)]	Semiconductor Property P of the pure material		pure A (y = 0)	1
bandgap (eV)		1.380		bandgap (eV)		2.260	
electron affinity (eV)		4.200		electron affinity (eV)		4.200	
dielectric permittivity	(relative)	12.500		dielectric permittivity (relative)		10.000	
CB effective density	of states (1/cm^3)	1.450E+18		CB effective density of states (1/cm ³)		2.000E+17	
VB effective density of	of states (1/cm^3)	1.600E+18		VB effective density of states (1/cm ³)		6.000E+17	
electron thermal velo	city (cm/s)	1.000E+7		electron thermal velo	city (cm/s)	1.000E+7	
hole thermal velocity	(cm/s)	1.000E+7		hole thermal velocity (cm/s)		1.000E+7	
electron mobility (cm	²/Vs)	1.300E+2		electron mobility (cm²/Vs)		1.000E+2	
hole mobility (cm²/Vs	;)	5.670E+1		hole mobility (cm²/Vs	5)	5.000E+1	
	effective mass of electron:	1.000E+0		Allow Tuppeling	effective mass of electron:	1.000E+0	
Allow Tunneling	effective mass of holes	1.000E+0		Allow Full to any	effective mass of holes	1.000E+0	
no ND grading (uniform)			-	no ND grading (unifo	orm)		-
shallow uniform donor density ND (1/cm3) 0.00		0.000E+0		shallow uniform donor density ND (1/cm3) 1.000E+1		1.000E+17	
no NA grading (uniform)			-	no NA grading (unifo	rm)		-
shallow uniform acc	eptor density NA (1/cm3)	4.000E+16		shallow uniform acceptor density NA (1/cm3) 0.000E+0			

Figure S1 The input parameters for the SnSe (left) and for TiO₂ (right) in SCAPS-1D.

Table S2. Set of parameters (z_i) (with 5 variables, face-centered alpha =1.56508) using central composite design (CCD).

Sr. No.	Z ₁	Z ₂	Z ₃	Z_4	Z_5
1	-1	-1	-1	-1	-1
2	1	-1	-1	-1	-1
3	-1	1	-1	-1	-1
4	1	1	-1	-1	-1
5	-1	-1	1	-1	-1
6	1	-1	1	-1	-1
7	-1	1	1	-1	-1
8	1	1	1	-1	-1
9	-1	-1	-1	1	-1
10	1	-1	-1	1	-1
11	-1	1	-1	1	-1
12	1	1	-1	1	-1
13	-1	-1	1	1	-1
14	1	-1	1	1	-1
15	-1	1	1	1	-1
16	1	1	1	1	-1
17	-1	-1	-1	-1	1
18	1	-1	-1	-1	1
19	-1	1	-1	-1	1
20	1	1	-1	-1	1
21	-1	-1	1	-1	1
22	1	-1	1	-1	1
23	-1	1	1	-1	1
24	1	1	1	-1	1

25	-1	-1	-1	1	1
26	1	-1	-1	1	1
27	-1	1	-1	1	1
28	1	1	-1	1	1
29	-1	-1	1	1	1
30	1	-1	1	1	1
31	-1	1	1	1	1
32	1	1	1	1	1
33	-1.56058	0	0	0	0
34	1.56058	0	0	0	0
35	0	-1.56058	0	0	0
36	0	1.56058	0	0	0
37	0	0	-1.56058	0	0
38	0	0	1.56058	0	0
39	0	0	0	-1.56058	0
40	0	0	0	1.56058	0
41	0	0	0	0	-1.56058
42	0	0	0	0	1.56058
43	0	0	0	0	0
44	0	0	0	0	0
45	0	0	0	0	0
46	0	0	0	0	0
47	0	0	0	0	0
48	0	0	0	0	0
49	0	0	0	0	0
50	0	0	0	0	0

Table S3 Input parameters using the CCD for the simulation and their efficiency after simulation by SCAPS-1D

Sr.	Band Gap	Shallow Acceptor	$CPO(\mathbf{x})$		Temp.	Efficiency
No.	(x ₁)	Density (x_2)	$CDO(X_3)$	W.F. (x_4)	(X ₅)	(R)
	eV	1/cm ³	eV	eV	K	%
1	1	9 x10 ⁺¹⁵	-0.1	4.8	275	15.77
2	1.5	9x10 ⁺¹⁵	-0.1	4.8	275	9.02
3	1	$4x10^{+16}$	-0.1	4.8	275	17.12
4	1.5	$4x10^{+16}$	-0.1	4.8	275	9.84
5	1	9x10 ⁺¹⁵	0.3	4.8	275	16.54
6	1.5	9x10 ⁺¹⁵	0.3	4.8	275	9.17
7	1	4x10 ⁺¹⁶	0.3	4.8	275	18.21
8	1.5	$4x10^{+16}$	0.3	4.8	275	10.23

9	1	9x10 ⁺¹⁵	-0.1	5.4	275	27.31
10	1.5	9x10 ⁺¹⁵	-0.1	5.4	275	19.97
11	1	$4x10^{+16}$	-0.1	5.4	275	27.3
12	1.5	$4x10^{+16}$	-0.1	5.4	275	19.98
13	1	9x10 ⁺¹⁵	0.3	5.4	275	29.95
14	1.5	9x10 ⁺¹⁵	0.3	5.4	275	19.47
15	1	$4x10^{+16}$	0.3	5.4	275	29.95
16	1.5	4x10 ⁺¹⁶	0.3	5.4	275	20.01
17	1	9x10 ⁺¹⁵	-0.1	4.8	320	14.99
18	1.5	9x10 ⁺¹⁵	-0.1	4.8	320	9.23
19	1	$4x10^{+16}$	-0.1	4.8	320	16.22
20	1.5	4x10 ⁺¹⁶	-0.1	4.8	320	10.18
21	1	9x10 ⁺¹⁵	0.3	4.8	320	14.68
22	1.5	9x10 ⁺¹⁵	0.3	4.8	320	8.85
23	1	$4x10^{+16}$	0.3	4.8	320	16.1
24	1.5	$4x10^{+16}$	0.3	4.8	320	9.98
25	1	9x10 ⁺¹⁵	-0.1	5.4	320	26.44
26	1.5	9x10 ⁺¹⁵	-0.1	5.4	320	18.8
27	1	4x10 ⁺¹⁶	-0.1	5.4	320	26.44
28	1.5	$4x10^{+16}$	-0.1	5.4	320	18.85
29	1	9x10 ⁺¹⁵	0.3	5.4	320	27.18
30	1.5	9x10 ⁺¹⁵	0.3	5.4	320	17.94
31	1	$4x10^{+16}$	0.3	5.4	320	27.18
32	1.5	4x10 ⁺¹⁶	0.3	5.4	320	18.42
33	0.85873	2.45x10 ⁺¹⁶	0.1	5.1	297.5	23.09
34	1.64127	2.45x10 ⁺¹⁶	0.1	5.1	297.5	13.26
35	1.25	2.4126x10 ⁺¹⁴	0.1	5.1	297.5	16.16
36	1.25	4.87587x10 ⁺¹⁶	0.1	5.1	297.5	20.21
37	1.25	2.45x10 ⁺¹⁶	-0.213	5.1	297.5	16.7
38	1.25	2.45x10 ⁺¹⁶	0.413	5.1	297.5	17.82
39	1.25	2.45x10 ⁺¹⁶	0.1	4.63048	297.5	9.31
40	1.25	2.45x10 ⁺¹⁶	0.1	5.56952	297.5	29.94
41	1.25	2.45x10 ⁺¹⁶	0.1	5.1	262.286	21.69
42	1.25	2.45x10 ⁺¹⁶	0.1	5.1	332.714	18.1
43	1.25	2.45x10 ⁺¹⁶	0.1	5.1	297.5	19.98
44	1.25	2.45x10 ⁺¹⁶	0.1	5.1	297.5	19.98
45	1.25	2.45x10 ⁺¹⁶	0.1	5.1	297.5	19.98
46	1.25	$2.45 \times 10^{+16}$	0.1	5.1	297.5	19.98
47	1.25	2.45x10 ⁺¹⁶	0.1	5.1	297.5	19.98
48	1.25	2.45x10 ⁺¹⁶	0.1	5.1	297.5	19.98
49	1.25	2.45x10 ⁺¹⁶	0.1	5.1	297.5	19.98
50	1.25	$2.45 \times 10^{+16}$	0.1	5.1	297.5	19.98

Tablx10 S4. Actual value of the efficiency from SCAPS-1D software and the predicted value of the efficiency by RSM model and their Residual.

Run Order	Actual Value of Efficiency	Predicted Value of Efficiency	Residual
1	18.10	18.84	-0.7404
2	9.98	9.36	0.6159
3	19.98	19.86	0.1225
4	18.21	18.26	-0.0487
5	9.84	10.38	-0.5394
6	27.30	28.02	-0.7165
7	10.18	10.05	0.1303
8	16.10	15.99	0.1110
9	18.80	19.09	-0.2909
10	19.98	19.86	0.1225
11	9.23	8.59	0.6389
12	10.23	10.70	-0.4688
13	23.09	24.51	-1.42
14	9.02	8.92	0.0992
15	15.77	15.23	0.5392
16	16.22	15.42	0.7954
17	29.94	28.40	1.54
18	16.54	16.80	-0.2602
19	19.98	19.81	0.1709
20	9.17	9.24	-0.0702
21	13.26	12.91	0.3522
22	19.98	19.86	0.1225
23	16.70	17.45	-0.7504

24	19.98	19.86	0.1225
25	16.16	18.00	-1.84
26	20.01	20.13	-0.1185
27	27.31	27.63	-0.3180
28	20.21	19.44	0.7661
29	14.99	13.97	1.02
30	17.12	16.69	0.4307
31	21.69	20.87	0.8155
32	26.44	26.75	-0.3118
33	19.47	19.74	-0.2700
34	18.85	19.48	-0.6294
35	8.85	7.91	0.9444
36	19.98	19.86	0.1225
37	29.95	29.59	0.3641
38	14.68	14.53	0.1495
39	19.98	19.86	0.1225
40	19.97	19.42	0.5495
41	17.94	18.41	-0.4653
42	27.18	27.32	-0.1362
43	27.18	26.93	0.2523
44	9.31	11.32	-2.01
45	17.82	18.14	-0.3220
46	19.98	19.86	0.1225
47	26.44	26.36	0.0767
48	19.98	19.86	0.1225
49	29.95	29.20	0.7526
50	18.42	18.79	-0.3738

SCAPS 3.3.10 Layer Prope	erties Panel							
LAYER 1			SnSe	SCAPS 3.3.10 Layer Properties Panel				
thickness (µm)	•	1.200		LAYER 2		TiO2		
		uniform pure A	(v=0)	thickness (µm)	•	0.100		
The layer is pure A: $y = 0$, uniform		0.000				uniform pure A (y=0)		
Semiconductor Pro	operty P of the pure mater	pure A (y = 0)	The layer is pure A: y = 0, uniform		0.000			
				Semiconductor Pr	operty P of the pure mater	pure A $(y = 0)$		
bandgap (eV)		1.000						
electron affinity (e)	V)	4.200		bandgap (eV)		2.260		
dielectric permittivi	ity (relative)	12.500		electron affinity (e)	V)	4.364		
CB effective densit	ty of states (1/cm ³)	1.450E+18		dielectric permittiv	ity (relative)	10.000		
VB effective densit	ty of states (1/cm ³)	1.600E+18		CB effective density of states (1/cm ³)		2.000E+17		
electron thermal velocity (cm/s)		1.000E+7		VB effective density of states (1/cm ³)		6.000E+17		
hole thermal velocity (cm/s)		1.000E+7		electron thermal v	electron thermal velocity (cm/s)			
electron mobility (cm²/Vs)		1.300E+2	hole thermal velocity (cm/s)		1.000E+7			
hole mobility (cm ² /	Vs)	5.670E+1		electron mobility (cm²/Vs)	1.000E+2		
Allow	effective mass of electro	1.000E+0		hole mobility (cm²/Vs)		5.000E+1		
, alon	effective mass of holes	1.000E+0	Allow		effective mass of electro	1.000E+0		
no ND grading (un	niform)		-	Allow	effective mass of holes	1.000E+0		
shallow uniform do	onor density ND (1/cm3)	0.000E+0		no ND grading (uniform)			-	
no NA grading (un	iform)		-	shallow uniform donor density ND (1/cm3) 1.000E+17				
shallow uniform ac	cceptor density NA (1/cm3)	2.890E+16		no NA grading (uniform)				
Absorption interp	polation model		<u></u>	shallow uniform acceptor density NA (1/cm3) 0.000E+0				
alpha pure A material (y=0) from file from model Set absorption model List of absorption submodels present: sqrt(hv-Eg) law (SCAPS traditional)				Absorption interpolation model alpha pure A material (y=0) from file from model Set absorption model List of absorption submodels present: sqrt(hv-Eg) law (SCAPS traditional)				

Figure S2. Input panel for the (left) SnSe, and (right) TiO₂.

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