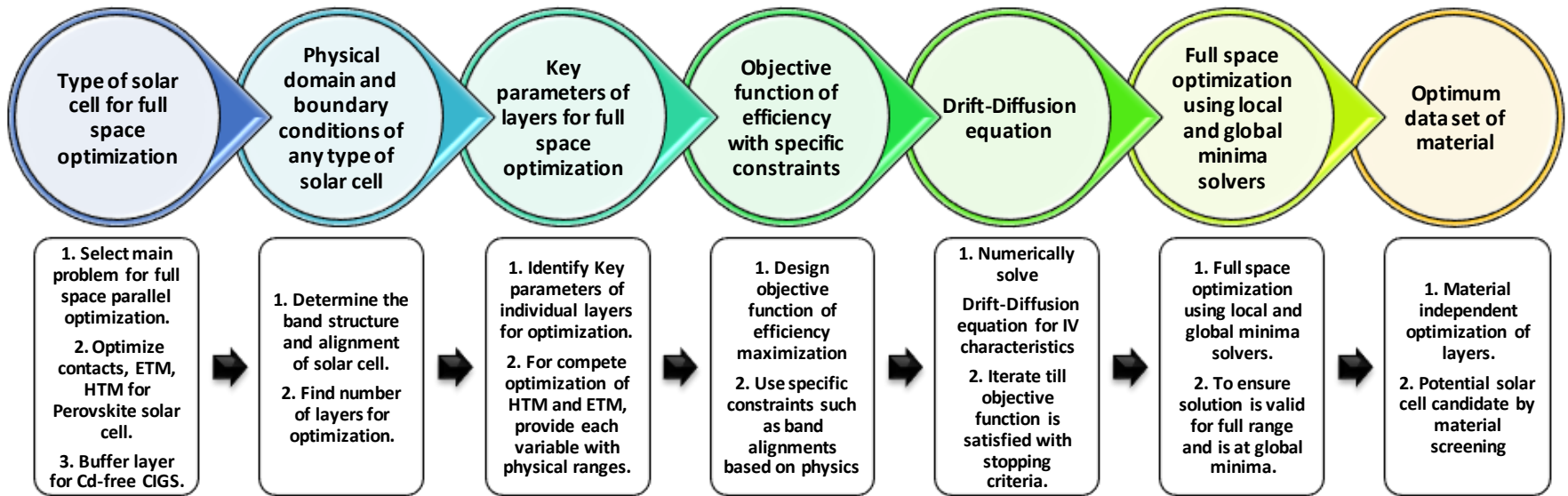


Full Space Device Optimization for Solar Cells

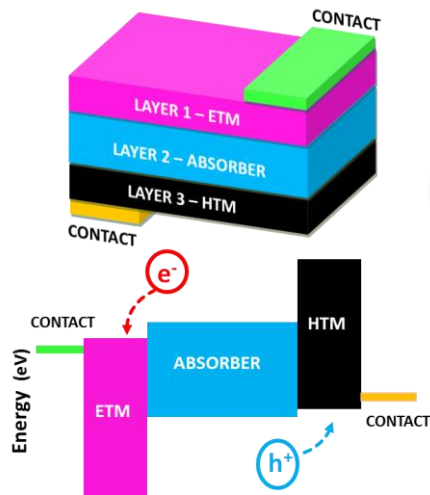
Ahmer A.B. Baloch, Shahzada P. Aly, Mohammad I. Hossain, Fedwa El Mellouhi,
Nouar Tabet, and Fahhad H Alharbi

Supplementary Material

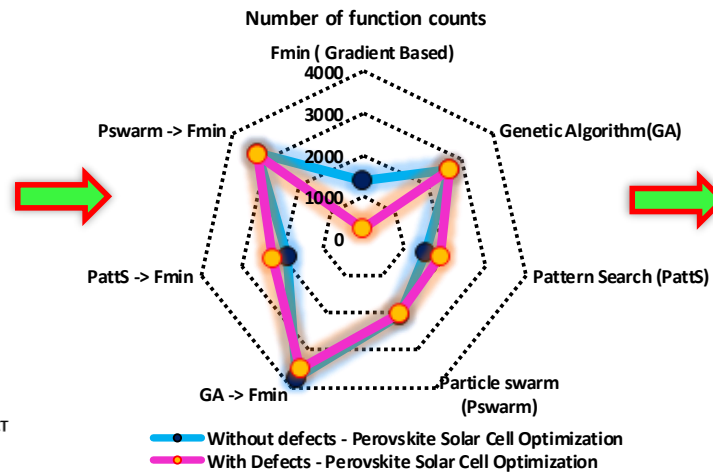
Supplementary Material



Arbitrary device structure



Local and Global Optimizers



Optimized material dataset and IV curve

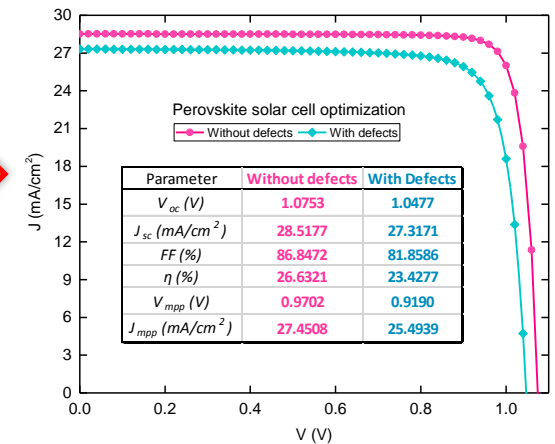


Figure S1: Detailed framework for full space optimization with schematics and results from simulation.

Table S1

Full space optimized parameters for PSC with Defects.

PSC with Defects		Optimization Algorithms						
Variable	Unit	fmin	GA	PattS	Particle Swarm	GA to Fmin	PattS to Fmin	Pswarm to Fmin
Front Contact Work function	eV	4.0964	3.9137	4.1000	4.0021	3.9170	4.1000	4.0021
Back Contact Work function	eV	5.1738	5.3478	5.2250	5.3900	5.3425	5.2250	5.3900
Thickness ETM	μm	0.1707	0.3906	0.0750	0.0500	0.3694	0.0750	0.0500
Donor Conc. ETM	1/cm ³ (10 ^{value})	18.568 5	17.406 0	18.531 0	18.1480	17.3525	18.5310	18.1480
Energy Gap ETM	eV	3.9375	3.6517	4.0000	4.0000	3.6606	4.0000	4.0000
Electron Mobility ETM	cm ² /V.s	175.49 44	1.4204	200.00 00	233.9900	2.8493	200.0000	233.9900
Hole Mobility ETM	cm ² /V.s	5.4444	0.3584	1.0000	3.3803	0.2875	1.0000	3.3803
Absorbtion Coeff. ETM	1/cm.eV ^{1/2}	125.74 77	126.32 81	125.89 25	1557.0408	138.6756	125.8925	1557.0408
CB DOS ETM	1/cm ³ (10 ^{value})	18.568 6	18.168 0	18.531 0	18.1640	18.1694	18.5310	18.1640
VB DOS ETM	1/cm ³ (10 ^{value})	18.524 1	18.121 0	18.000 0	18.0880	18.0934	18.0000	18.0880
Affinity Energy ETM	eV	4.0303	3.9117	4.0000	3.9913	3.9091	4.0000	3.9913
Dielectric Perm. ETM	-	7.3402	5.6484	6.5000	6.0039	5.7548	6.5000	6.0039
Thickness Perovskite	μm	0.7321	0.7291	0.7324	0.7324	0.7375	0.7324	0.7324
Thickness HTM	μm	0.4989	0.0743	0.4500	0.5000	0.0742	0.4500	0.5000
Acceptor Conc. HTM	1/cm ³ (10 ^{value})	18.206 6	18.048 0	19.000 0	18.0000	18.0672	19.0000	18.0000
Energy Gap HTM	eV	3.3645	2.8238	2.8996	2.9872	2.8235	2.8999	2.9872
Electron Mobility HTM	cm ² /V.s	4.9727	1.8524	2.0000	3.8813	1.5428	2.0000	3.8813
Hole Mobility HTM	cm ² /V.s	436.13 25	155.83 00	200.00 00	230.8800	176.6236	200.0000	307.7459
Absorbtion Coeff. HTM	1/cm.eV ^{1/2}	8529.0 370	211.54 37	1258.9 254	1737.0007	213.8454	1258.9254	1737.0007
CB DOS HTM	1/cm ³ (10 ^{value})	19.958 9	18.061 0	18.000 0	18.2750	18.0673	18.0000	18.2750
VB DOS HTM	1/cm ³ (10 ^{value})	18.207 0	18.058 0	19.000 0	18.0000	18.0674	19.0000	18.0000
Affinity Energy HTM	eV	2.0355	2.5767	2.5000	2.4128	2.5765	2.5000	2.4128
Dielectric Perm. HTM	-	16.161 2	4.9913	20.000 0	20.0000	7.2553	20.0000	20.0000

Table S2

Full space optimized parameters for PSC without Defects.

PSC without Defects			Optimization Algorithms					
Variable	Unit	fmin	GA	PattS	Particle Swarm	GA to Fmin	PattS to Fmin	Pswarm to Fmin
Front Contact Work function	eV	4.0763	4.114 2	4.1000	4.0763	4.0398	4.1000	4.0763
Back Contact Work function	eV	5.3759	5.144 9	5.3500	5.3758	5.2561	5.3500	5.3758
Thickness ETM	μm	0.5000	0.123 9	0.0594	0.5000	0.0703	0.0594	0.5000
Donor Conc. ETM	1/cm ³ (10 ^{value})	17.779 1	16.39 00	17.828 0	17.7790	16.3652	17.8280	17.7790
Energy Gap ETM	eV	4.0000	3.319 5	4.0000	4.0000	3.4842	4.0000	4.0000
Electron Mobility ETM	cm ² /V.s	191.35 61	2.621 4	200.00 00	191.3800	19.4276	200.0000	191.3800
Hole Mobility ETM	cm ² /V.s	5.4391	4.054 8	1.0000	5.4389	3.6442	1.0000	5.4389
Absorbtion Coeff. ETM	1/cm.eV ^{1/2}	2.0000	2.200 6	2.0375	2.0000	2.0277	2.0375	2.0000
CB DOS ETM	1/cm ³ (10 ^{value})	18.748 9	19.45 80	20.000 0	18.7490	19.5973	20.0000	18.7500
VB DOS ETM	1/cm ³ (10 ^{value})	18.037 9	19.09 20	18.000 0	18.0380	18.8936	18.0000	18.0380
Affinity Energy ETM	eV	4.0692	3.937 8	4.0000	4.0692	3.9354	4.0000	4.0692
Dielectric Perm. ETM	-	8.3914	3.476 2	19.000 0	8.3917	3.8342	19.0000	8.3917
Thickness Perovskite	μm	1.1024	1.099 3	1.1094	1.1017	1.1104	1.1094	1.1019
Thickness HTM	μm	0.4995	0.442 5	0.4969	0.5000	0.4393	0.4969	0.4993
Acceptor Conc. HTM	1/cm ³ (10 ^{value})	17.999 9	18.69 60	19.000 0	18.0000	18.7599	19.0000	18.0000
Energy Gap HTM	eV	3.3337	3.601 6	2.8996	3.3337	3.6004	2.8996	3.3337
Electron Mobility HTM	cm ² /V.s	4.5182	0.275 5	2.0000	4.5184	1.2107	2.0000	4.5184
Hole Mobility HTM	cm ² /V.s	361.03 23	3.357 7	200.00 00	360.9900	3.7668	200.0000	360.9900
Absorbtion Coeff. HTM	1/cm.eV ^{1/2}	3.7570	3.061 3	3.1000	3.7569	2.9416	3.1000	3.7569
CB DOS HTM	1/cm ³ (10 ^{value})	19.342 1	19.35 60	18.000 0	19.3420	19.4116	18.0000	19.3420
VB DOS HTM	1/cm ³ (10 ^{value})	18.000 0	18.69 80	19.000 0	18.0000	18.7610	19.0000	18.0000
Affinity Energy HTM	eV	2.0663	1.793 2	2.5000	2.0663	1.7996	2.5000	2.0663
Dielectric Perm. HTM	-	20.000 0	4.124 1	20.000 0	20.0000	4.5051	20.0000	20.0000

Table S3

Full space optimized parameters for CIGS

CIGS for non-toxic ETM		Optimization - Gradient based (fmin)	
Variable	Unit	Without thickness of CIGS absorber	With thickness of CIGS absorber
Thickness ETM	μm	0.010001	0.010124
Donor Conc. ETM	$1/\text{cm}^3 (10^{\text{value}})$	18.998	18.957
Acceptor Conc. ETM	$1/\text{cm}^3 (10^{\text{value}})$	1.4922	0.72606
Energy Gap ETM	eV	2.9982	3.2456
Affinity Energy ETM	eV	4.2035	4.2138
Dielectric Perm. ETM	-	14.857	7.3719
Electron Mobility ETM	$\text{cm}^2/\text{V.s}$	12.484	18.676
Hole Mobility ETM	$\text{cm}^2/\text{V.s}$	382.09	12.841
VB DOS ETM	$1/\text{cm}^3 (10^{\text{value}})$	18.362	18.824
CB DOS ETM	$1/\text{cm}^3 (10^{\text{value}})$	18.001	18.763
Absorbtion Coeff. ETM	$1/\text{cm.eV}^{1/2}$	1001.5	18381
Front Contact Work function	eV	4.2035	4.2138
Thickness CIGS Absorber	μm		3.9999