SURGE'21 Project Abstract for the End-term Report

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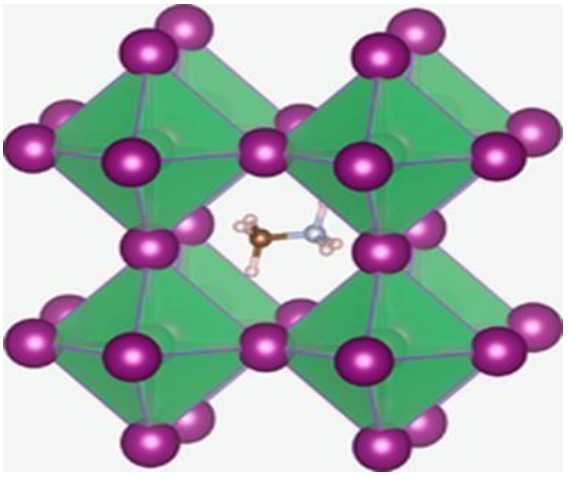
The organic molecule as additives to improve the stability of perovskite solar cells by defect passivation.

A perovskite solar cell is a hybrid type of solar cell that includes a perovskite structured compound, of organic-inorganic lead or tin halid-based material as the light-harvesting active layer.



Crystal structure $CH_3NH_3PbX_3$ perovskites.

The crystal structure of perovskite is of ABX3, Here where A and B are cations and X is halogen ion like Iodide, Bromide, and chloride. The integration of both organic and inorganic hybrid perovskite solar cells had shown great advancement in the efficiency of solar cells in this half-decade.

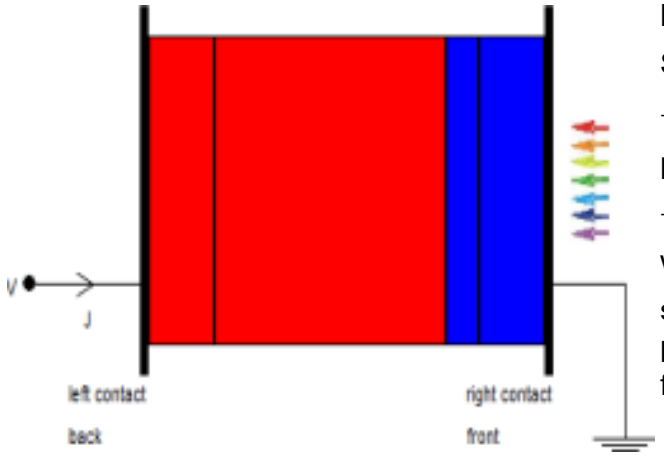
CAS-Cl(Cysteamine hydrochloride) was found to passivate the perovskite solar cell also exhibiting a high-efficiency approach of 21% also it could operate in the open air for a longer period of time and the efficiency of perovskite solar cells remains almost the same.

To get on practical result for this efficiency and all different parameter of a perovskite solar cell which are essential to design an effective and household use it must be stable at the open environment and the efficiency must be retained but due to some defects this is not possible to use and for this, we try to learn SCAPS-1D software through which we get the stimulation of perovskite solar cell different layers with desirable parameter analysis like efficiency, short circuit current density, fill factor, open-circuit voltage. Table 1, in this different parameters and materials, we used in the stimulation of perovskite solar cells

Table1. Stimulation Parameter for SCAPS1-D

Parameter	CuI	CH3NH3SnI3	TiO2	ZnO: Al
Thickness (μm)	0.200	0.700	0.100	0.200

Bandgap(eV)	3.100	1.30	3.260	3.300
Electron affinity(eV)	2.100	4.170	4.200	4.600
Dielectric Permittivity	6.5	6.50	10.0	9.000
CB effective density of states (1/cm3)	2.200E+19	1.000E+18	2.200E+18	2.200E+18
VB effective density of states (1/cm3)	1.800E+19	1.000E+19	1.800E+19	1.800E+19
Electron thermal velocity(cm/S)	1.00E+7	1.00E+6	1.00E+7	1.00E+7
Hole thermal velocity(cm/S)	1.00E+7	1.00E+6	1.00E+7	1.00E+7
Electron mobility(cm2/VS)	1.00E+2	1.60E-+0	1.00E+2	1.00E+2
Hole mobility(cm2/VS)	4.390E+1	1.600E+0	2.500E+1	2.500E+1
Shallow uniform donor density ND (1/cm3)	0	0	1.00E+19	1.00E+18
Shallow uniform acceptor density NA(1/cm3)	1.00E+18	3.200 E+15	0	0



Map for SCAPS-1d simulation:

Start → set illumination state, temperature →set different layers → put different properties (primary and secondary) →Electrical and optical properties along with secondary properties → run stimulation → result (batch calculation for large set of values.) Now extract the python file data to

analyze using MATLAB.

Output

On changing temperature keeping all parameters the same

Temperature(K)	Voc(V)	Jsc(mA/cm2)	FF(%)	Efficiency(%)
300	1.0959	33.774487	81.87	30.30
320	1.0753	33.777699	80.83	29.36
350	1.0435	33.784927	79.17	27.91

On changing HTM layer(CuI) band gap keeping all parameter same

Bandgap(eV)	Voc(V)	Jsc(mA/cm2)	FF(%)	Efficiency(%)
3.100	1.0959	33.774487	81.87	30.30
2.8	1.0960	33.771665	74.09	27.43
2.4	1.0495	33.760658	45.37	16.08

On changing ETM layer() bandgap keeping all parameters same

Bandgap(eV)	Voc(V)	Jsc(mA/cm2)	FF(%)	Efficiency(%)
3.100	1.0959	33.774487	81.87	30.30
3.4	1.0961	33.888587	81.87	30.41
3.6	1.0962	33.968913	81.87	30.49
2.8	1.0941	32.604209	81.87	29.21
2.6	1.0926	31.651596	81.88	28.31

We are further looking to extend this analysis to COMSOL for the 2d solar cell as SCAPS-1d was of one dimension solar cell simulation software so to get better result and analysis with our own physical and material properties to get optimum result on COMSOL as it accept user based designing and manipulation of its different properties of solar cell to get better efficiency and stability to solar cells.

Keywords: Perovskite solar cell, SCAPS-1D, COMSOL, Defects passivation, solar cell.

References :

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