Optimization and Simulation of Perovskite Based Solar Cells: Performance Analysis & Material Selection by SCAPS 1-D

A DISSERTATION

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OF

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IN
PHYSICS

Submitted by:

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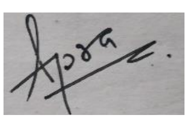

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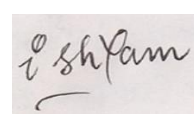

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CERTIFICATE

We hereby certify that the Project Dissertation titled **"Optimization and Simulation of Perovskite Based Solar Cells: Performance Analysis & Material Selection by SCAPS 1-D"** which is submitted by Apra Sancerwal, 2K19/MSCMAT/15, and, Ikshvaku Shyam, 2K19/MSCPHY/16, of Department of Applied Mathematics, Delhi Technological University, Delhi in partialfulfillment of the requirement for the award of the degree of Master of Science, is a record of the project work carried out by the students under my supervision. to the best of our knowledge, this work has not been submitted in part or full for any Degree or Diploma to this University or elsewhere.

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ABSTRACT

There has been a significant efficiency jump in photovoltaic research of Perovskite Solar Cells, which can be credited to Perovskite's optoelectronic properties like tunable band gap and high absorption coefficient. Efficiency depends upon exciton generation, as it is a product function, which in turn depends on the material i.e., a material with low band gap will absorb the light in near IR range. Even though Perovskite materials have high efficiency but they have stability issues in ambient conditions, in addition metal-halide perovskite like $CH_3NH_3PbI_3$ is preferred but lead (Pb) is a toxic element, hence it should be substituted with safer elements like Bismuth or Silicon. In this study, several other perovskite materials ($CH_3NH_3GeI_3$, Cs_2TiBr_6, Cs_2TiI_6 and Cs_2TiCl_6) have been considered and their power conversion efficiency was calculated by numerical simulation using Solar Cell Capacitance Simulator (SCAPS- 1D) software. Other than the perovskite materials itself, the thickness of the materials, defect density and device temperature have also been varied to optimize the parameters. Finally, comparisons have been made to determine the suitable perovskite material against their defect density, layer thickness and device temperature.

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LIST OF ABBREVIATIONS

ETL: Electron Transfer Layer
HTL: Hole Transfer Layer
PVK: Perovskite
PVSC: Perovskite Solar Cell
SCAPS: Solar Cell Capacitance Simulator

CHAPTER 1 INTRODUCTION

1.1 OVERVEIW

Power is an important ingredient to meet the daily need of today's world. The consumption of energy has significantly changed from 1965 to present. In 1965, the major part of North America, Europe and Euro-Asia was responsible for 80% of the world energy consumption. However, after 2015 the Asia pacific region shares a 42% consumption of energy while the America, Europe and Euro Asia together consume a 43% of total energy. The population jumped from 3 billion in 1965 to more than 7 billion today. The increasing population of the world also claims a large amount of energy consumption which results in an increment of 45% average energy consumption throughout the world.

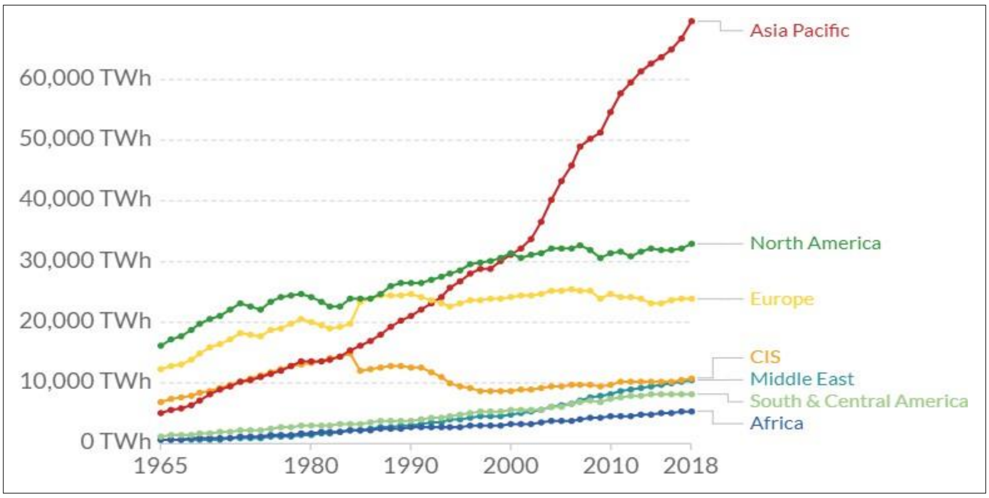

Figure 1.1.1: Primary energy consumption by world region (TWh /year)

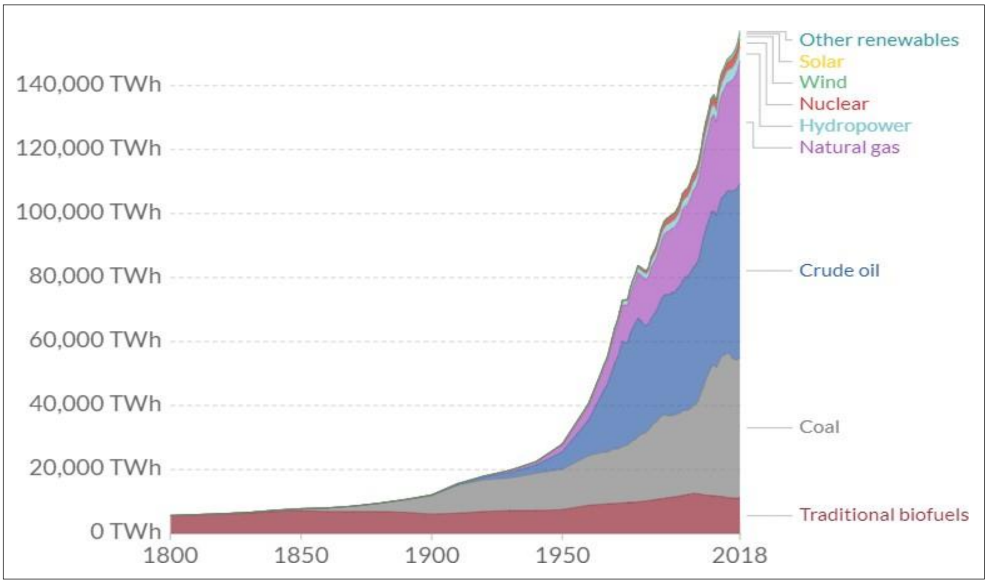

Figure 1.1.2: Global primary energy consumption (TWh /year)

To achieve the required amount of energy we are mainly dependent on the fossil fuels inwhich Oil and coal are the main source of energy. They both constitute a total 60-80% share in energy production. However, we are having a very limited amount of available fossil fuels which requires a huge amount of extracting and refinery cost.

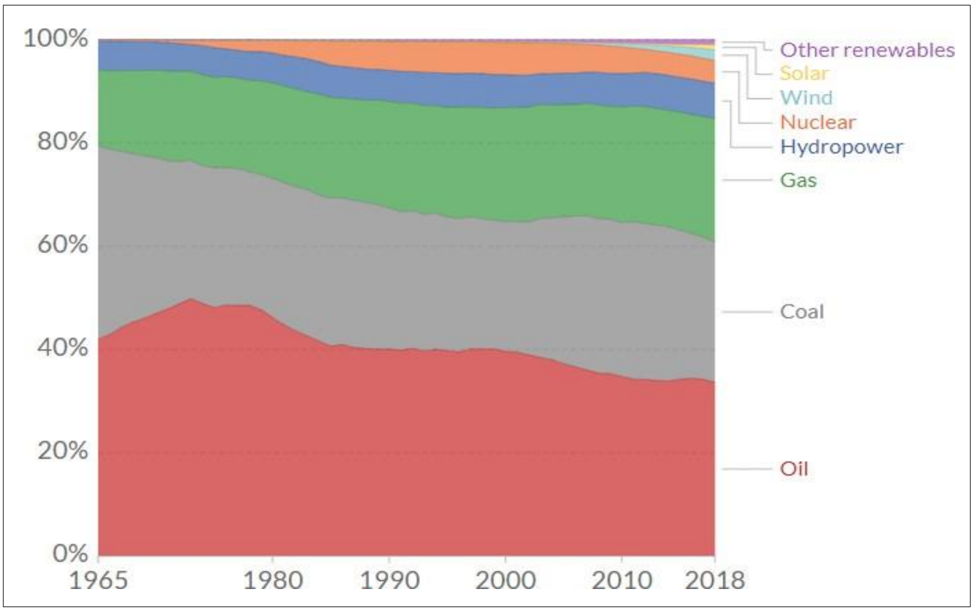

Figure 1.1.3: Energy consumption by source in percentage

In addition of this, they are less efficient and have adverse effect on environment and living beings. The emission of various greenhouse gases like CO_2, Methane etc. leads usto various climatic disadvantages. These gases are the main reason for the globalwarming on earth and depletion of Ozone layer. These consequences of using fossil fuels made researchers to find an alternative. The researchers develop various methods of using renewable energy resources. These resources are nature friendly and can be repeatedly used and replaced naturally.

Solar energy emerged as one of the leading power sources after discovery of photovoltaic (PV) cell. Solar energy has now become the third most source of power generation in the world because it converts the solar radiation into electricity directly. Solar photovoltaic energy shares a 25% of contribution in energy production making it the rapidly evolving power resource. Solar panels are now being used in industries, institutions and households.

1.2 PEROVSKITE SOLAR CELLS

A perovskite is a material that has the same crystal structure as the mineral calcium titanium oxide, the first-discovered perovskite crystal. Generally, perovskite compounds have a chemical formula ABX_3, where ‘A’ and ‘B’ represent cations and X is an anion that bonds to both. A large number of different elements can be combined together to form perovskite structures. Using this compositional flexibility, scientists can design perovskite crystals to have a wide variety of physical, optical, and electrical characteristics. Perovskite crystals are found today in ultrasound machines, memory chips, and now – solar cells.

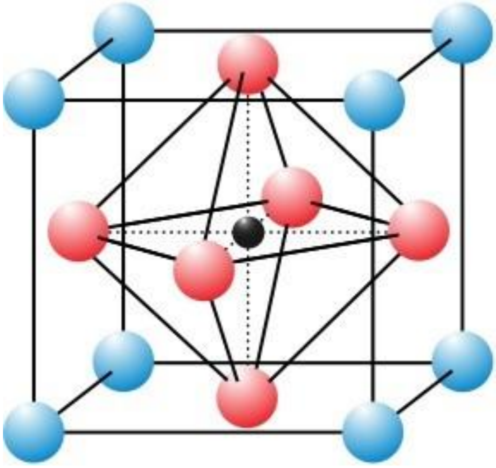

Figure 1.2.1: A schematic structure of a perovskite structure

Perovskites are a group of materials having a unique crystal structure that is named by the mineral that has it. They have showed potential for great performance and inexpensive production costs when utilized to make solar cells.

Absorber materials based on methylammonium lead halide have dominated contemporary research on perovskite solar cells. Despite the fact that perovskite materials have been studied for over a century, research on methylammonium lead halides for semiconductor applications only began in the last twenty years. Perovskite absorbers were first used in solar cells in 2006, and the results were published in 2009. However, because they relied on a corrosive liquid phase that steadily destroyed other layers inside the device, these cells were inefficient (less than 4% efficiency) and unstable. By 2012, liquid-phase components had been replaced with solid-state connections, resulting in a 10% increase in efficiency.

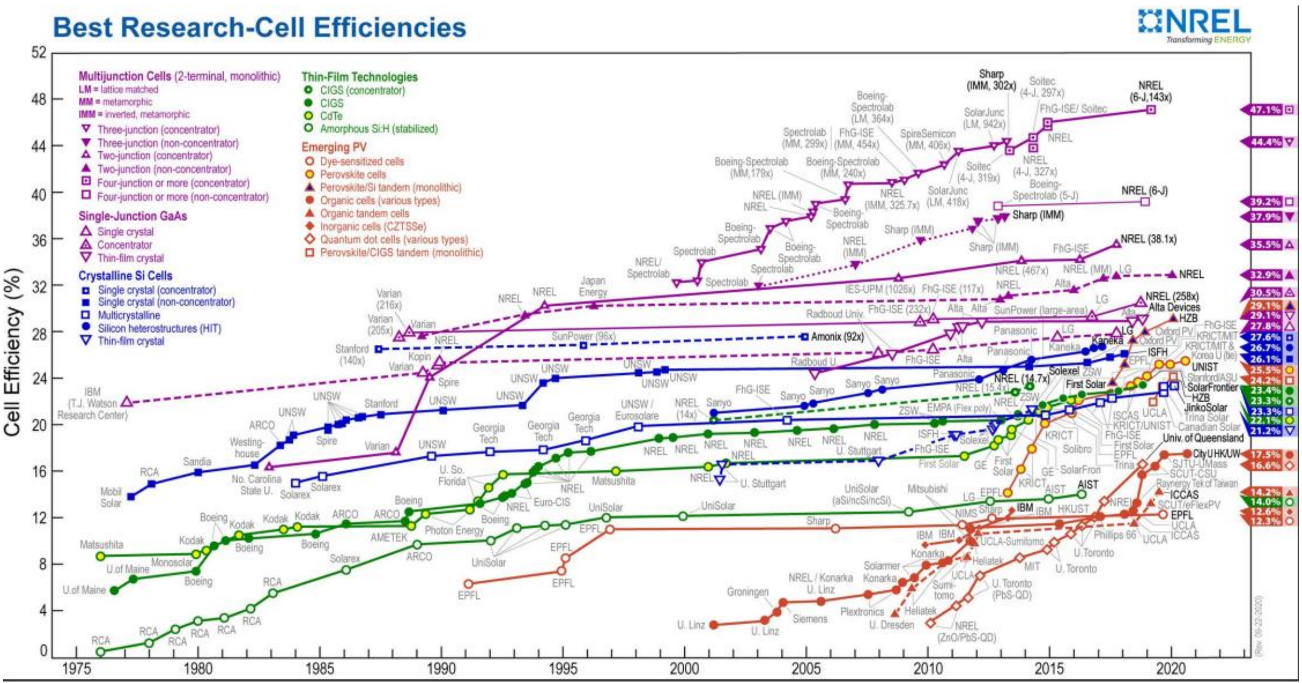

Figure 1.2.2: Solar cells efficiencies over the years

Perovskite Solar Cells (PVSCs) have potential for electricity generation as exhibited by recent findings considering their relatively economical fabrication as compared to conventional solar cells (SLAMI, BOUCHAOUR, & MERAD, 2019). Hence, the research work in this field is flourishing. $CH_3NH_3PbI_3$, especially, is used as a fruitful light harvester (Mandadapu, Vedanayakam, & Thyagarajan, 2017) because of its characteristics like long diffusion length, ideal band gap, fine carrier transport mechanism, easily fabricated on a suitable substrate and tunable band gap (Mola, 2014; Dong, et al., 2015; Xing, et al., 2013; Stranks, et al., 2013). Also, the efficiency of PVSCs has escalated quickly from 3.8% to around 20% in a decade (NREL, Best Research-Cell Efficiencies Chart.). Large scale use of lead halide-based PVSCs is still not prevalent as these cells have toxic Pb; which can be, favorably, swapped with Sn and Ge based halide substances (Abdelaziz, Zekry, Shaker, & Abouelatta, 2020; Singh, Agarwal, & Agarwal , 2020; Nagane, et al., 2018; Huiying, 2019; Serrano-Lujan, et al., 2015). Prior research substantiates the belief that due to the multi-layered structure of PVSCs, junction regulates both the stability and the efficiency of the solar cell (SLAMI, BOUCHAOUR, & MERAD, 2019). This study looks into the effects of different layer properties (thickness, defect densities) and the impact of device temperature on different PVSCs is observed. It is based on numerical simulation by SCAPS-1D software as simulation saves experimental effort (Burgelman, Decock, Niemegeers, Verschraegen, & Degrave, 2020; Hima, Nacereddine, & ACHOUR, Effect of Electron Transporting Layer on Power Conversion Efficiency of Perovskite-Based Solar Cell: Comparative Study, 2019; Husainat, Ali, Cofie, Attia, & Fuller, 2019).

CHAPTER 2 SCAPS 1-D AND SIMULATION

SCAPS (a Solar Cell Capacitance Simulator) is a one-dimensional solar cell simulation programme developed at the. Department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium. SCAPS is a 1-D solar cell simulation software, which is used to simulate the behavior of photovoltaic structures (Burgelman, Decock, Niemegeers, Verschraegen, & Degrave, 2020). It has distinct electrical calibrations for dark and light mode of illumination and different temperatures. Using this program, the values at variable temperatures can be easily estimated.

Figure 2.1: SCAPS 1-D working process

SCAPS is a Windows-oriented program, developed with LabWindows/CVI of National Instruments. We use here the LW/CVI terminology of a 'Panel' (names used in other softwares are: a window, a page, a pop-up…). SCAPS opens with the 'Action Panel'.

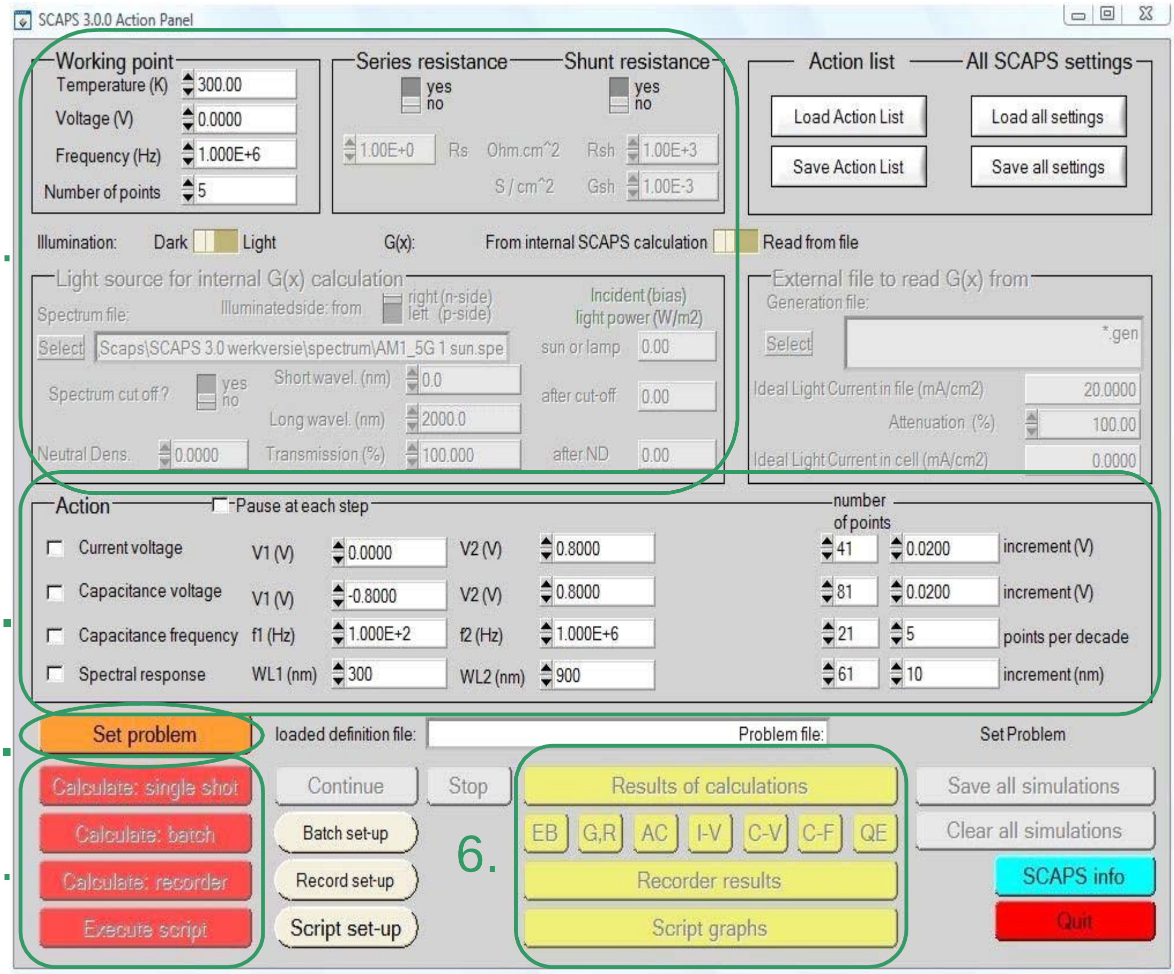

Figure 2.2: SCAPS 1-D Action Panel

There are dedicated panels for the basic actions:

1. Run SCAPS
2. Define the problem, thus the geometry, the materials, all properties of your solar cell
3. Indicate the circumstances in which you want to do the simulation, i.e. specify the working point
4. Indicate what you will calculate, i.e. which measurement you will simulate.
5. Start the calculation(s)
6. Display the simulated curves

The Action Panel of SCAPS 1-D, where initial parameters like temperature and solar spectrum are set before creating junction solar layered solar cell. To create layers in solar cells, “Set problem” is used.

To create layers the parameters of all the layers inserted and the layer is created by pressing "Add".

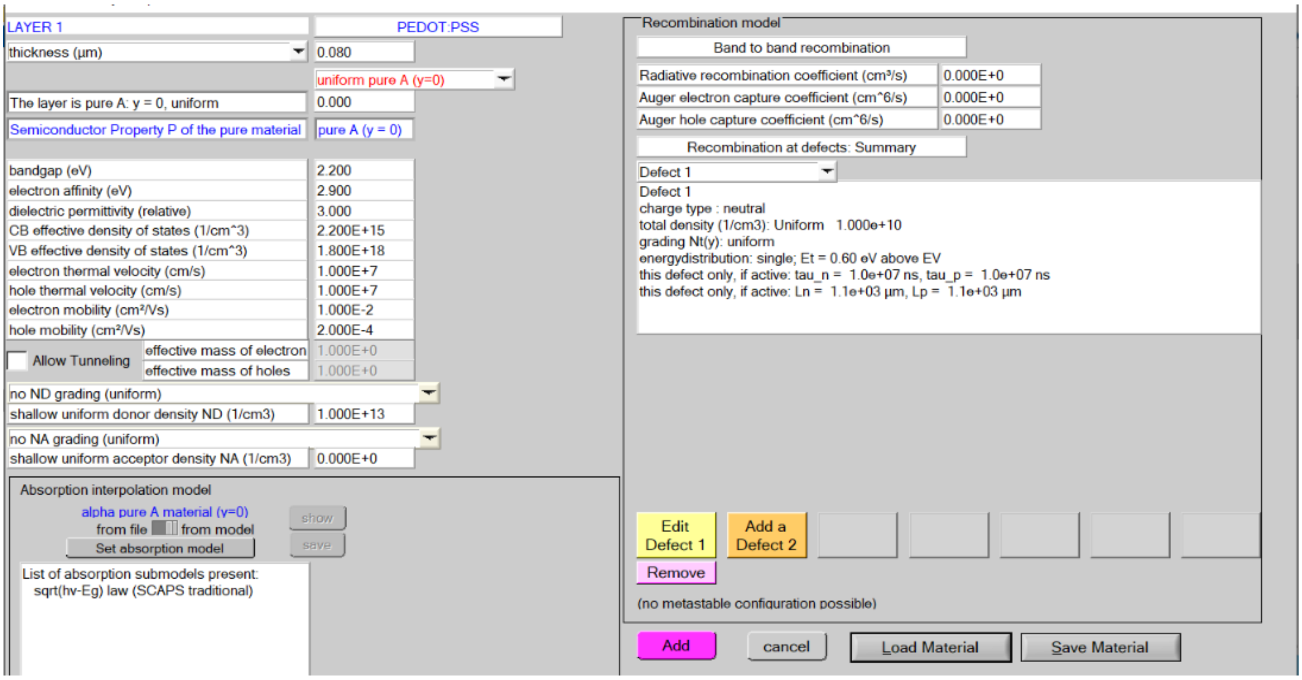

Figure 2.3: Layer Creation in SCAPS 1-D

After layers are created and direction of the light rays falling in the solar cells are decided. The layers are saved and loaded in solar cell definition panel.

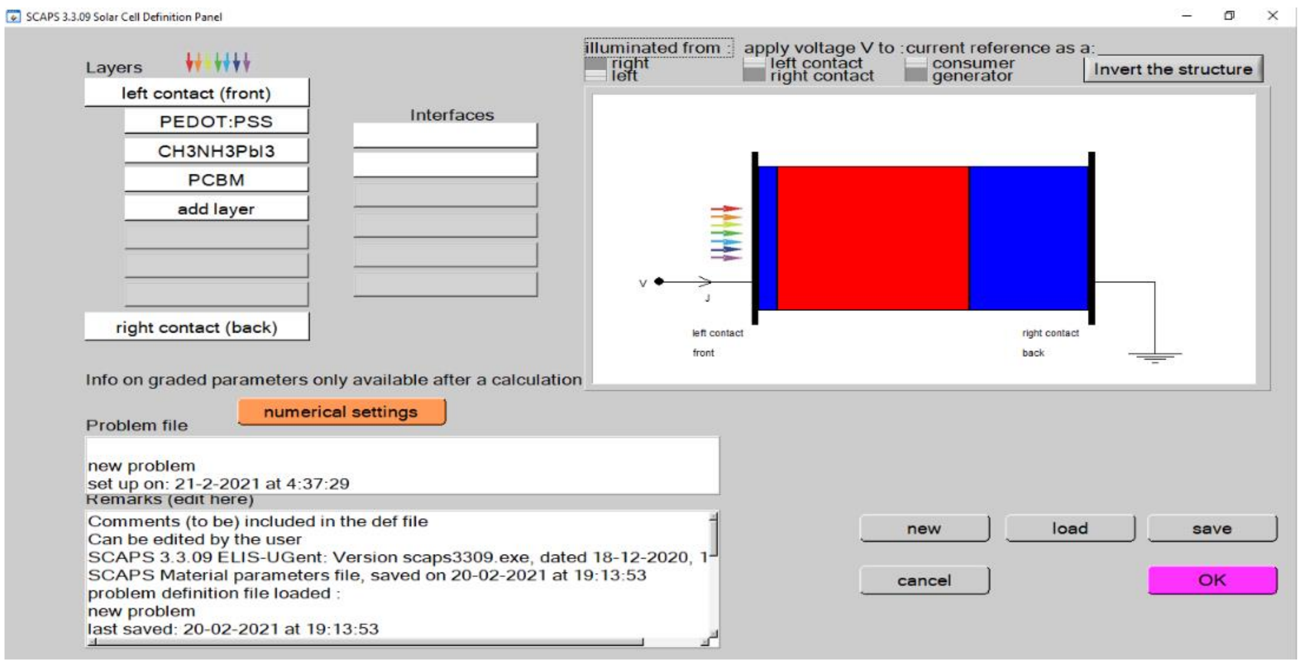

Figure 2.4: Solar Cell Definition Panel

After we create all our layers and load it to SCAPS 1-D, we press “calculate single shot” from Action Panel to optimize the layered solar cell.

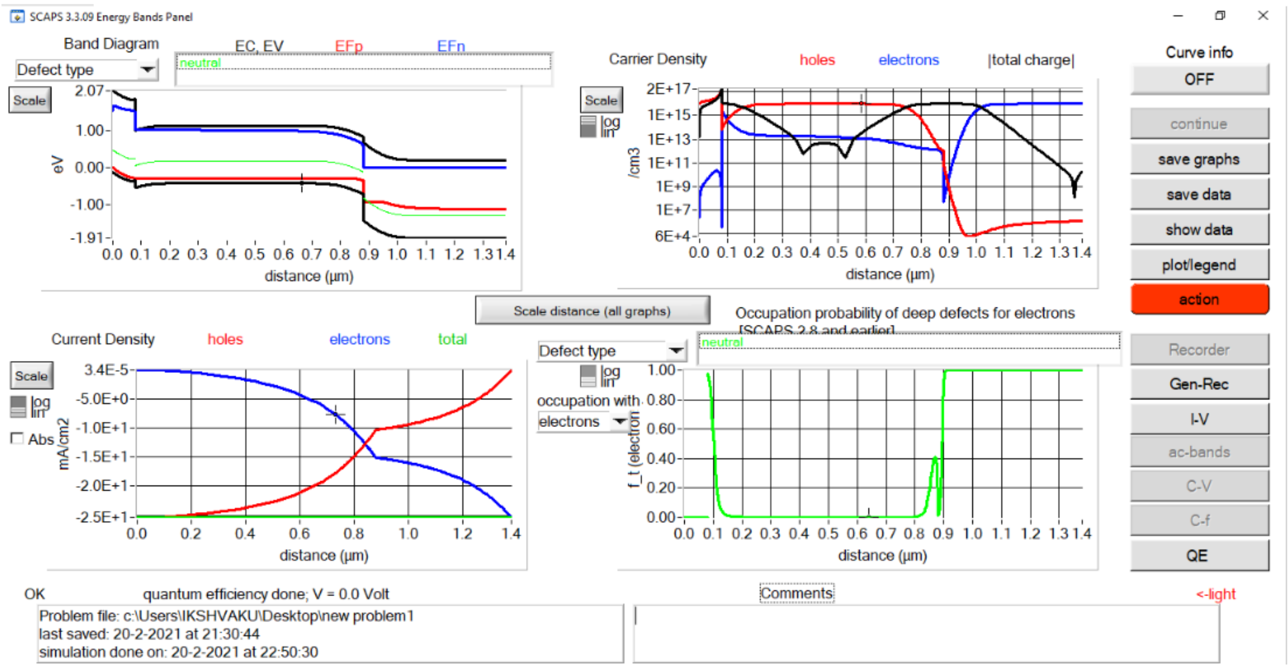

Figure 2.5: Energy Band Panel

Depending on the number of layers the solar cell has, it takes some and optimizes the solar cell and shows efficiency, fill factors etc.

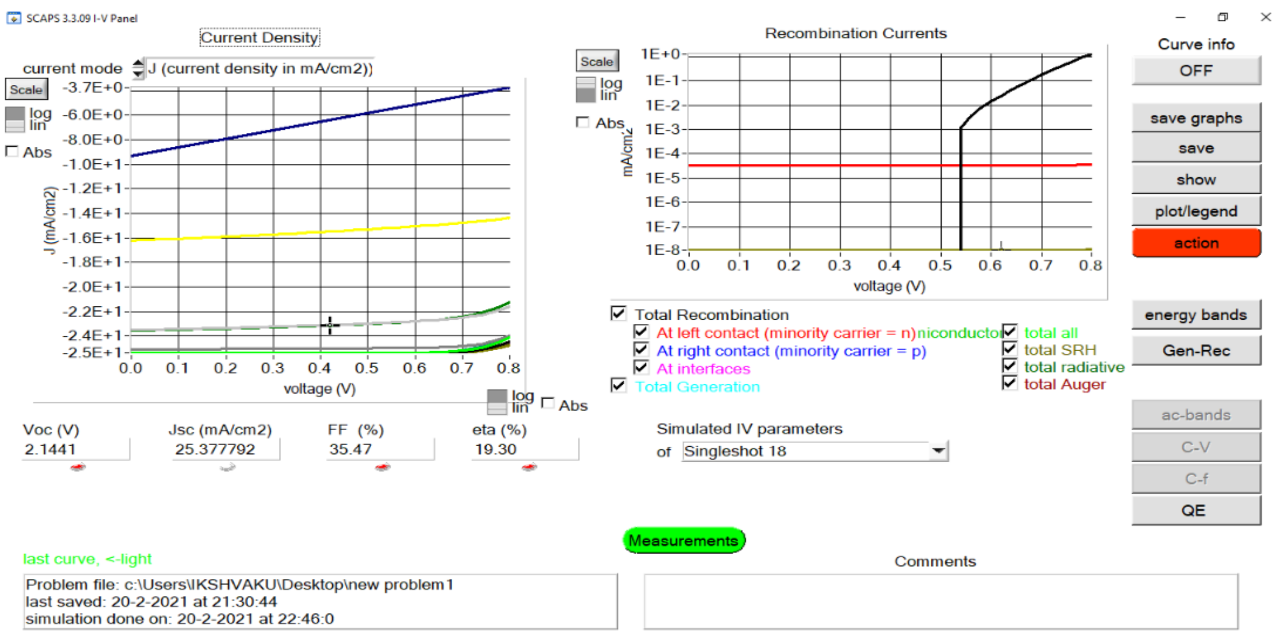

Figure 2.6: Results Panel

The detailed report is obtained from the result panel.

Select scaps3309

```
SCAPS 3.3.09 ELIS-UGent: Version scaps3309.exe, dated 18-12-2020, 16:03:28

Simulation of I-V curves

Single shot simulation #        7

Calculation started :   28-5-2021 at 20:45:20


problem definition file :       new problem

last saved:     28-05-2021 at 20:49:25


Calculation under illumination

Optical generation from internal SCAPS calculation

Illumination spectrum read from file

spectrum file :

C:\Users\spectrum\AM1_5G 1 sun.spe  last saved:        22-05-2009 at 14:59:48

Neutral density filter: ND        0.0000

Transmission of ND filter:        1.0000e+00

Power from spectrum:      100.0000      mW/cm2

Incident power on solar cell structure    100.0000      mW/cm2


Working point conditions

Temperature       300.00        K

Workpoint bias voltage      0.0000      Volt

Frequency         1.0000e+06    Hz
```

scaps3309

```
Voltage reference convention: voltage referred to right contact, voltage V applied to left contact

Current reference convention: current positive when entering the left contact
Power generated by the cell: = -V*I; power consumed by the cell = +V*I


    v(V)        jtot(mA/cm2)    j_total_rec(mA/cm2)     j_total_gen(mA/cm2)        jbulk(mA/cm2)        jifr(mA/cm2)            jminor_left(mA/cm2)     jminor_right(mA/
cm2)    j_SRH(mA/cm2)    j_Radiative(mA/cm2)     j_Auger(mA/cm2)


   0.000000        -1.62216082e+01           9.16709894e+00     2.53881968e+01         8.77623667e+00         0.00000000e+00         3.90863154e-01         -8.81
160249e-07           8.77623667e+00       0.00000000e+00     0.00000000e+00

   0.020000        -1.61909191e+01           9.19785979e+00     2.53881968e+01         8.80611122e+00         0.00000000e+00         3.91749443e-01         -8.81
013798e-07           8.80611122e+00       0.00000000e+00     0.00000000e+00

   0.040000        -1.61598699e+01           9.22890899e+00     2.53881968e+01         8.83627239e+00         0.00000000e+00         3.92637480e-01         -8.80
863636e-07           8.83627239e+00       0.00000000e+00     0.00000000e+00

   0.060000        -1.61284558e+01           9.26032436e+00     2.53881968e+01         8.86678491e+00         0.00000000e+00         3.93540338e-01         -8.80
709021e-07           8.86678491e+00       0.00000000e+00     0.00000000e+00

   0.080000        -1.60966609e+01           9.29211885e+00     2.53881968e+01         8.89766092e+00         0.00000000e+00         3.94458811e-01         -8.80
549212e-07           8.89766092e+00       0.00000000e+00     0.00000000e+00

   0.100000        -1.60644785e+01           9.32430430e+00     2.53881968e+01         8.92891173e+00         0.00000000e+00         3.95393451e-01         -8.80
383011e-07           8.92891173e+00       0.00000000e+00     0.00000000e+00

   0.120000        -1.60318875e+01           9.35689296e+00     2.53881968e+01         8.96054901e+00         0.00000000e+00         3.96344830e-01         -8.80
208076e-07           8.96054901e+00       0.00000000e+00     0.00000000e+00

   0.140000        -1.59988819e+01           9.38989761e+00     2.53881968e+01         8.99258494e+00         0.00000000e+00         3.97313547e-01         -8.80
021301e-07           8.99258494e+00       0.00000000e+00     0.00000000e+00

   0.160000        -1.59654509e+01           9.42333199e+00     2.53881968e+01         9.02503262e+00         0.00000000e+00         3.98300245e-01         -8.79
817533e-07           9.02503262e+00       0.00000000e+00     0.00000000e+00

   0.180000        -1.59315659e+01           9.45721119e+00     2.53881968e+01         9.05790645e+00         0.00000000e+00         3.99305619e-01         -8.79
588417e-07           9.05790645e+00       0.00000000e+00     0.00000000e+00
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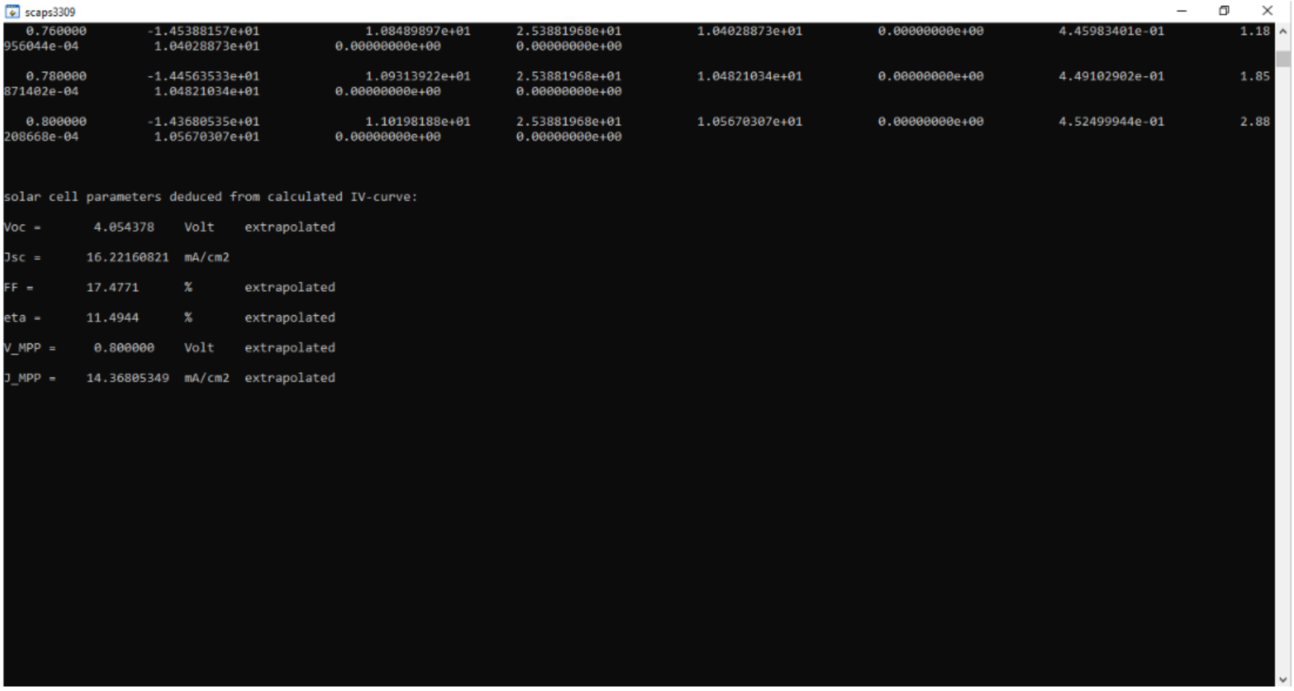


Figure 2.7: Detailed readings after optimization of solar cell

CHAPTER 3 OPTIMISING PEROVSKITE SOLAR CELLS

There are 3 layers in the solar cells under consideration: PEDOT:PSS (Hole Transfer Layer), PVK layer (Perovskite layer) and PCBM (Electron Transfer layer).

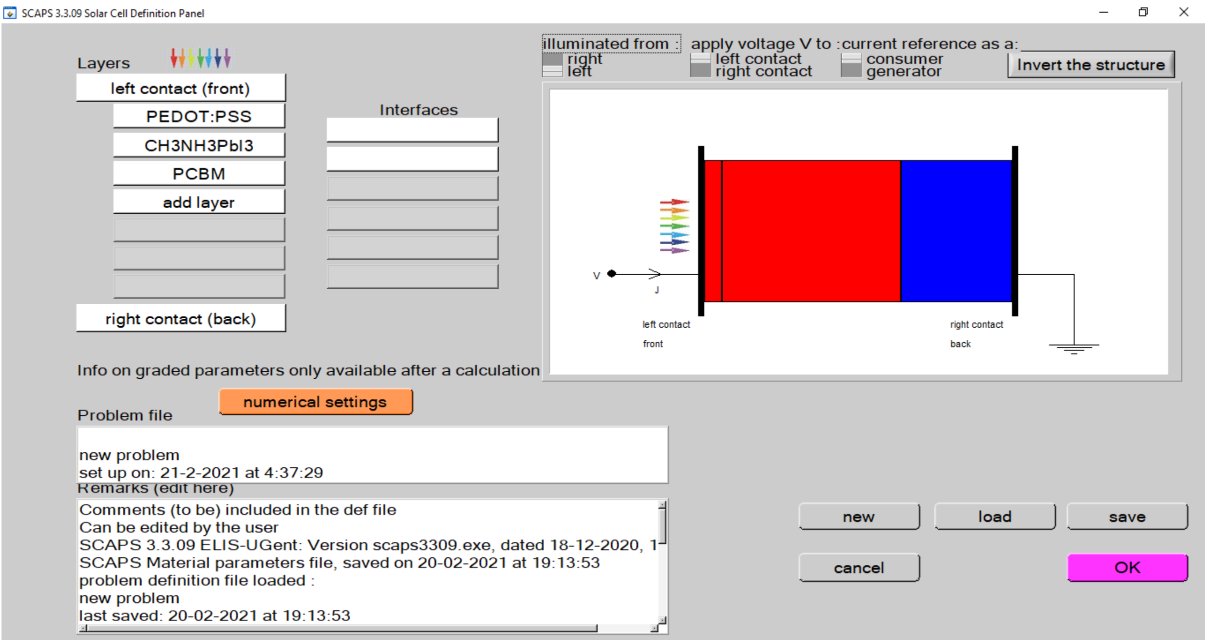


Figure 3.1: Light Coming from Left-Hand Side to the solar cell

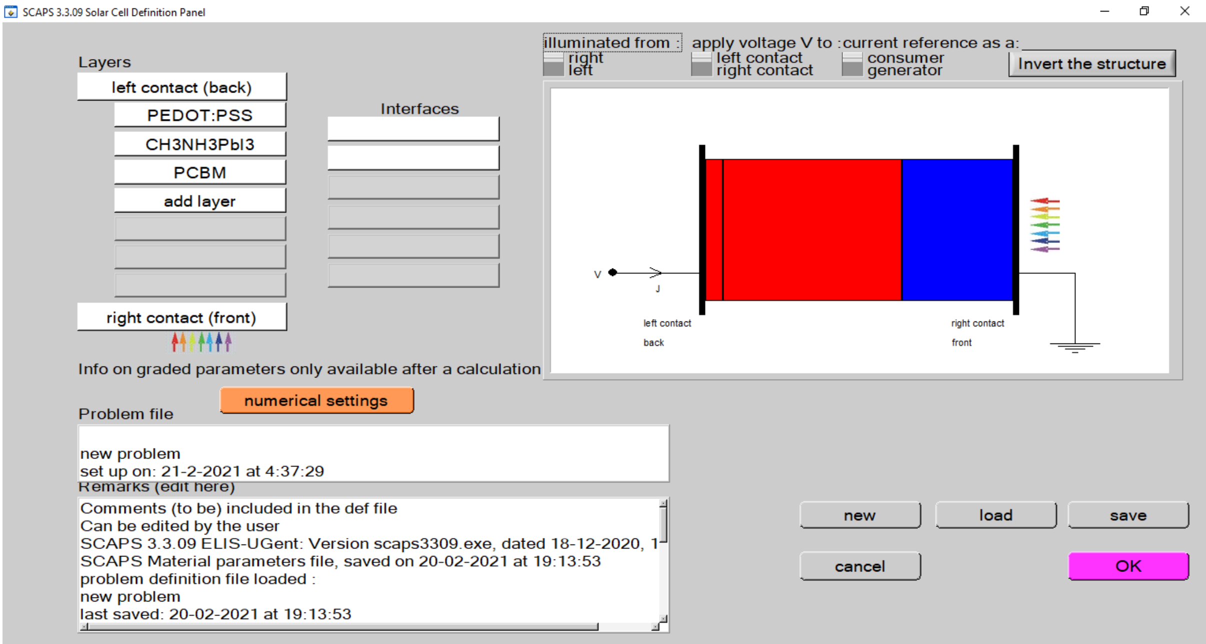


Figure 3.2: Light Coming from Right-Hand Side to the solar cell

The perovskite solar cells were step by step optimized and their variation were noted to study the efficiency of the solar cell on layer thickness, defect density and device temperature.

3.1. LEAD PEROVSKITE ($CH_3NH_3PbI_3$)

(a) Study of dependence of defect density vs efficiency.

TABLE:3.1.1 PVK variation of efficiency vs defect density, keeping the defect density of HTL=0 and ETL =0 when light is coming from ETL side

Defect Density(1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
10000000000		25.147912		20.12
1E+11		25.146742		20.12
1E+12		25.135051		20.1
1E+13		25.018641		19.97
1E+14		23.902836		18.76
1E+15	4.1281	23.902836	17.17	11.46

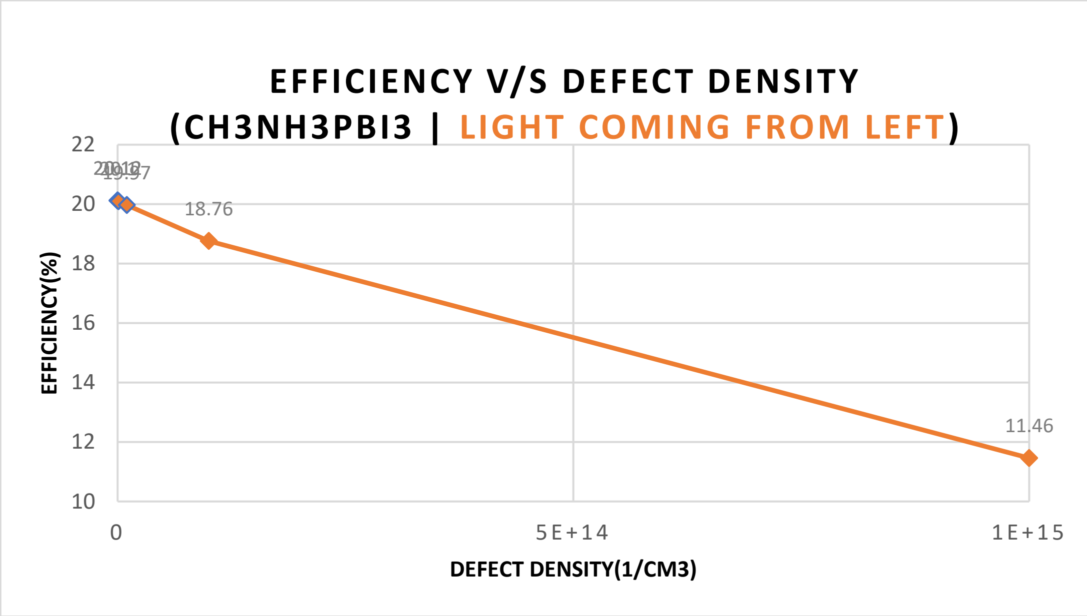


Figure 3.1.1: Efficiency-Defect density graph in $CH_3NH_3PbI_3$ when light is coming from Left-Hand Side to the solar cell

TABLE:3.1.2 PVK variation of efficiency vs defect density, keeping the defect density of HTL=0 and ETL =0 when light is coming from HTL side

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
10000000000	2.1441	25.377762	35.47	19.3
1E+11	2.1441	25.377495	35.47	19.3
1E+12	2.144	25.374823	35.47	19.3
1E+13	2.1428	25.348269	35.46	19.26
1E+14	2.1326	25.097613	35.39	18.94
1E+15	1.993	24.559817	35.21	18.91

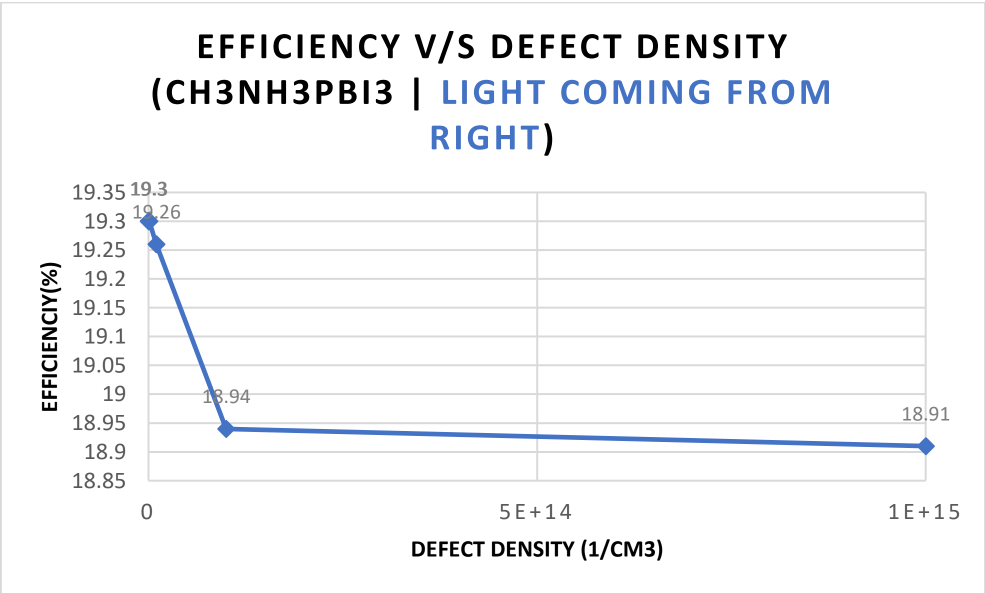


Figure 3.1.2: Efficiency-Defect graph in $CH_3NH_3PbI_3$ when light is coming from Right-Hand Side to the solar cell

(b) Solar cell variation of efficiency vs defect density.

TABLE:3.1.3 Solar cell variation of efficiency vs defect density, keeping the defect density when light coming from ETL side

Defect Density(1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	eta (%)
10000000000		25.141044		20.11
1E+11		25.139823		20.11
1E+12		25.127624		20.1
1E+13		25.006145		19.96
1E+14		23.841036		18.71
1E+15	4.0602	15.786278	17.44	11.18

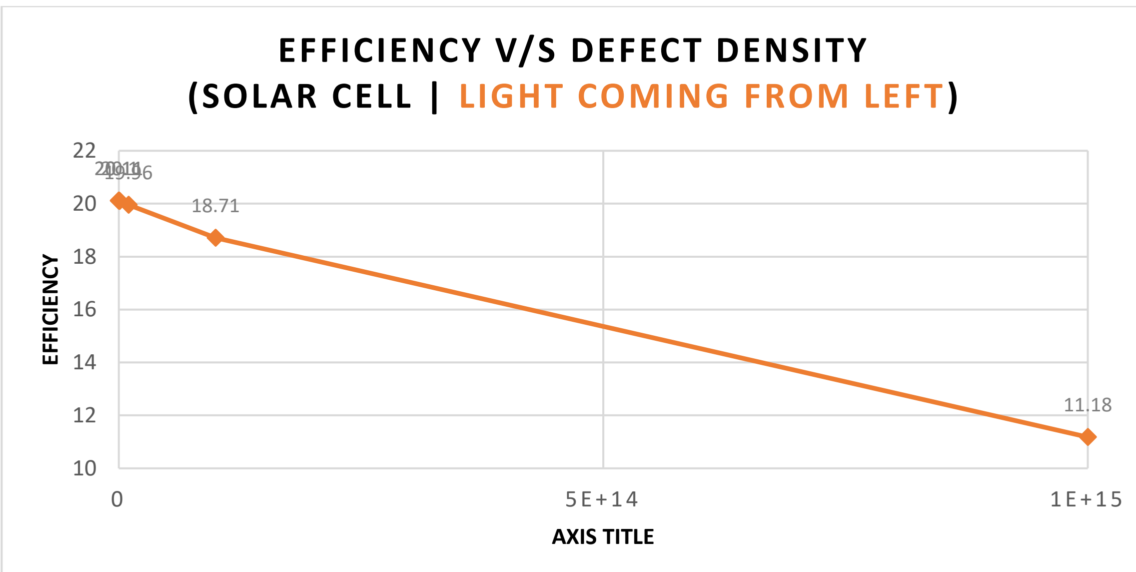


Figure 3.1.3: Efficiency-Defect density graph in Solar cell when light is coming from Left-Hand Side to the solar cell

TABLE:3.1.4 Solar cell variation of efficiency vs defect density, keeping the defect density when light coming from HTL side

Defect Density(1/cm^3)	V_{oc}	Jsc (mA/cm^2)	FF(%)	eta (%)
10000000000	2.0852	25.37777	36.33	19.23
1E+11	2.0852	25.377505	36.33	19.23
1E+12	2.0852	25.374853	36.33	19.22
1E+13	2.0838	25.348492	36.33	19.19
1E+14	2.0727	25.09959	36.27	18.87
1E+15	2.0438	23.560599	35.41	17.05

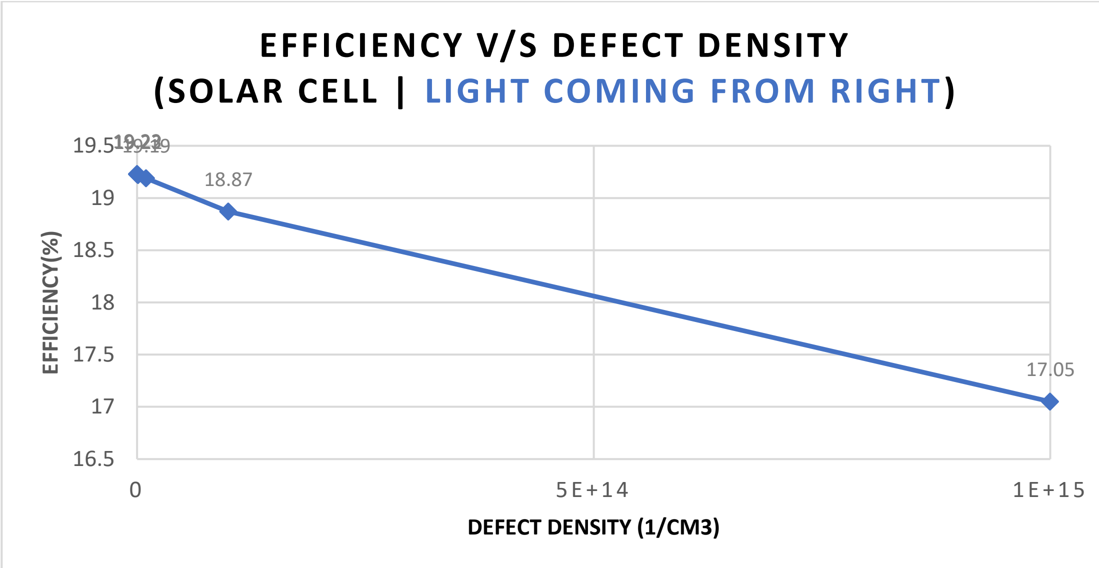


Figure 3.1.4: Efficiency-Defect density graph in solar cell when light is coming from Right-Hand Side to the solar cell

OBSERVATION

The efficiency of the solar cell and the respective layers decreases with gradual increase in defect density. The maximum efficiency is observed at $1 * 10^{10}\ (cm^{-3})$ defect density in each layer and in the whole solar cell.

(c) Study of dependence of efficiency vs thickness

At temperature = 298 K and defect density = $1 * 10^{10}\ (cm^{-3})$, since maximum efficiency in previous observations is observed at $1 * 10^{10}\ (cm^{-3})$.

TABLE: 3.1.5 PVK variation of efficiency vs thickness, keeping the thickness of HTL= 0.05 µm and ETL =0.5 µm when light is coming from ETL side

Thickness (µm)	Voc	Jsc(mA/cm2)	FF(%)	eta(%)
0.3		20.991258		16.78
0.4		22.463132		17.96
0.5		23.451225		18.76
0.6		24.12828		19.3
0.7		24.601877		19.68
0.8		24.939718		19.95
0.8		25.185051		20.15
1		25.366435		20.29

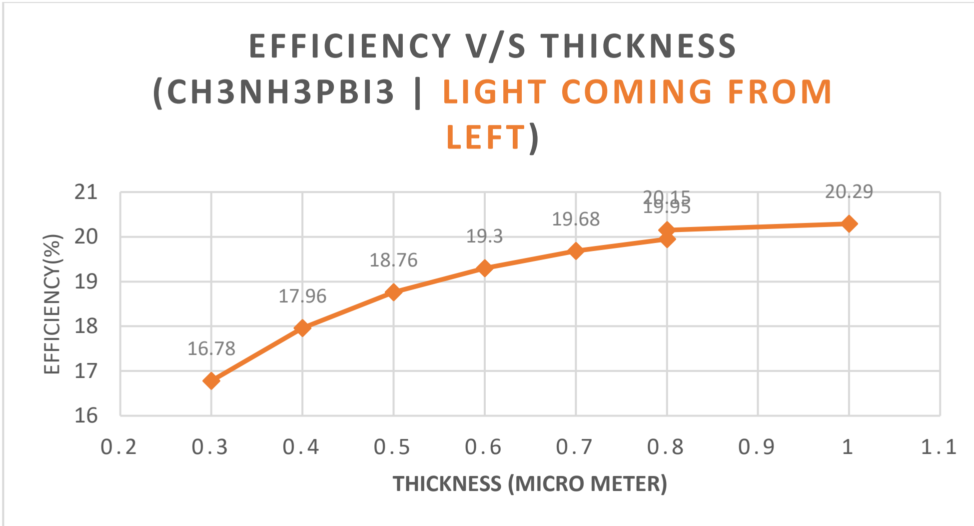


Figure 3.1.5: Efficiency-Thickness graph in $CH_3NH_3PbI_3$ layer when light is coming from Left-Hand Side to the solar cell

TABLE: 3.1.6 PVK variation of efficiency vs thickness, keeping the thickness of HTL= 0.05 µm and ETL =0.5 µm when light is coming from HTL side

Thickness (µm)	Voc	Jsc(mA/cm2)	FF(%)	eta(%)
0.3		21.502597		17.16
0.4		22.946273		18.31
0.5		23.915299		19.08
0.6		24.579918		19.6
0.7		25.045286		19.97
0.8		25.377542		20.24
0.9		25.619209		20.45
1		25.797463		20.57

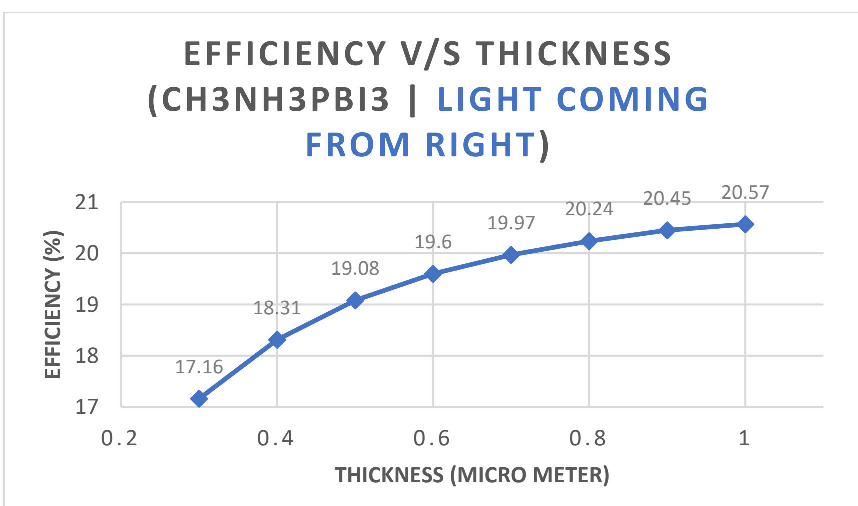


Figure 3.1.6: Efficiency-thickness density graph in $CH_3NH_3PbI_3$ layer when light is coming from Left-Hand Side to the solar cell

(d) Study of dependence of efficiency vs temperature

At defect density = $1 * 10^{10}$ (cm^{-3}), since, maximum efficiency in previous observations is observed at $1 * 10^{10}$ (cm^{-3}).
At thickness of HTL=0.07 µm, PVK=1.0 µm and ETL= 0.3 µm.

TABLE: 3.1.7 Solar cell variation of efficiency vs temperature when light is coming from ETL side

Temperature (K)	Voc	Jsc(mA/cm2)	FF(%)	eta(%)
263		25.590808		20.47
268		25.583791		20.47
273		25.576813		20.46
278		25.569732		20.46
283		25.562554		20.46
288		25.553111		20.44
293		25.54797		20.44
298		25.540566		20.43
303		25.533104		20.43
308		25.525601		20.42
313		25.518102		20.41
318		25.510566		20.41

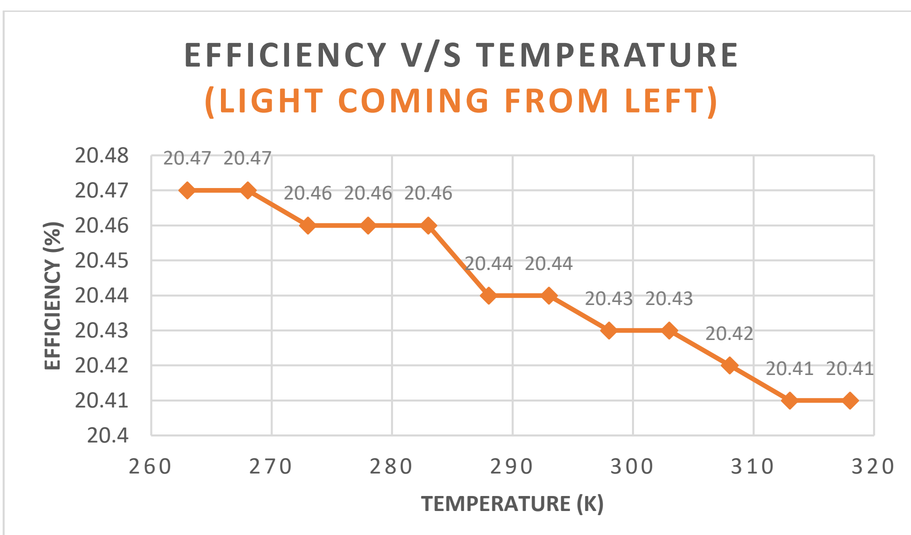


Figure 3.1.7: Efficiency-temperature graph in solar cell when light is coming from Left-Hand Side to the solar cell

TABLE: 3.1.8 Solar cell variation of efficiency vs temperature when light is coming from HTL side

Temperature (K)	Voc	Jsc(mA/cm2)	FF(%)	eta(%)
263	7.0334	25.795935	11.2	20.47
268	7.6578	25.795936	10.37	20.48
273	8.3314	25.795954	9.54	20.49
278	9.0299	25.79611	8.8	20.5
283	9.7663	25.79612	8.14	20.51
288		25.796121		20.52
293		25.796169		20.53
298		25.796169		20.54
303		25.796175		20.54
308	3.3825	25.796172	23.08	20.14
313	3.6054	25.707047	21.7	20.18
318	3.841	25.797048	20.4	20.21

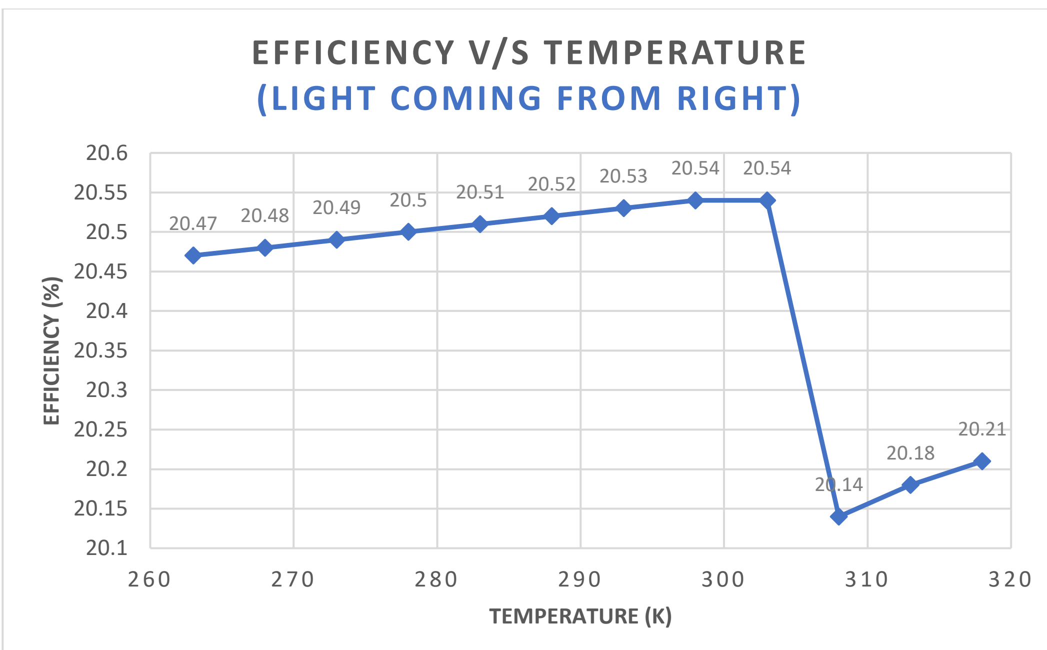


Figure 3.1.8: Efficiency-temperature graph in solar cell when light is coming from Right-Hand Side to the solar cell

OBSERVATION

The efficiency of the solar cell decreases with gradual increase in the temperature.

3.2. BROMINE PEROVSKITE (Cs_2TiBr_6)

(a) Study of dependence of defect density vs efficiency.

At temperature = 298 K, HTL thickness (0.08 µm), PVK thickness (200 nm) andETL thickness (0.5 µm).

TABLE: 3.2.1 PVK variation of efficiency vs defect density, keeping the defect density of HTL=0 and ETL =0 when light is coming from HTL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
1.00E+09		4.420862		3.53
1.00E+10		4.420855		3.53
1.00E+11		4.420788		3.53
1.00E+12		4.420116		3.53
1.00E+13		4.413407		3.52
1.00E+14		4.347327		3.47
1.00E+15		3.774729		3.01

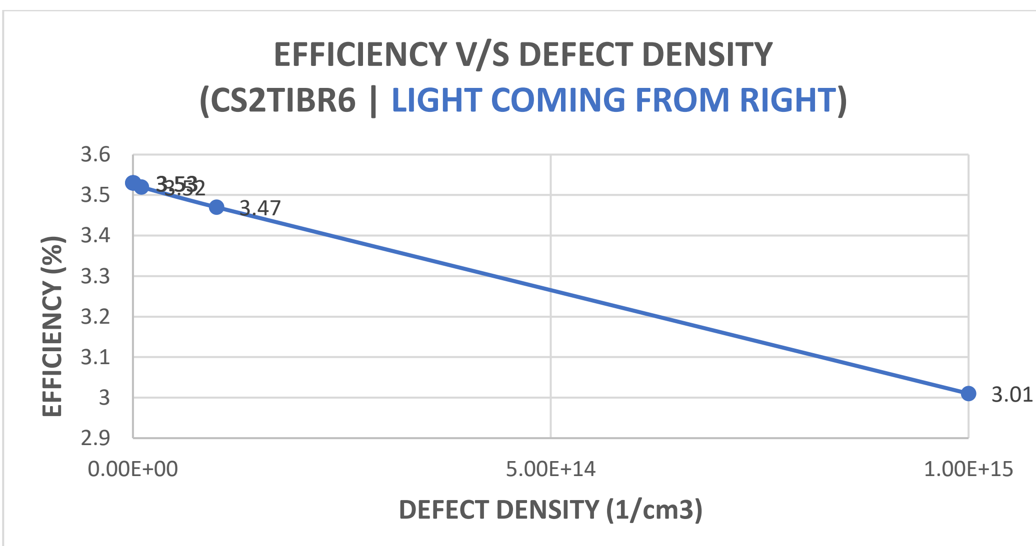


Figure 3.2.1: Efficiency-Defect density graph in Cs_2TiBr_6 when light is coming from Right-Hand Side to the solar cell.

TABLE: 3.2.2 PVK variation of efficiency vs defect density, keeping the defect density of HTL=0 and ETL =0 when light is coming from ETL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
1.00E+09	6.7518	9.669603	11.37	7.42
1.00E+10	6.7518	9.669596	11.37	7.42

1.00E+11	6.7517	9.66953	11.37	7.42
1.00E+12	6.7509	9.668874	11.37	7.42
1.00E+13	6.7425	9.662315	11.38	7.42
1.00E+14	6.6707	9.597638	11.5	7.36
1.00E+15	5.9863	9.029961	12.76	6.9

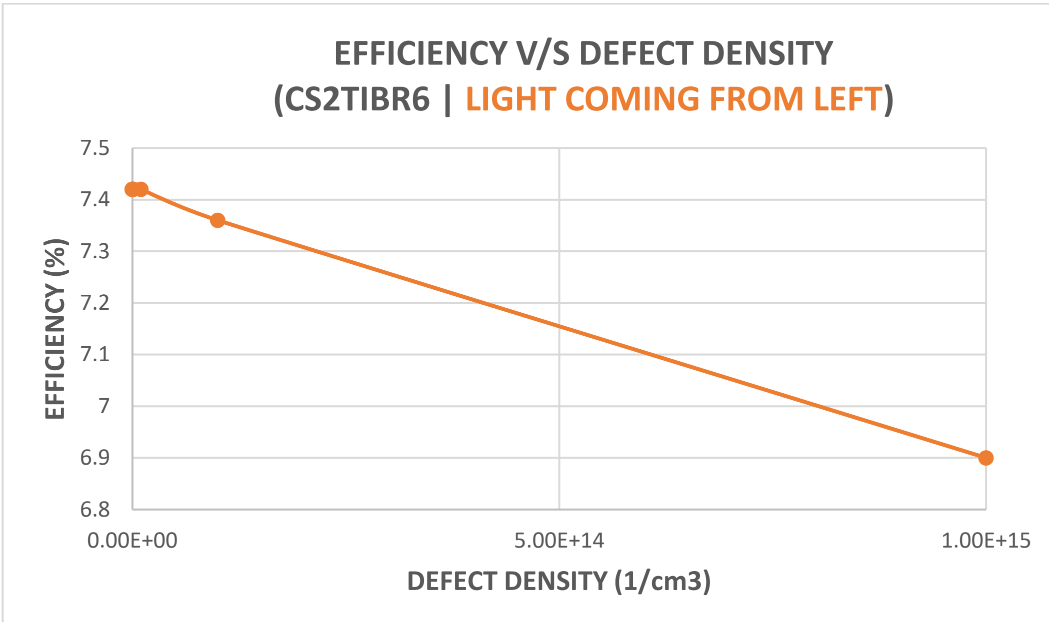


Figure 3.2.2: Efficiency-Defect density graph in Cs_2TiBr_6 layer when light is coming from Left-Hand Side to the solar cell.

(b) Solar cell variation of efficiency vs defect density.

TABLE:3.2.3 Solar cell variation of efficiency vs defect density, keeping the defect density when light coming from ETL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
1.00E+09	6.7518	9.669602	11.37	7.42
1.00E+10	6.7517	9.669595	11.37	7.42
1.00E+11	6.7508	9.66952	11.37	7.42
1.00E+12	6.7414	9.668775	11.39	7.42
1.00E+13	6.6492	9.661329	11.54	7.41
1.00E+14	5.8927	9.587812	12.97	7.33
1.00E+15	3.3755	8.934843	21.84	6.59

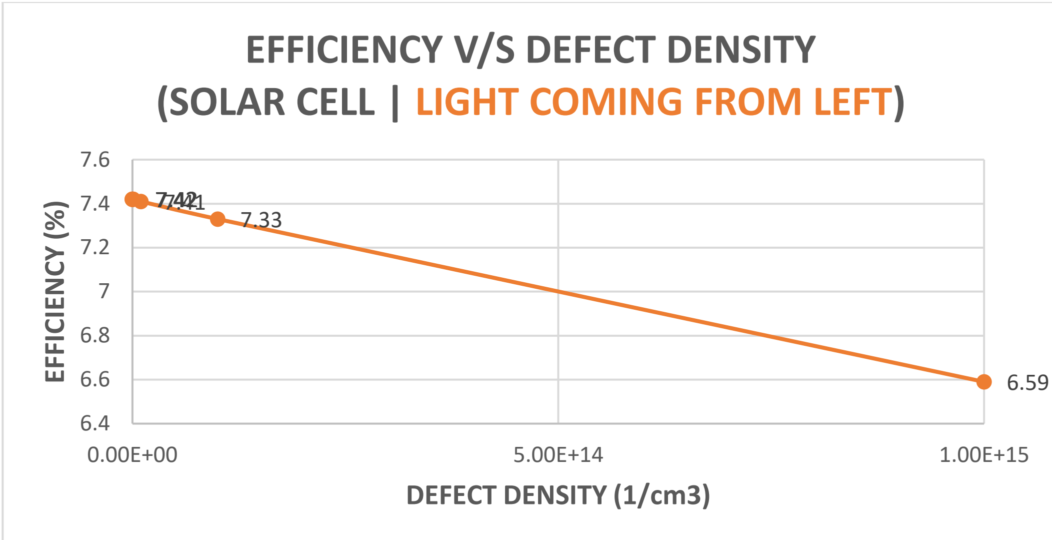


Figure 3.2.3: Efficiency-Defect density graph in Solar cell when light is coming from Left-Hand Side to the solar cell

TABLE:3.2.4 Solar cell variation of efficiency vs defect density, keeping the defect density when light coming from HTL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
1.00E+09		4.420862		3.53
1.00E+10		4.420855		3.53
1.00E+11		4.420787		3.53
1.00E+12		4.420105		3.53
1.00E+13		4.413295		3.52
1.00E+14		4.346237		3.47
1.00E+15		3.765821		3

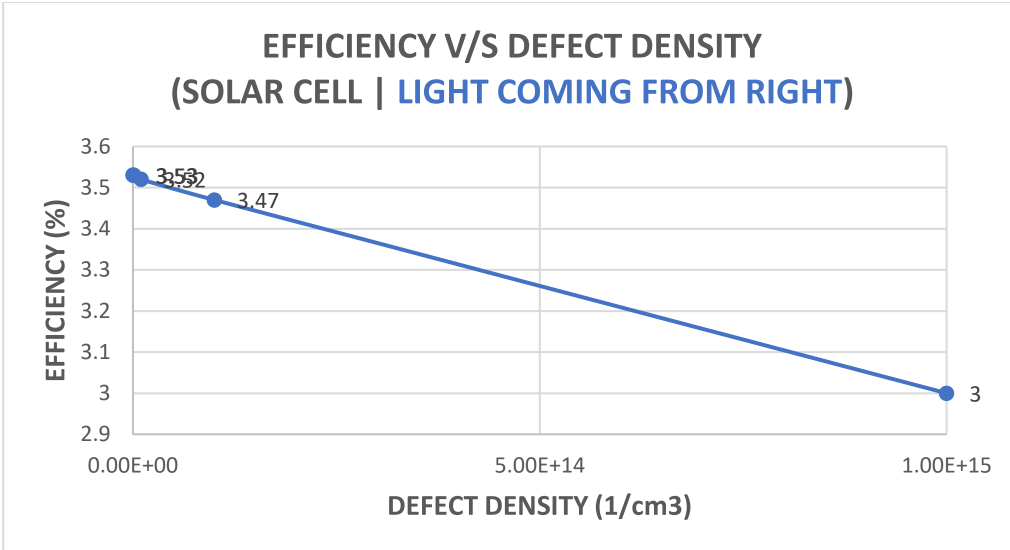


Figure 3.2.4: Efficiency-Defect density graph in Solar cell when light is coming from Right-Hand Side to the solar cell

OBSERVATION

The efficiency of the solar cell and the respective layers decreases with gradual increase in defect density. The maximum efficiency is observed at $1 * 10^{10}$ (cm^{-3}) defect density in each layer and in the whole solar cell.

(b) Study of dependence of efficiency vs thickness.

At temperature = 298 K and defect density = $1 * 10^{10}$ (cm^{-3}), since maximumefficiency in previous observations is observed at $1 * 10^{10}$ (cm^{-3}).

TABLE: 3.2.5 PVK variation of efficiency vs thickness, keeping the thickness of HTL= 0.5 μm and ETL =0.5 μm when light is coming from ETL side.

Thickness (nm)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
100		10.941967		8.63
150	8.2502	11.453473	9.5	8.98
200	6.4997	11.941324	11.98	9.3
250	5.4776	12.390839	14.09	9.56
300	4.7406	12.800154	16.13	9.79
350	4.4302	13.171234	17.11	9.98
400	4.1717	13.507378	18.01	10.15
450	3.9823	13.811856	18.71	10.29
500	3.8363	14.088162	19.27	10.41
550	3.7578	14.339453	19.53	10.52
800	3.5384	15.308645	20.18	10.93

1000	3.4861	15.8455	20.2	11.16
1100	3.4457	16.060572	20.32	11.25
1500	3.438	16.689988	20.1	11.53
2000	3.448	17.17094	19.88	11.77
2500	3.4716	17.478255	19.69	11.95

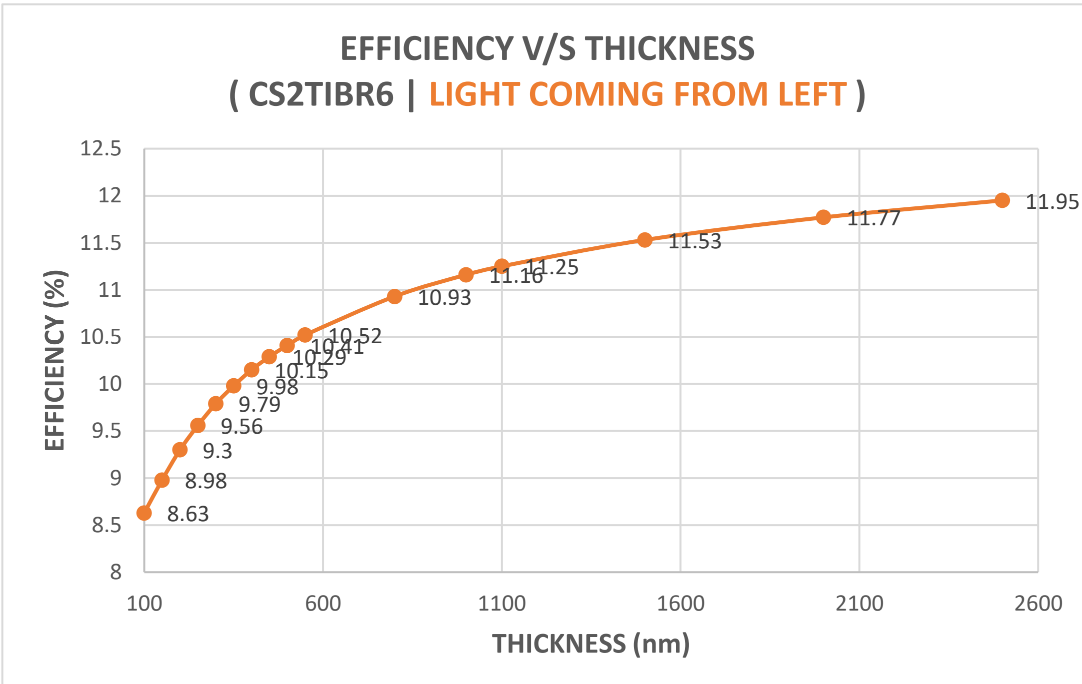


Figure 3.2.5: Efficiency-thickness density graph in Cs_2TiBr_6 layer when light is coming from Left-Hand Side to the solar cell

TABLE: 3.2.6 PVK variation of efficiency vs thickness, keeping the thickness of HTL= 0.5 µm and ETL =0.5 µm when light is coming from HTL side.

Thickness (nm)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
100	1.7916	5.331154	38.25	3.65
150	1.9531	4.864339	37.06	3.52
200	2.1589	4.602129	34.49	3.43
250	2.3933	4.428488	31.65	3.35
300	2.697	4.296059	28.43	3.29
350	3.11	4.183392	24.89	3.24
400	3.6968	4.080246	21.09	3.18
450	4.5236	3.98167	17.34	3.12
500	5.6899	3.885339	13.85	3.06
550	7.3164	3.790271	10.81	3
800		3.331843		2.66
1000		2.997186		2.39
1100		2.843833		2.27

1500		2.325959		1.86
2000		1.859592		1.49
2500		1.532817		1.23

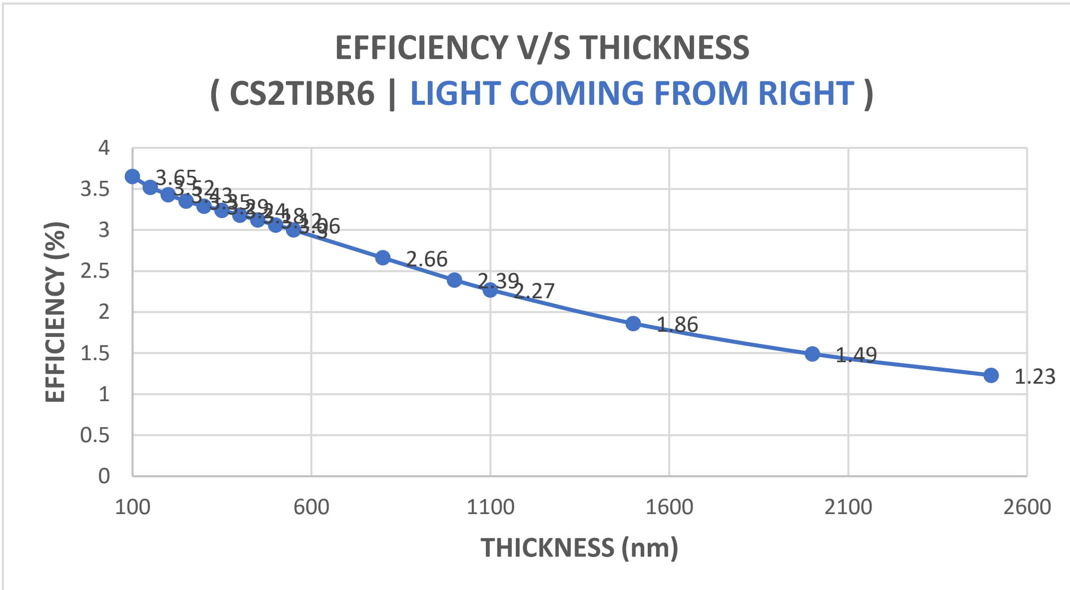


Figure 3.2.6: Efficiency-thickness density graph in Cs_2TiBr_6 layer when light is coming from Right-Hand Side to the solar cell.

(c) Study of dependence of efficiency vs temperature.

At defect density = $1 * 10^{10}$ (cm^{-3}), since, maximum efficiency in previousobservations is observed at $1 * 10^{10}$ (cm^{-3}).

At thickness of HTL=0.5 µm, PVK=400 nm and ETL= 0.3 µm.

TABLE: 3.2.7 Solar cell variation of efficiency vs temperature when light is coming from ETL side.

Temperature (K)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
263	6.0636	13.66795	12.51	10.37
268	5.7775	14.096773	13.1	10.67
273	5.5973	13.962187	13.54	10.58
278	5.3585	13.843001	14.15	10.49
283	5.0635	13.738417	14.96	10.41
288	4.7498	13.647058	15.92	10.32
293	4.4493	13.56745	16.95	10.23
298	4.1733	13.498123	18.01	10.14

303	3.9368	13.437574	19.01	10.05
308	3.7178	13.384724	20.03	9.97
313	3.5465	13.338339	20.89	9.88
318	3.384	13.326403	21.77	9.82

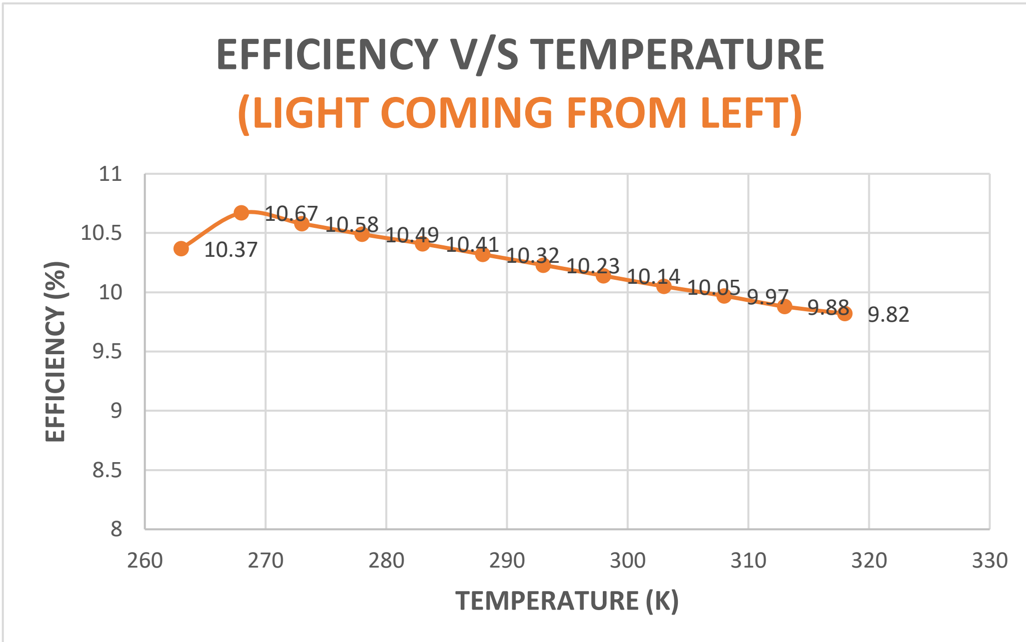


Figure 3.2.7: Efficiency-temperature graph in solar cell when light is coming from Left-Hand Side to the solar cell.

TABLE: 3.2.8 Solar cell variation of efficiency vs temperature when light is coming from HTL side.

Temperature (K)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
263	1.6838	7.492188	31.55	3.98
268	1.6834	6.894461	33.88	3.93
273	1.6938	6.365553	35.95	3.88
278	1.715	5.904479	37.64	3.81
283	1.7577	5.506385	38.63	3.74
288	1.8317	5.164977	38.67	3.66
293	1.9603	4.873508	37.38	3.57
298	2.194	4.625356	34.26	3.48
303	2.5446	4.414364	30.09	3.38
308	3.0597	4.235001	25.33	3.28
313	3.0538	4.219926	25.4	3.27
318	4.4988	3.952433	17.46	3.1

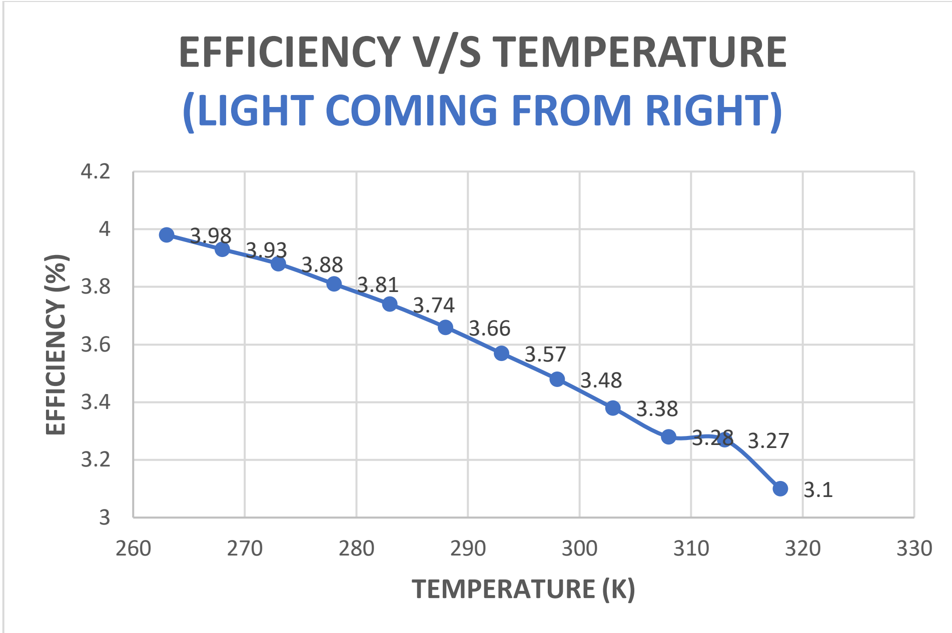


Figure 3.2.9: Efficiency-temperature graph in solar cell when light is coming from Right-Hand Side to the solar cell.

OBSERVATION

The efficiency of the solar cell decreases with gradual increase in the temperature.

3.3. Cs_2TiI_6

(a) Study of dependence of defect density vs efficiency.

At temperature = 298 K, HTL thickness (0.08 µm), PVK thickness (2 µm) and ETLthickness (0.5 µm).

TABLE: 3.3.1. PVK variation of efficiency vs defect density, keeping the defect density of HTL=0 and ETL =0 when light is coming from ETL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
1.00E+10	3.7269	18.701133	20.59	14.35
1.00E+11	3.657	18.701061	20.95	14.33
1.00E+12	3.1147	18.700339	24.24	14.12
1.00E+13	1.6871	18.693128	39.28	12.39
1.00E+14	1.034	18.621872	41.15	7.92
1.00E+15	0.9466	17.981992	29.02	4.94

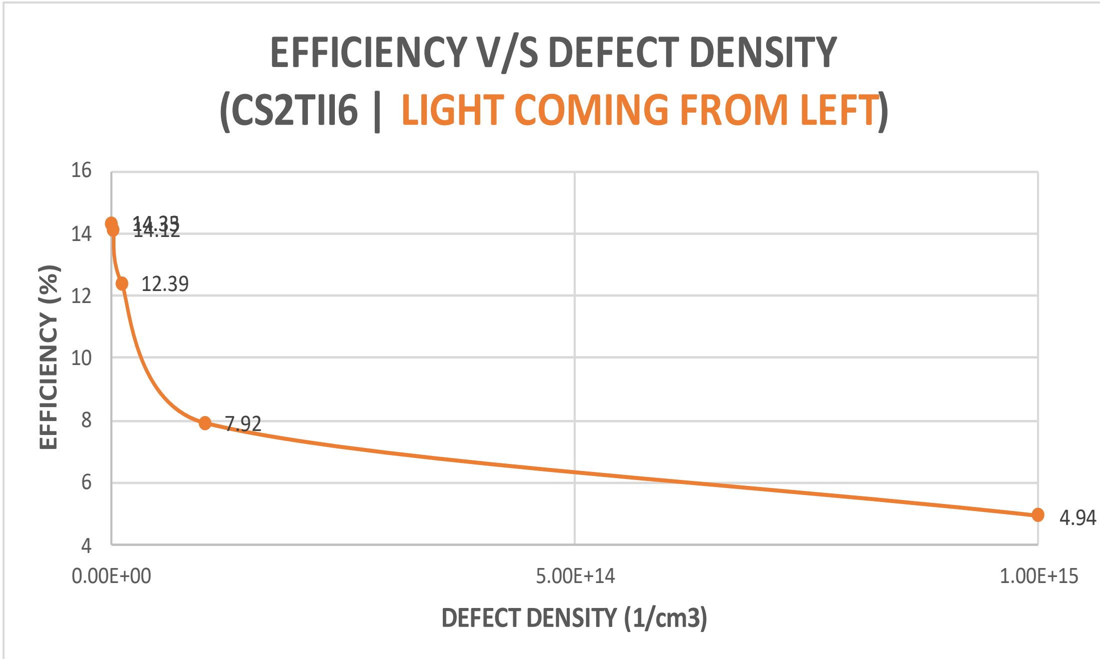


Figure 3.3.1: Efficiency-Defect density graph in Cs_2TiI_6 when light is coming from Left-Hand Side to the solar cell.

TABLE: 3.3.2. PVK variation of efficiency vs defect density, keeping the defect density of HTL=0 and ETL =0 when light is coming from HTL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
1.00E+10	6.1768	18.960863	12.69	14.86
1.00E+11	5.9637	18.960554	13.12	14.83
1.00E+12	4.5289	18.957458	17	14.6
1.00E+13	1.9567	18.926591	34.25	12.68
1.00E+14	1.0985	18.626574	34.31	7.02
1.00E+15	0.9054	16.242378	19.06	2.8

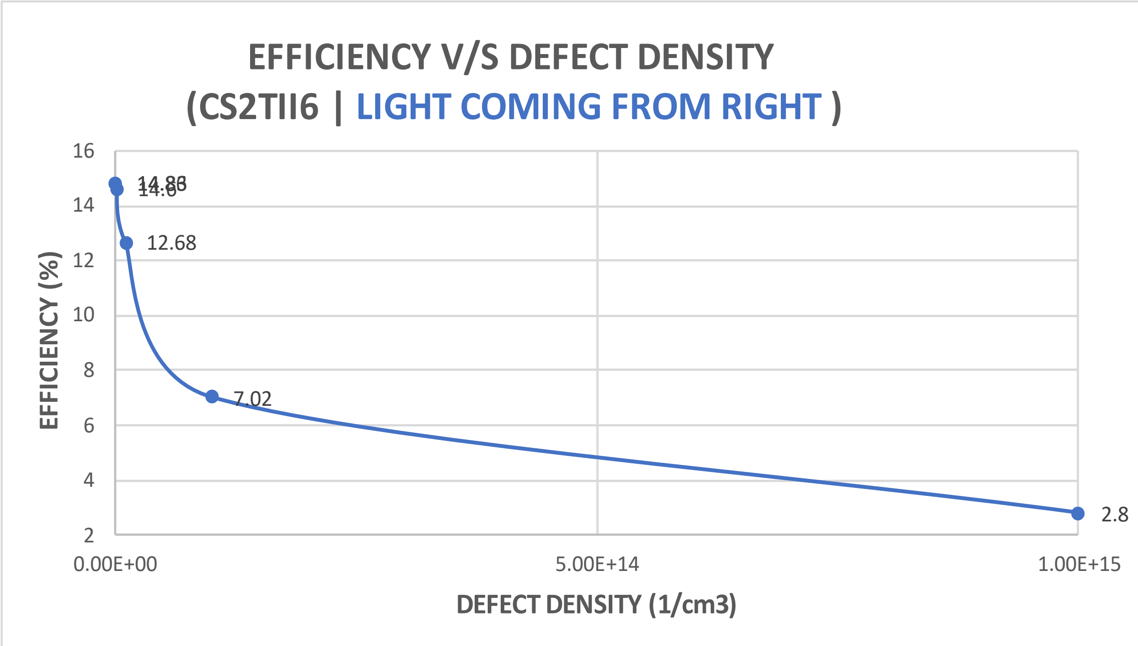


Figure 3.3.2: Efficiency-Defect density graph in Cs_2TiI_6 later when light is coming from Right-Hand Side to the solar cell.

(c) Solar cell variation of efficiency vs defect density.

TABLE: 3.3.3. Solar cell variation of efficiency vs defect density, keeping the defect density when light coming from ETL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
1.00E+10	3.7275	18.701129	20.58	14.35
1.00E+11	3.6559	18.701023	20.95	14.33
1.00E+12	3.1043	18.699963	24.31	14.11
1.00E+13	1.6779	18.689376	39.37	12.34
1.00E+14	1.0393	18.58479	40.64	7.85
1.00E+15	0.9561	17.650801	28.16	4.75

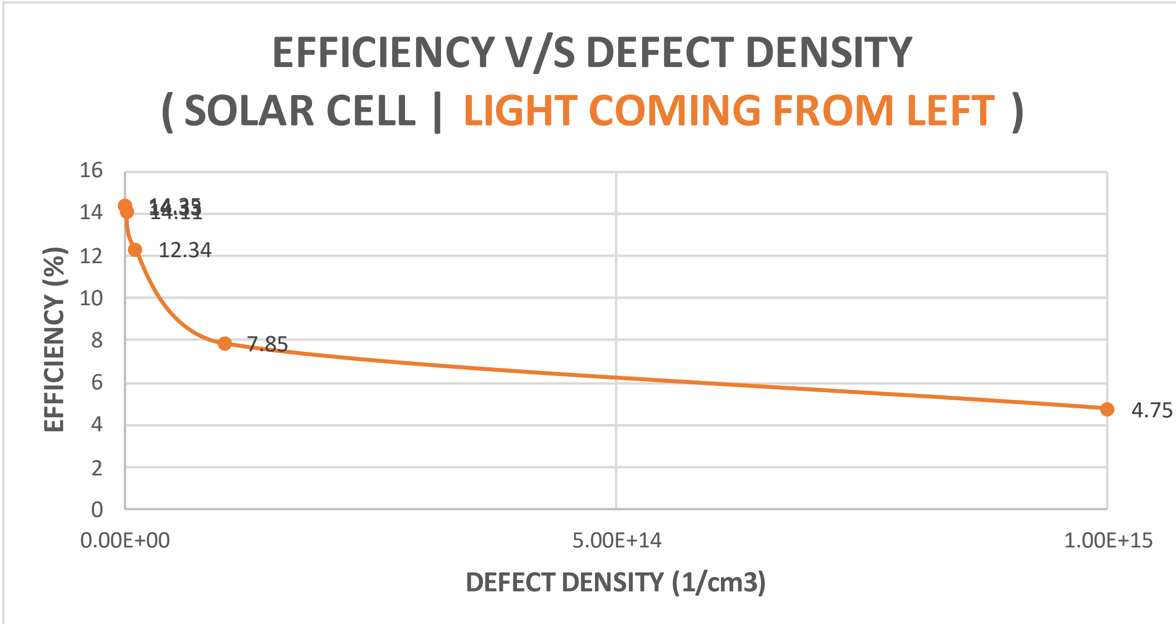


Figure 3.3.3: Efficiency-Defect density graph in Solar cell when light is coming from Left-Hand Side to the solar cell

TABLE: 3.3.4. Solar cell variation of efficiency vs defect density, keeping the defect density when light coming from HTL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
1.00E+10	6.1768	18.960863	12.69	14.86
1.00E+11	5.9637	18.960553	13.12	14.83
1.00E+12	4.5286	18.957455	17	14.6
1.00E+13	1.9566	18.926561	34.25	12.68
1.00E+14	1.0985	18.626287	34.31	7.02
1.00E+15	0.9054	16.240137	19.06	2.8

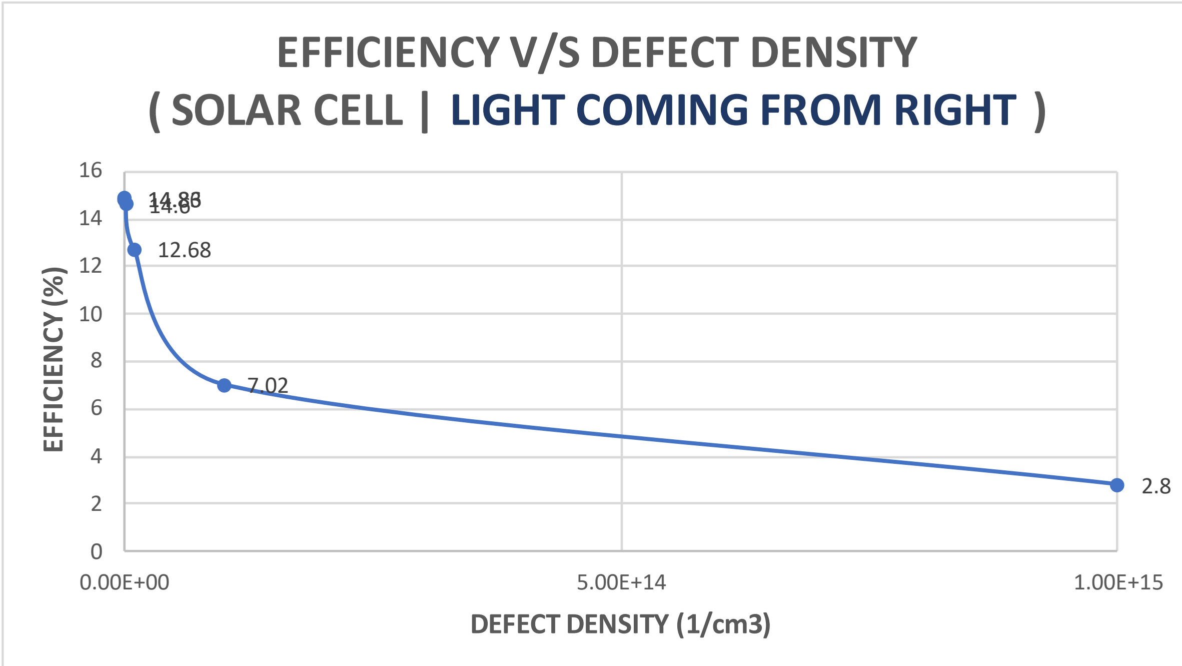


Figure 3.3.4: Efficiency-Defect density graph in Solar cell when light is coming from Right-Hand Side to the solar cell

OBSERVATION

The efficiency of the solar cell and the respective layers decreases with gradual increase in defect density. The maximum efficiency is observed at $1 * 10^{10}$ (cm^{-3}) defect density in each layer and in the whole solar cell.

(b) Study of dependence of efficiency vs thickness.

At temperature = 298 K and defect density = $1 * 10^{10}$ (cm^{-3}), since maximumefficiency in previous observations is observed at $1 * 10^{10}$ (cm^{-3}).

TABLE: 3.3.5. PVK variation of efficiency vs thickness, keeping the thickness of HTL= 0.05 µm and ETL =0.5 µm when light is coming from ETL side.

Thickness (µm)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
0.5	4.5145	16.89031	16.37	12.49
1	4.6578	18.197912	16.03	13.59
1.5	4.7212	18.53935	15.86	13.88
2	4.7697	18.646928	15.72	13.98
2.5	4.8129	18.685794	15.59	14.02
3	4.8568	18.701732	15.45	14.04
3.5	4.9004	18.709298	15.32	14.05
4	4.9455	18.718383	15.19	14.06

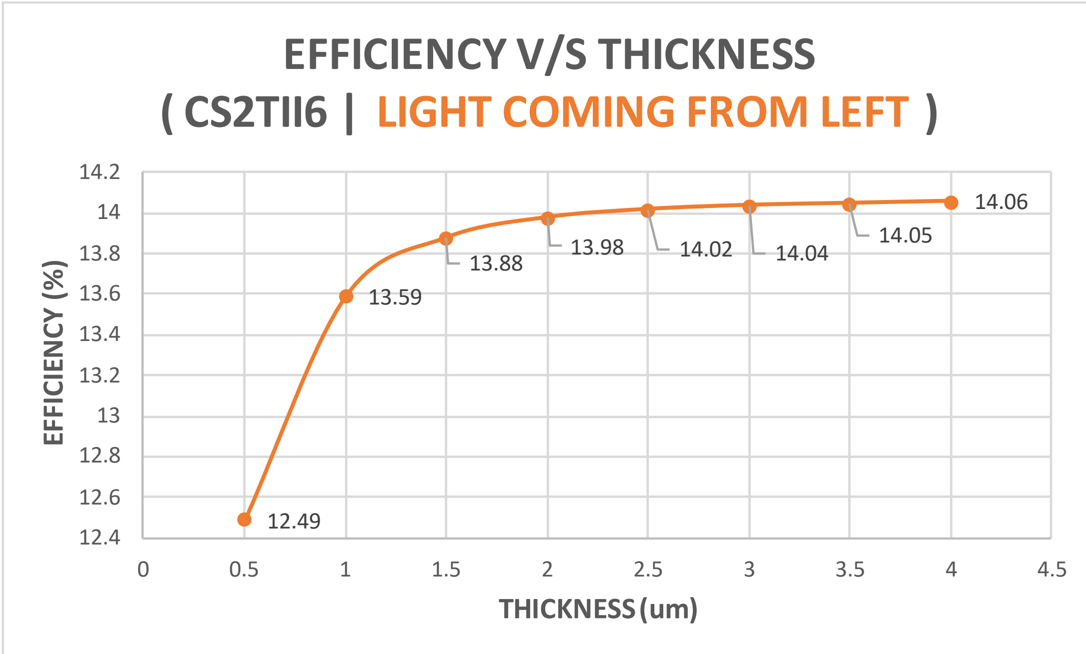


Figure 3.3.5: Efficiency-thickness density graph in Cs_2TiI_6 layer when light is coming from Left-Hand Side to the solar cell.

TABLE: 3.3.6. PVK variation of efficiency vs thickness, keeping the thickness of HTL= 0.05 µm and ETL =0.5 µm when light is coming from HTL side.

Thickness (µm)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
0.5		17.130501		13.62
1		18.484335		14.69
1.5		18.845233		14.97
2		18.9616		15.05
2.5		19.004718		15.08
3		19.021354		15.09
3.5		19.029697		15.09
4		19.034269		15.08

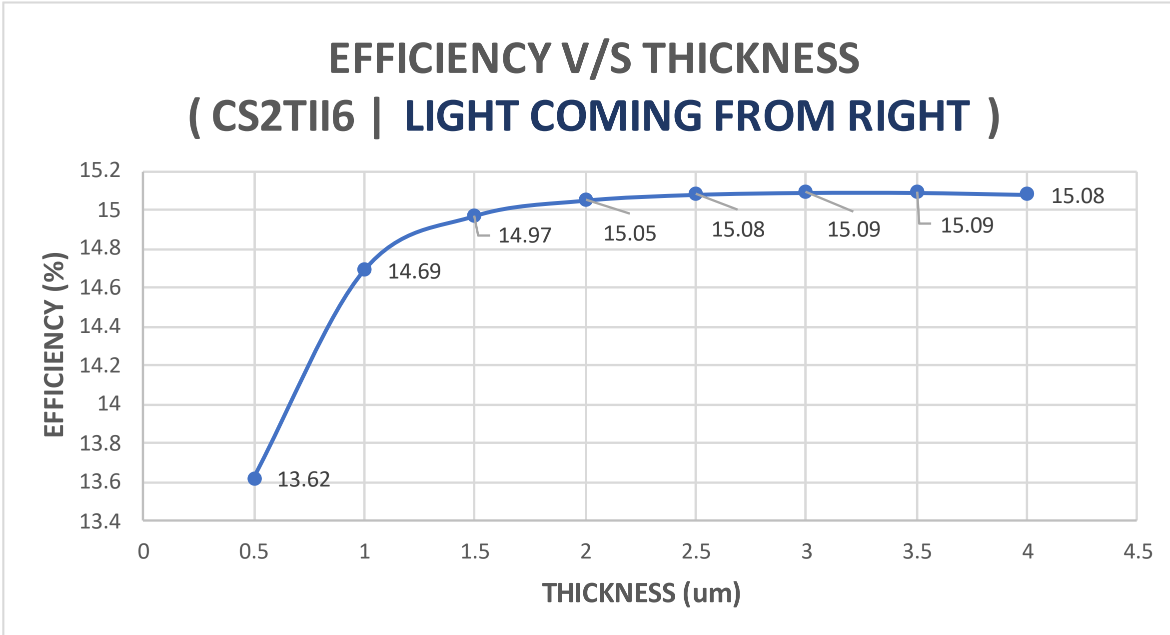


Figure 3.3.6: Efficiency-thickness density graph in Cs_2TiI_6 layer when light is coming from Right-Hand Side to the solar cell.

(c) Study of dependence of efficiency vs temperature.

At defect density = $1 * 10^{10}$ (cm^{-3}), since, maximum efficiency in previousobservations is observed at $1 * 10^{10}$ (cm^{-3}).

At thickness of HTL=0.07 µm, PVK=2.5 µm and ETL= 0.3 µm.

TABLE: 3.3.7 Solar cell variation of efficiency vs temperature when light is coming from ETL side

Temperature (K)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
283	4.1246	18.755563	18.62	14.4
288	3.8919	18.747921	19.65	14.34
293	4.5365	18.746127	16.95	14.42
298	3.5147	18.732286	21.56	14.19
303	3.5089	18.72856	21.55	14.16
308	3.2213	18.719548	23.29	14.04
313	3.096	18.711281	24.1	13.96
318	2.9816	18.706221	24.89	13.88
323	2.8764	18.697698	25.65	13.8
328	2.7784	18.689096	26.4	13.71

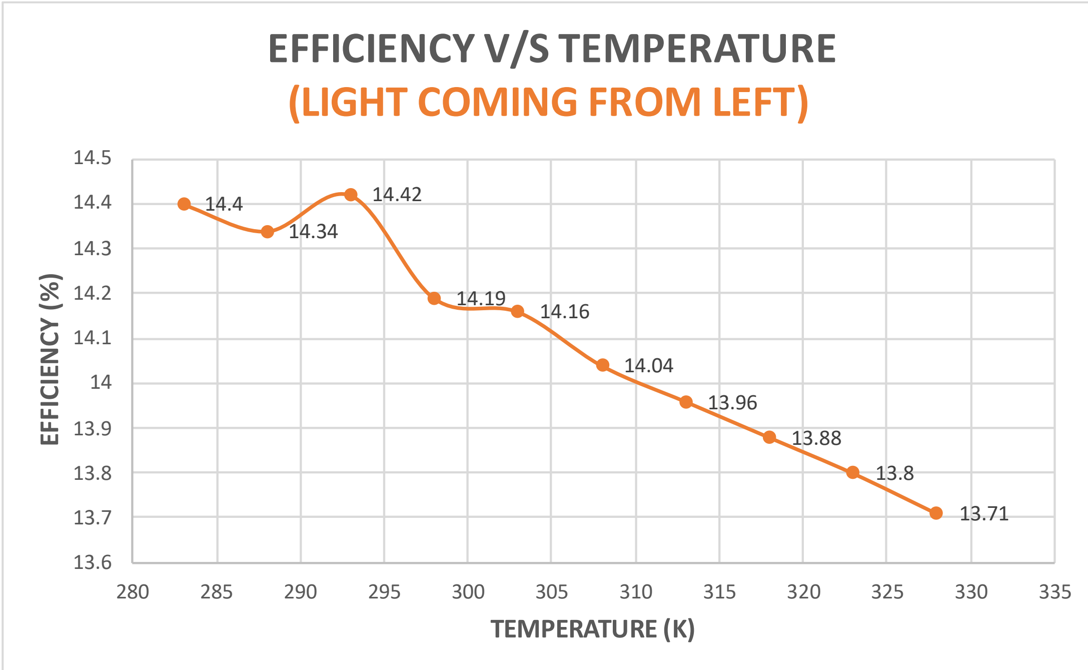


Figure 3.3.7: Efficiency-temperature graph in solar cell when light is coming from Left-Hand Side to the solar cell

TABLE: 3.3.8 Solar cell variation of efficiency vs temperature when light is coming from HTL side.

Temperature (K)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
283		19.008151		15.07
288		19.007335		15.04
293	9.9677	19.006387	7.93	15.01
298	8.707	19.006842	9.05	14.98
303	7.6639	19.005582	10.26	14.94
308	6.7857	19.004124	11.55	14.9
313	6.0558	19.004155	12.9	14.85
318	5.4389	19.002266	14.31	14.79
323	4.9175	19.000128	15.77	14.73
328	4.4768	18.999477	17.25	14.67

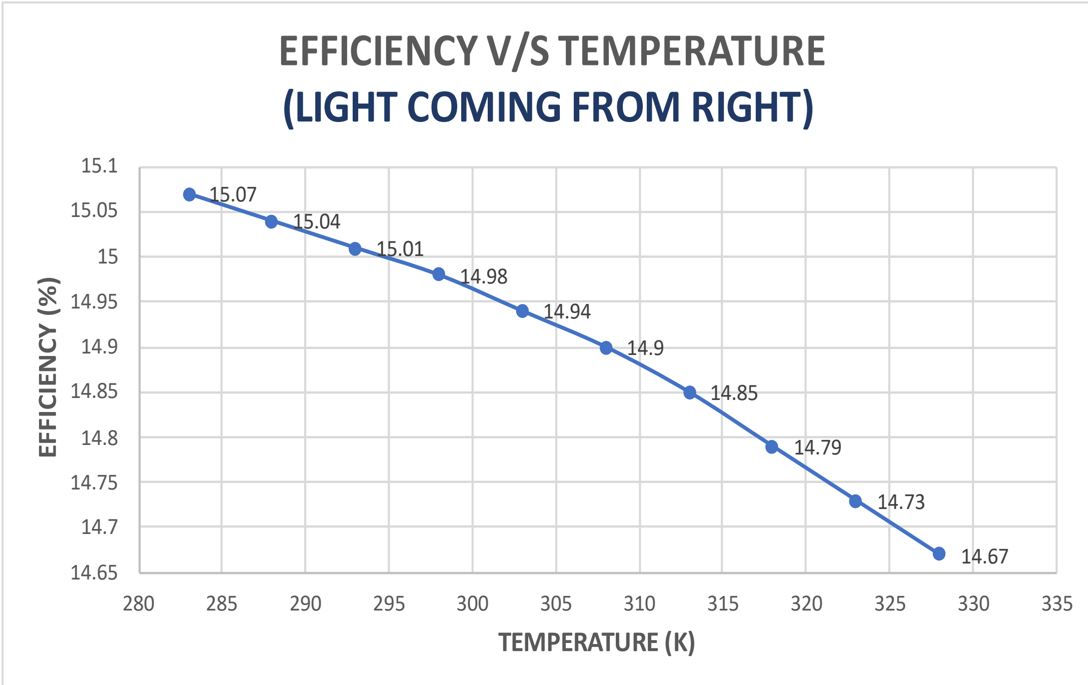


Figure 3.3.8: Efficiency-temperature graph in solar cell when light is coming from Right-Hand Side to the solar cell.

OBSERVATION

The efficiency of the solar cell decreases with gradual increase in thetemperature.

3.4. Cs_2TiCl_6

(a) Study of dependence of defect density vs efficiency.

At temperature = 298 K, HTL thickness (0.08 µm), PVK thickness (2 µm) and ETLthickness (0.5 µm).

TABLE.3.4.1. PVK variation of efficiency vs defect density, keeping the defect density of HTL=0 and ETL =0 when light is coming from ETL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
10000000000	1.0893	9.832106	51.66	5.53
1E+11	1.0892	9.832086	51.66	5.53
1E+12	1.089	9.83189	51.64	5.53
1E+13	1.0871	9.829925	51.46	5.5
1E+14	1.0712	9.810361	49.95	5.25
1E+15	1.042	9.622679	43.38	4.35

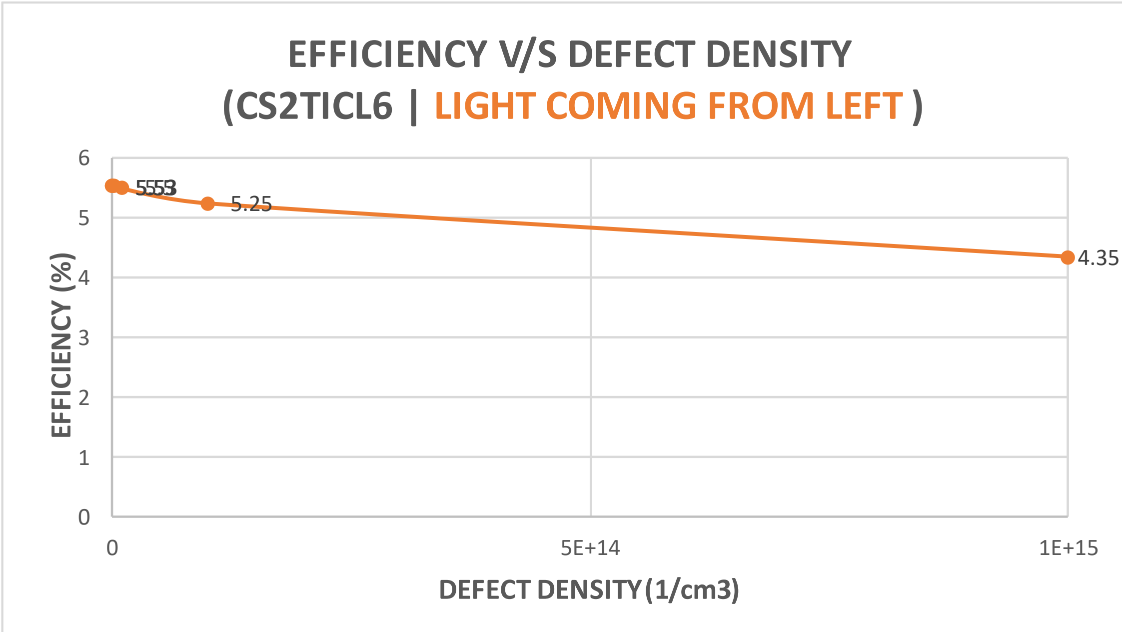


Figure 3.4.1: Efficiency-Defect density graph in Cs_2TiCl_6 when light is coming from Left-Hand Side to the solar cell.

TABLE.3.4.2. PVK variation of efficiency vs defect density, keeping the defect density of HTL=0 and ETL =0 when light is coming from HTL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
10000000000	0.991	9.46E-01	49.49	0.46
1E+11	0.9909	9.46E-01	49.49	0.46
1E+12	0.9904	9.46E-01	49.47	0.46
1E+13	0.9854	9.46E-01	49.27	0.46
1E+14	0.9521	9.42E-01	47.22	0.42
1E+15	0.9003	9.05E-01	35.47	0.29

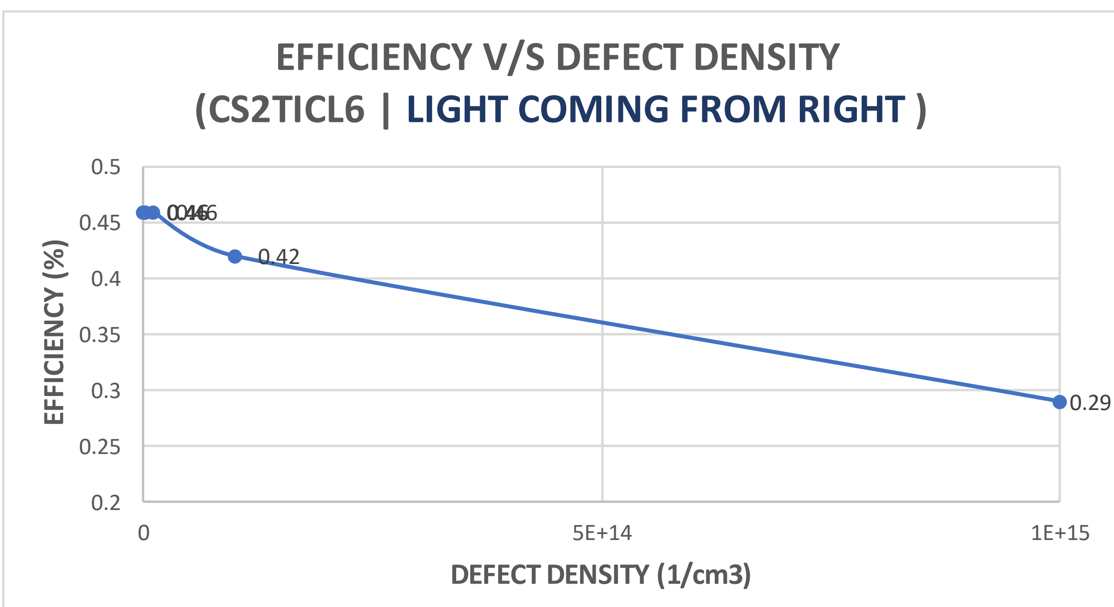


Figure 3.4.2: Efficiency-Defect density graph in Cs_2TiCl_6 when light is coming from Right-Hand Side to the solar cell.

Solar cell variation of efficiency vs defect density.

TABLE.3.4.3. Solar cell variation of efficiency vs defect density, keeping the defect density when light coming from ETL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
10000000000	1.0893	9.832102	51.66	5.53
1E+11	1.0892	9.832046	51.66	5.53
1E+12	1.089	9.831488	51.64	5.53
1E+13	1.0867	9.825916	51.46	5.49
1E+14	1.0678	9.770796	49.97	5.21
1E+15	1.0282	9.273939	43.12	4.11

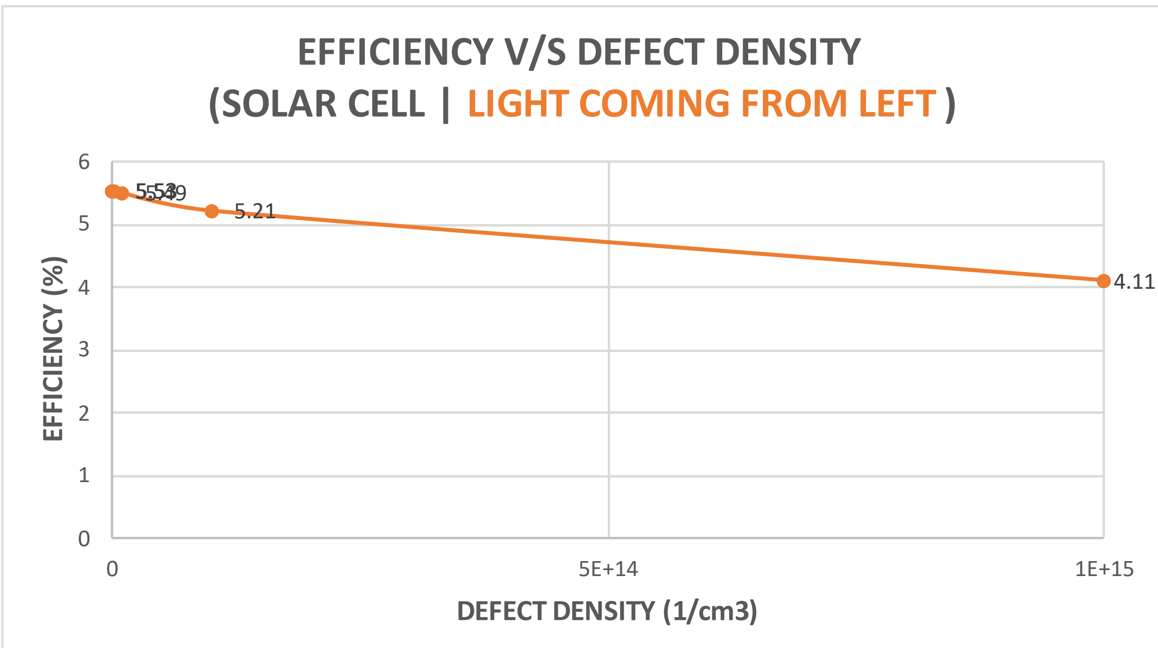


Figure 3.4.3: Efficiency-Defect density graph in Solar cell when light is coming from Left-Hand Side to the solar cell

TABLE.3.4.4. Solar cell variation of efficiency vs defect density, keeping the defect density when light coming from HTL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
10000000000	0.991	9.46E-01	49.49	0.46
1E+11	0.9909	9.46E-01	49.49	0.46
1E+12	0.9904	9.46E-01	49.47	0.46
1E+13	0.9854	9.46E-01	49.27	0.46
1E+14	0.9521	9.42E-01	47.22	0.42
1E+15	0.9	9.05E-01	35.48	0.29

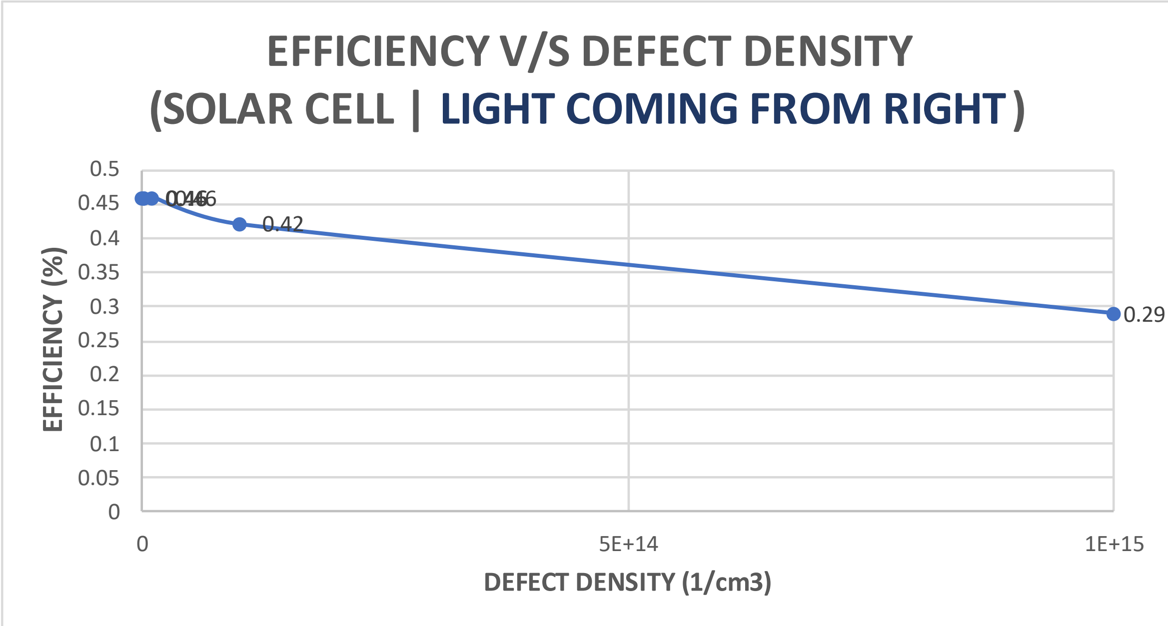


Figure 3.4.4: Efficiency-Defect density graph in Solar cell when light is coming from Right-Hand Side to the solar cell

OBSERVATION

The efficiency of the solar cell and the respective layers decreases with gradual increase in defect density. The maximum efficiency is observed at $1 * 10^{10}$ (cm^{-3}) defect density in each layer and in the whole solar cell.

(b) Study of dependence of efficiency vs thickness.

At temperature = 298 K and defect density = $1 * 10^{10}$ (cm^{-3}), since maximumefficiency in previous observations is observed at $1 * 10^{10}$ (cm^{-3}).

TABLE.3.4.5. PVK variation of efficiency vs thickness, keeping the thickness of HTL= 0.05 µmand ETL =0.5 µm when light is coming from ETL side.

Thickness (µm)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
0.5	1.0861	8.341641	49.61	4.49
1	1.0731	9.400075	53.44	5.39
1.5	1.0799	9.716638	54.38	5.71
2	1.0947	9.833624	54.52	5.87
2.5	1.1124	9.883619	54.4	5.98
3	1.1311	9.905802	54.2	6.07
3.5	1.1504	9.914863	53.94	6.15
4	1.1706	9.917674	53.61	6.22

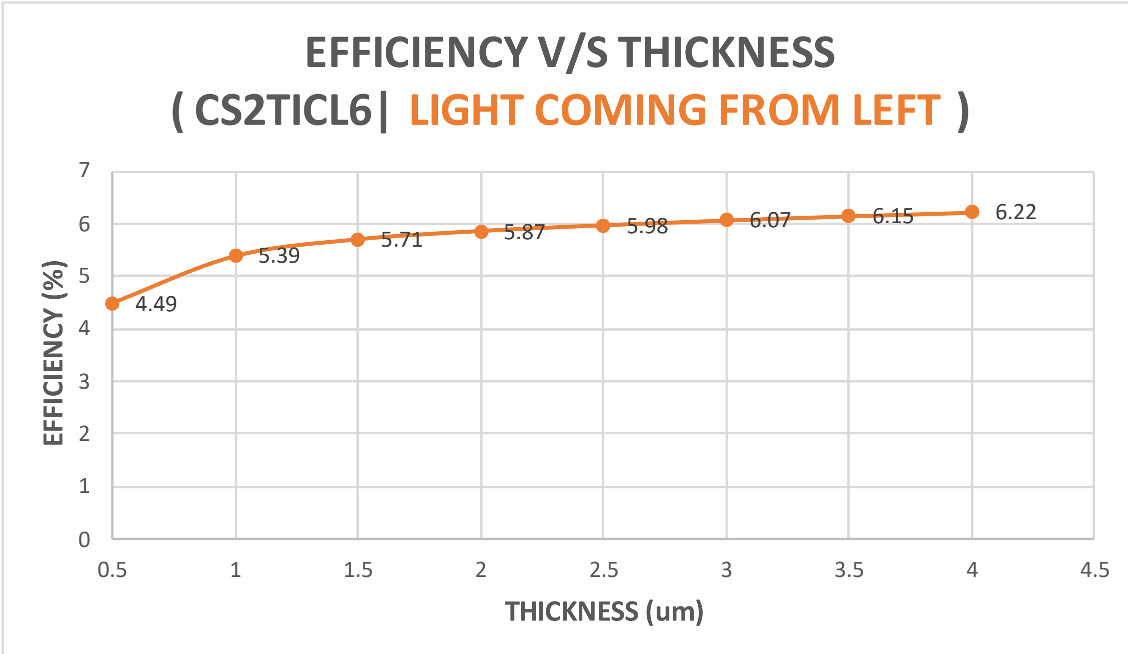


Figure 3.4.5: Efficiency-thickness density graph in Cs_2TiCl_6 layer when light is coming from Left-Hand Side to the solar cell.

TABLE.3.4.6. PVK variation of efficiency vs thickness, keeping the thickness of HTL= 0.05 µm and ETL =0.5 µm when light is coming from HTL side.

Thickness (µm)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
0.5	1.034	1.318133	27.16	0.37
1	1.0005	9.10E-01	48.66	0.44
1.5	0.9923	9.40E-01	49.64	0.46
2	0.99	9.47E-01	49.97	0.47
2.5	0.9895	9.43E-01	50.16	0.47
3	0.99	9.35E-01	50.25	0.46
3.5	0.9909	9.25E-01	50.23	0.46
4	0.9921	9.15E-01	50.11	0.45

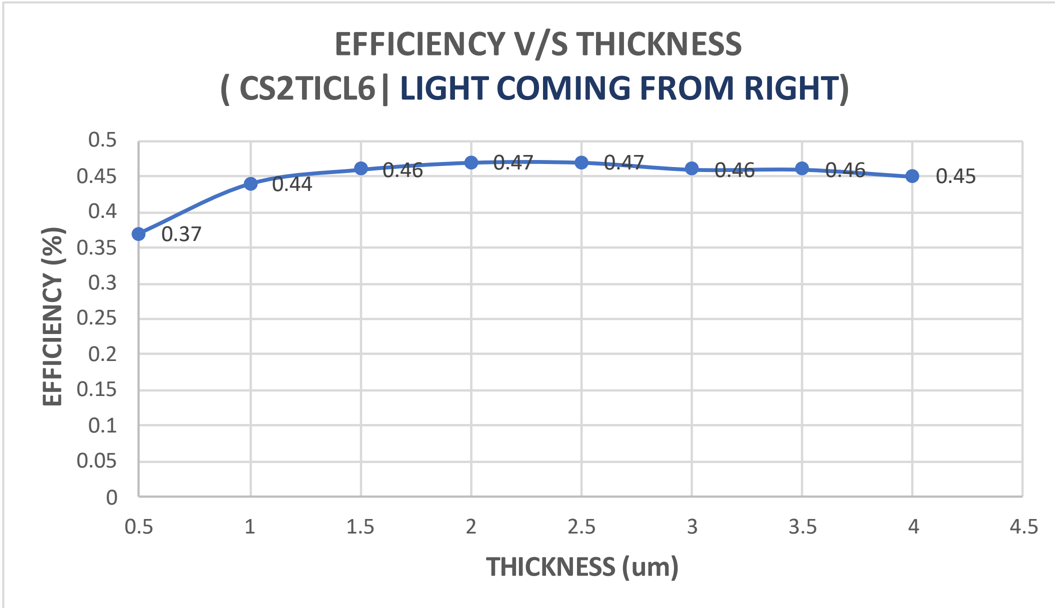


Figure 3.4.6: Efficiency-thickness density graph in Cs_2TiCl_6 layer when light is coming from Right-Hand Side to the solar cell.

(c) Study of dependence of efficiency vs temperature.

At defect density = $1 * 10^{10}$ (cm^{-3}), since, maximum efficiency in previousobservations is observed at $1 * 10^{10}$ (cm^{-3}).

At thickness of HTL=0.07 µm, PVK=2.5 µm and ETL= 0.3 µm.

TABLE: 3.4.7 Solar cell variation of efficiency vs temperature when light is coming from ETL side.

Temperature (K)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
263	1.1571	9.962409	54.27	6.26
268	1.1463	9.951707	54.19	6.18
273	1.1365	9.940726	54.08	6.11
278	1.1274	9.929625	53.92	6.04
283	1.1192	9.918716	53.72	5.96
288	1.1117	9.908391	53.48	5.89
293	1.1049	9.897096	53.21	5.82
298	1.0987	9.885988	52.91	5.75
303	1.0931	9.87459	52.57	5.67
308	1.0882	9.863378	52.21	5.6
313	1.0838	9.853012	51.82	5.53
318	1.0798	9.841656	51.41	5.46

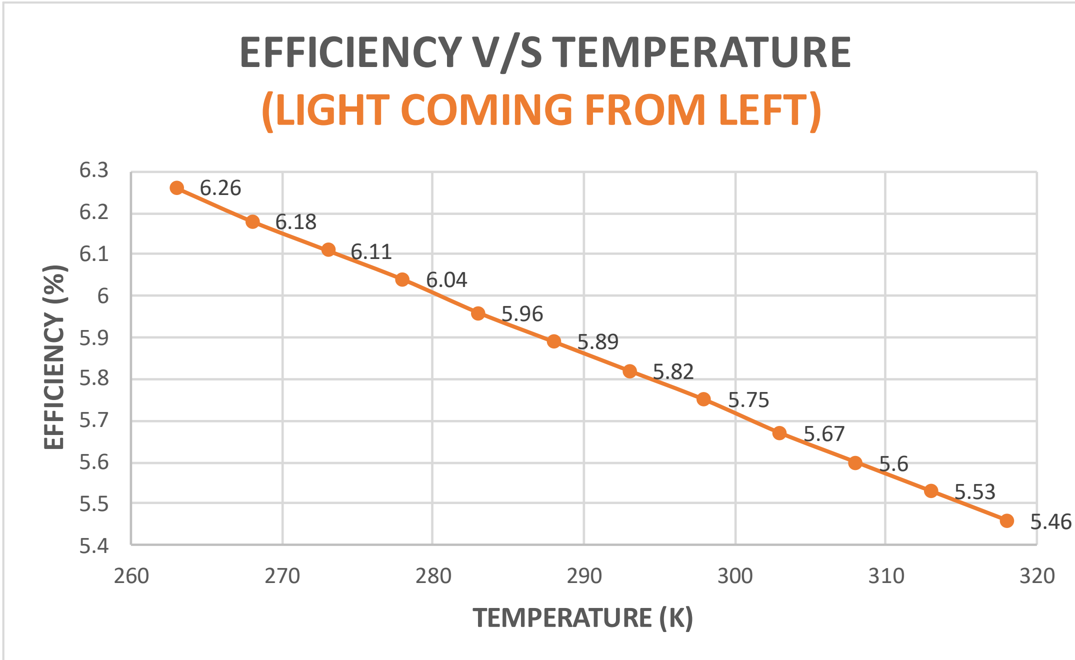


Figure 3.4.7: Efficiency-temperature graph in solar cell when light is coming from Left-Hand Side to the solar cell.

TABLE: 3.4.8 Solar cell variation of efficiency vs temperature when light is coming from HTL side.

Temperature (K)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
263	1.025	2.152932	50.73	1.12
268	1.019	2.144588	50.39	1.1
273	1.0137	2.136139	50.01	1.08
278	1.009	2.127709	49.61	1.07
283	1.0048	2.119329	49.19	1.05
288	1.0009	2.111718	48.8	1.03
293	0.9977	2.10242	48.27	1.01
298	0.9946	2.094043	47.78	1
303	0.9919	2.08556	47.28	0.98
308	0.9893	2.078138	46.84	0.96
313	0.9874	2.068622	46.25	0.94
318	0.9855	2.060156	45.72	0.93

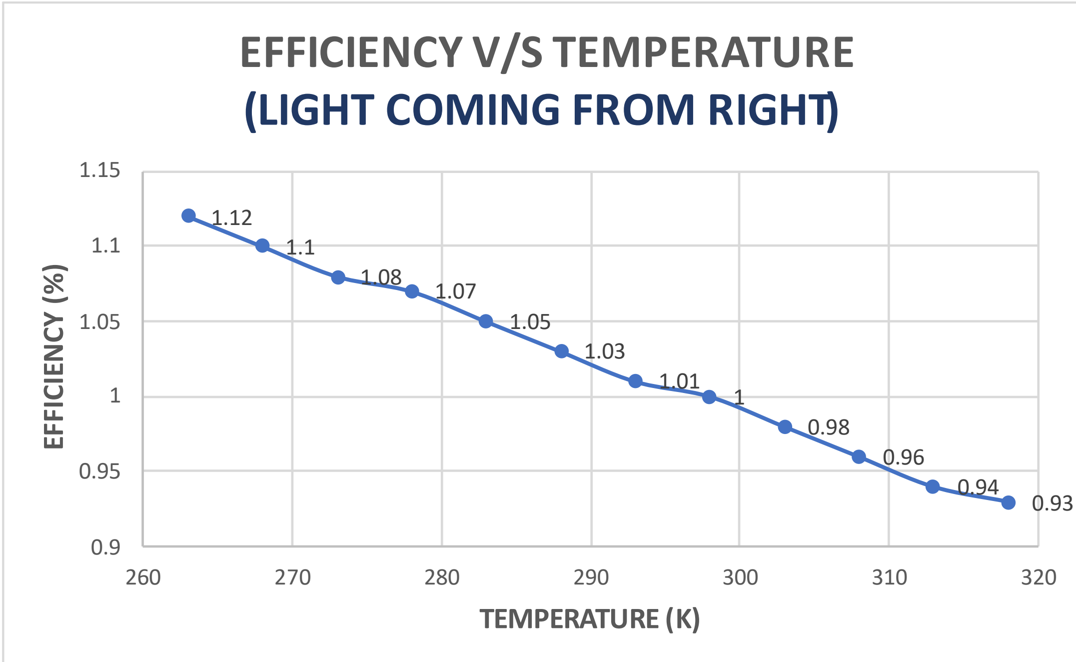


Figure 3.4.8: Efficiency-temperature graph in solar cell when light is coming from Right-Hand Side to the solar cell.

OBSERVATION

The efficiency of the solar cell decreases with gradual increase in thetemperature.

3.5. $CH_3NH_3GeI_3$

There are 3 layers in the solar cells under consideration: PEDOT:PSS (Hole Transfer Layer), $CH_3NH_3GeI_3$ (Perovskite layer) and PCBM (Electron Transfer layer)

(a) Study of dependence of defect density vs efficiency.

At temperature = 298 K, HTL thickness (0.08 µm), PVK thickness (0.4 µm) andETL thickness (0.5 µm).

TABLE 3.5.1. PVK variation of efficiency vs defect density, keeping the defect density of HTL=0 and ETL =0 when light is coming from ETL side.

Defect Density ($1/cm^3$)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
10000000000	1.5094	14.190043	46.15	9.89
1E+11	1.5094	14.190043	46.15	9.89
1E+12	1.5094	14.190043	46.15	9.89
1E+13	1.5094	14.190043	46.15	9.89
1E+14	1.5094	14.190043	46.15	9.89
1E+15	1.5087	14.190042	46.17	9.88

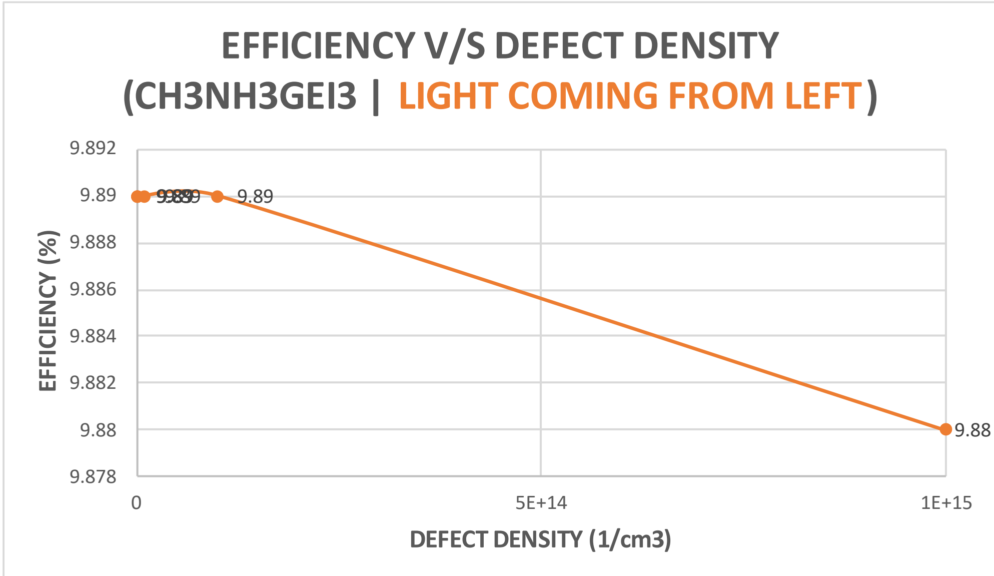


Figure 3.5.1: Efficiency-Defect density graph in $CH_3NH_3GeI_6$ when light is coming from Left-Hand Side to the solar cell.

TABLE 3.5.2. PVK variation of efficiency vs defect density, keeping the defect density of HTL=0 and ETL =0 when light is coming from HTL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
10000000000	2.5351	12.546877	11.97	3.81
1E+11	2.5351	12.546877	11.97	3.81
1E+12	2.5351	12.546877	11.97	3.81
1E+13	2.5351	12.546877	11.97	3.81
1E+14	2.5349	12.546877	11.98	3.81
1E+15	2.5333	12.546875	11.98	3.81

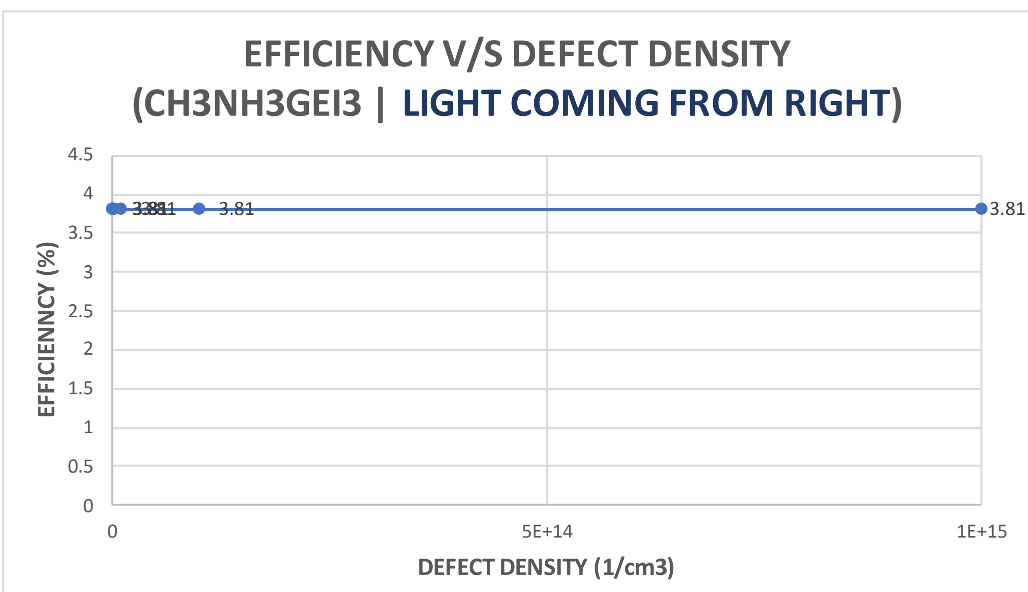


Figure 3.5.2: Efficiency-Defect density graph in $CH_3NH_3GeI_6$ when light is coming from Right-Hand Side to the solar cell.

Solar cell variation of efficiency vs defect density.

TABLE 3.5.3. Solar cell variation of efficiency vs defect density, keeping the defect density when light coming from ETL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
10000000000	1.5094	14.190041	46.15	9.89
1E+11	1.5094	14.190016	46.15	9.89
1E+12	1.5094	14.189775	46.15	9.88
1E+13	1.509	14.187362	46.15	9.88
1E+14	1.5049	14.163419	46.19	9.85
1E+15	1.4842	13.941592	46.17	9.55

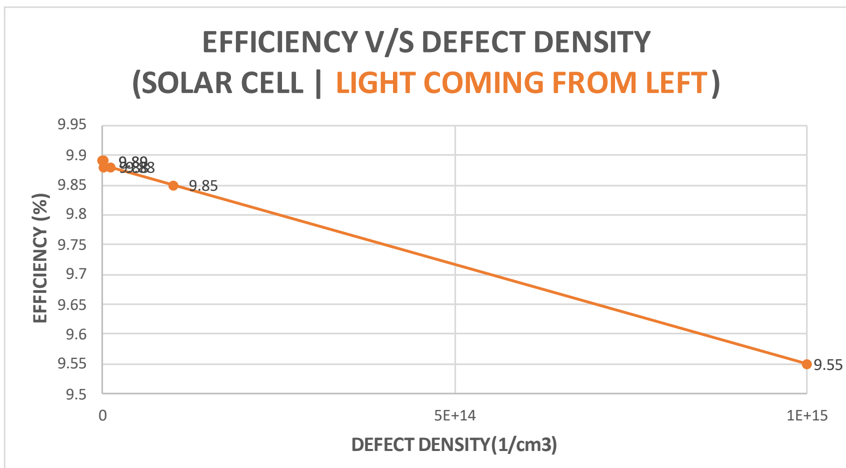


Figure 3.5.3: Efficiency-Defect density graph in Solar cell when light is coming from Left-Hand Side to the solar cell

TABLE 3.5.4. Solar cell variation of efficiency vs defect density, keeping the defect density when light coming from HTL side.

Defect Density (1/cm^3)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
10000000000	2.5351	12.546877	11.97	3.81
1E+11	2.5351	12.546875	11.97	3.81
1E+12	2.5351	12.546855	11.97	3.81
1E+13	2.5351	12.546657	11.97	3.81
1E+14	2.535	12.544676	11.98	3.81
1E+15	2.5352	12.525058	11.98	3.8

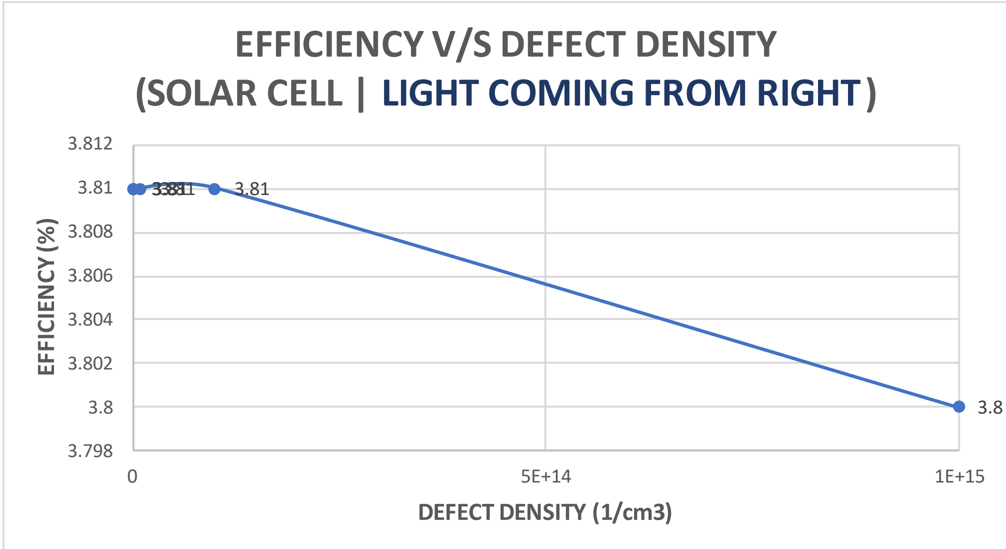


Figure 3.5.4: Efficiency-Defect density graph in Solar cell when light is coming from Right-Hand Side to the solar cell

OBSERVATION

The efficiency of the solar cell and the respective layers decreases with gradual increase in defect density. The maximum efficiency is observed at1 $* 10^{11}$ (cm^{-3}) defect density in each layer and in the whole solar cell.

(b) Study of dependence of efficiency vs thickness.

At temperature = 298 K and defect density = 1 $* 10^{11}$ (cm^{-3}), since maximumefficiency in previous observations is observed at 1 $* 10^{11}$ (cm^{-3}).

TABLE 3.5.5.PVK variation of efficiency vs thickness, keeping the thickness of HTL= 0.05 µm and ETL =0.5 µm when light is coming from ETL side.

Thickness (µm)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
0.2	3.9254	12.952791	15.59	7.92
0.4	3.7272	14.307398	19.59	10.44
0.6	3.1657	15.081463	24.19	11.55
0.8	2.8802	15.636152	26.89	12.11
1	2.7262	16.01173	28.48	12.43
1.2	2.6322	16.263025	29.51	12.63
1.4	2.5702	16.438201	30.22	12.77

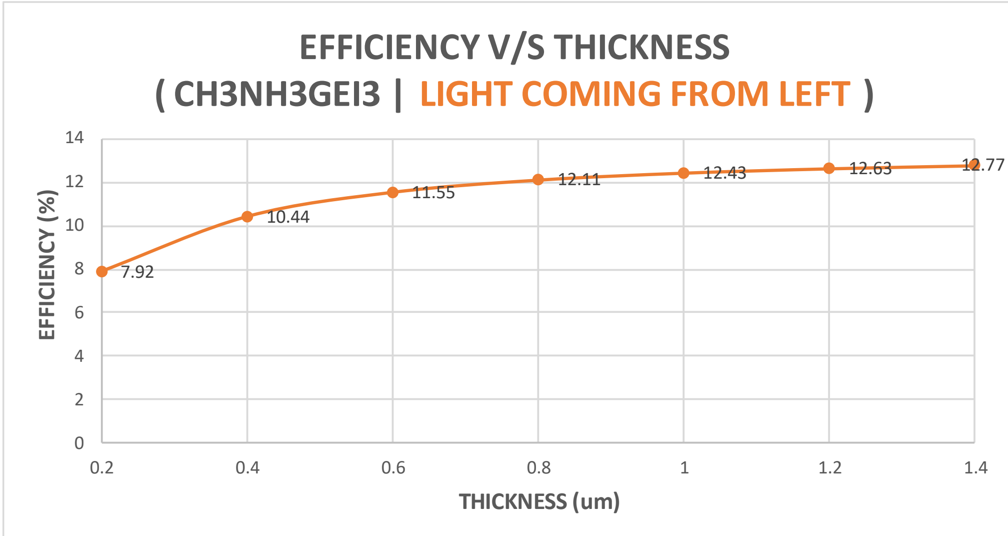


Figure 3.5.5: Efficiency-thickness density graph in $CH_3NH_3GeI_3$ layer when light is coming from Left-Hand Side to the solar cell

TABLE 3.5.6. PVK variation of efficiency vs thickness, keeping the thickness of HTL= 0.05 µm and ETL =0.5 µm when light is coming from HTL side.

Thickness (µm)	Voc	Jsc (mA/cm²)	FF(%)	η (%)
0.2	1.5554	13.151653	19.32	3.95
0.4	2.7123	13.801451	10.38	3.89
0.6	3.7873	11.928289	10.09	4.56
0.8	4.6072	10.070427	10.72	4.98
1	5.1806	9.053493	11.19	5.25
1.2	5.5654	8.540711	11.44	5.44
1.4	5.8199	8.27125	11.58	5.58

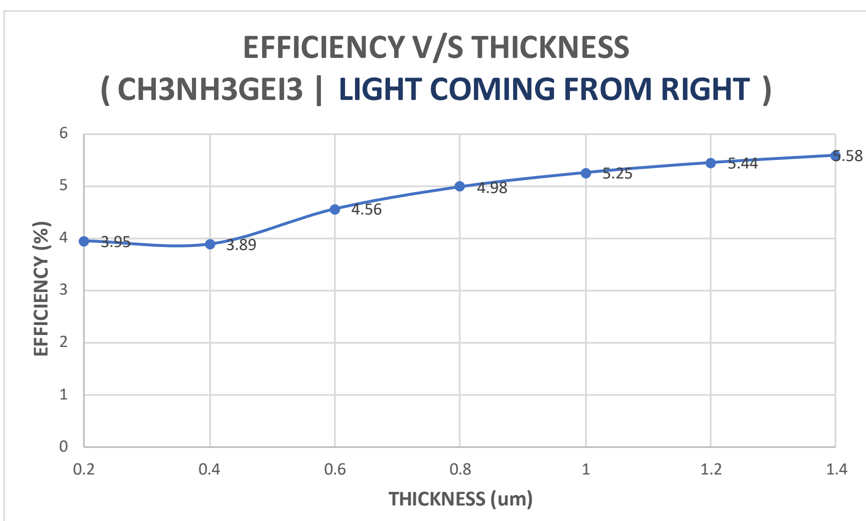


Figure 3.5.6: Efficiency-thickness density graph in $CH_3NH_3GeI_3$ layer when light is coming from Right-Hand Side to the solar cell.

(c) Study of dependence of efficiency vs temperature.

At defect density = $1 * 10^{11}$ (cm^{-3}), since, maximum efficiency in previousobservations is observed at $1 * 10^{11}$ (cm^{-3}).

At thickness of HTL=0.05 µm, PVK=0.8 µm and ETL= 0.3 µm.

TABLE: 3.5.7 Solar cell variation of efficiency vs temperature when light is coming from ETL side.

Temperature (K)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
263		15.683304		12.39
268	9.1754	15.674481	8.6	12.36
273	7.3231	15.665934	10.75	12.34
278	5.9112	15.657101	13.3	12.31
283	4.8331	15.648426	16.22	12.27
288	4.2643	15.645209	18.35	12.24
293	3.3723	15.630974	23.09	12.17
298	3.0372	15.627894	25.56	12.13
303	2.5	15.613838	30.83	12.04
308	2.2981	15.610437	33.4	11.98
313	1.9676	15.596542	38.62	11.85
318	1.8427	15.593369	40.99	11.78

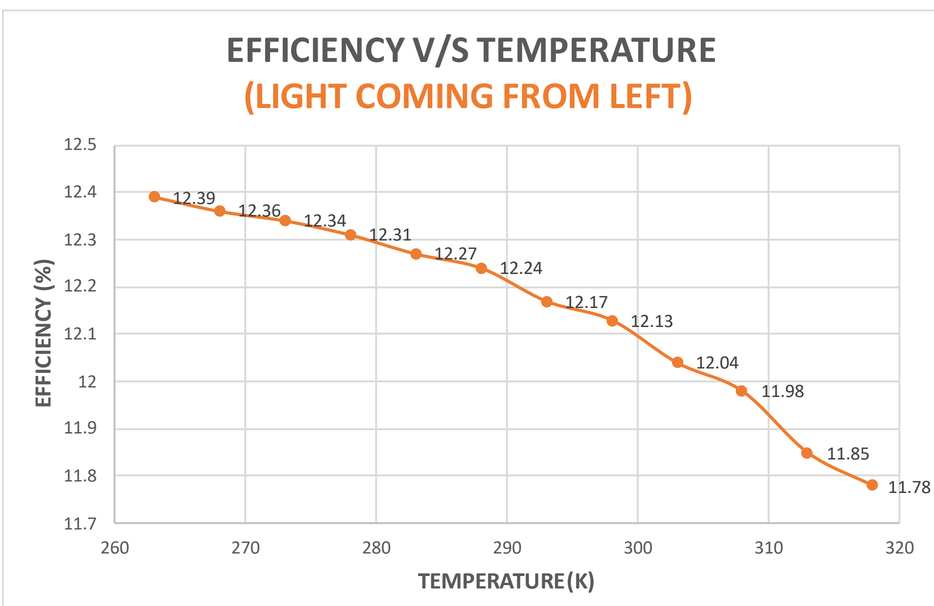


Figure 3.5.7: Efficiency-temperature graph in solar cell when light is coming from Left-Hand Side to the solar cell.

TABLE: 3.5.8 Solar cell variation of efficiency vs temperature when light is coming from HTL side.

Temperature (K)	Voc	Jsc (mA/cm^2)	FF(%)	η (%)
263	8.4669	11.896549	6.29	6.34
268	8.1891	11.758256	6.57	6.33
273	7.7978	11.62447	6.98	6.32
278	7.2886	11.495363	7.54	6.32
283	6.6945	11.370696	8.29	6.31
288	6.0448	11.250531	9.26	6.3
293	5.3795	11.134883	10.5	6.29
298	4.7346	11.02376	12.02	6.28
303	4.1408	10.91676	13.85	6.26
308	3.6093	10.813887	15.99	6.24
313	3.1488	10.715243	18.42	6.22
318	2.7592	10.620449	21.12	6.19

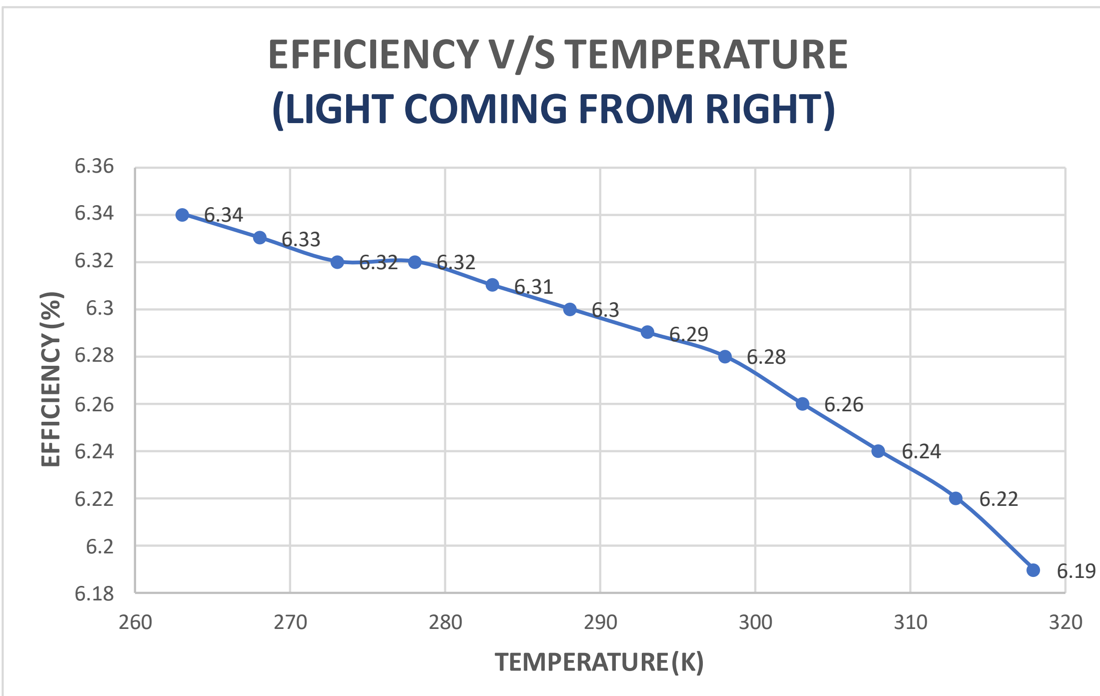


Figure 3.5.8: Efficiency-temperature graph in solar cell when light is coming from Right-Hand Side to the solar cell.

OBSERVATION

The efficiency of the solar cell decreases with gradual increase in the temperature.

CHAPTER 4 RESULTS AND DISCUSSION

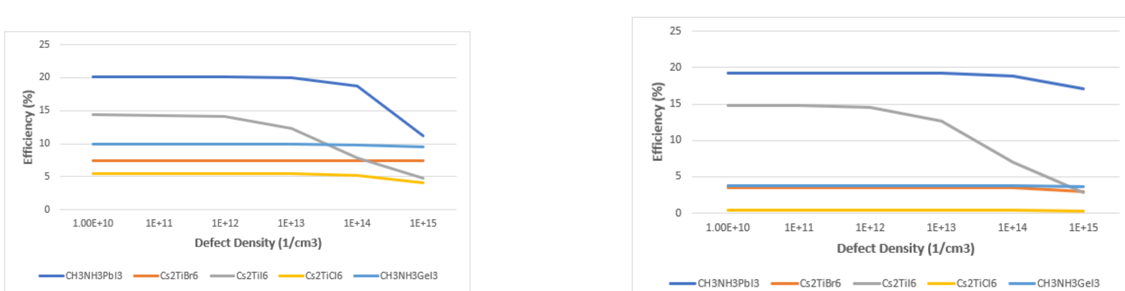
In this study, various critical parameters like defect density, thickness and temperature, that affect the perovskite solar cell performance for different perovskite based solar cells was considered, and its Power Conversion efficiency (η) was calculated. The simulation parameter values for different PVSCs are given in Table 4.1 (APPENDIX).

1. Effect of Defect Density of PVSC on PCE (η)

At device temperature 298 K, at constant thickness of HTL, PVK and ETL layers, the defect density of these layers was studied in 10^{10} cm^{-3} –10^{15} cm^{-3} defect density range, and the efficiencies (η %) variations of solar cells were noted.

TABLE 4.2: Defect Density variations on PCE (η) in various PVSCs

Defect Density ($1/cm^3$)	$CH_3NH_3PbI_3$ (η %)		Cs_2TiBr_6(η %)		Cs_2TiI_6(η %)		Cs_2TiCl_6(η %)		$CH_3NH_3GeI_3$(η %)	
	Left	**Right**	**Left**	**Right**	**Left**	**Right**	**Left**	**Right**	**Left**	**Right**
1E+10	**20.11**	*19.23*	**7.42**	*3.53*	**14.35**	**14.86**	**5.53**	0.46	**9.89**	*3.81*
1E+11	20.11	19.23	7.42	3.53	14.33	14.83	5.53	0.46	9.89	3.81
1E+12	20.1	19.22	7.42	3.53	14.11	14.6	5.53	0.46	9.88	3.81
1E+13	19.96	19.19	7.41	3.52	12.34	12.68	5.49	0.46	9.88	3.81
1E+14	18.71	18.87	7.33	3.47	7.85	7.02	5.21	0.42	9.85	3.81
1E+15	11.18	17.05	6.59	3	4.75	2.8	4.11	0.29	9.55	3.8



(i) (ii)

Graph 1. Efficiency v/s Defect Density curve for the Solar cells.
(i)when light comes from Left (HTL side), (ii) when light comes from right (ETL side).

It is observed that the power conversion efficiency (η) of all the PVSCs decrease with increase in defect densities in their layers. The reason being, defects decrease solar cell efficiency by allowing light to produce heat rather than electricity through new recombination pathways (loss). Deep energy levels in the semiconductor bandgap are caused by defects, which reduce the carrier lifetime and quantum efficiency of solar cells (Ullah, Marí, & Sánchez Ruiz, 2016).

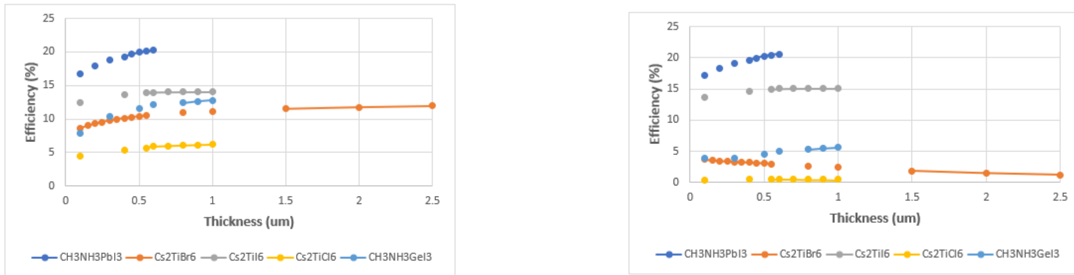
2. Effect of layer thickness of PVSC on PCE (η)

At device temperature 298K and defect density= 1E+10 cm^{-3} (for all other PVSCs) and 1E+11cm^{-3}(for $CH_3NH_3GeI_3$), thickness of PVK layer was varied and power conversion efficiency (η) was noted.

TABLE 4.3: Layer thickness variations on Power Conversion efficiency (η) in various PVSCs

Thickness(μm)	$CH_3NH_3PbI_3$ (η %)		Thickness (μm)	Cs_2TiI_6 (η %)		Thickness (μm)	Cs_2TiCl_6(η %)	
	Left	Right		Left	Right		Left	Right
0.3	16.78	17.16	0.5	12.49	13.62	0.5	4.49	0.37
0.4	17.96	18.31	1	13.59	14.69	1	5.39	0.44
0.5	18.76	19.08	1.5	13.88	14.97	1.5	5.71	0.46
0.6	19.3	19.6	2	13.98	15.05	2	5.87	0.47
0.7	19.68	19.97	2.5	14.02	15.08	2.5	5.98	0.47
0.8	19.95	20.24	3	14.04	15.09	3	6.07	0.46
0.9	20.15	20.45	3.5	14.05	15.09	3.5	6.15	0.46
1	20.29	20.57	4	14.06	15.08	4	6.22	0.45

Thickness (μm)	Cs_2TiBr_6(η %)		Thickness (μm)	$CH_3NH_3GeI_3$ (η %)	
	Left	Right		Left	Right
0.1	8.63	3.65	0.2	7.92	3.95
0.15	8.98	3.52	0.4	10.44	3.89
0.2	9.3	3.43	0.6	11.55	4.56
0.25	9.56	3.35	0.8	12.11	4.98
0.3	9.79	3.29	1	12.43	5.25
0.35	9.98	3.24	1.2	12.63	5.44
0.4	10.15	3.18	1.4	12.77	5.58
0.45	10.29	3.12			
0.5	10.41	3.06			
0.55	10.52	3			
0.8	10.93	2.66			
1	11.16	2.39			
1.5	11.53	1.86			
2	11.77	1.49			
2.5	11.95	1.23			



Graph 2. Efficiency v/s Thickness curve of PVK layer

(i) when light comes from Left (HTL side), (ii) when light comes from right (ETL side).

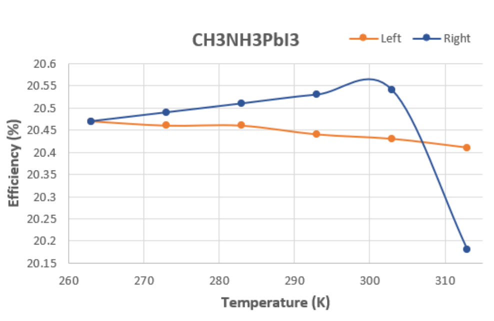
It is observed that the power conversion efficiency (η) of the PVSCs mostly increase with increase in their layer thickness. The reason being, with increase in layer thickness, the number of charge carrier in the solar cells also increases, due to which electricity is transferred efficiently and hence PCE increases (η) (TIVANOV, ASTASHENOK, FEDOTOV, & WĘGIEREK, 2012).

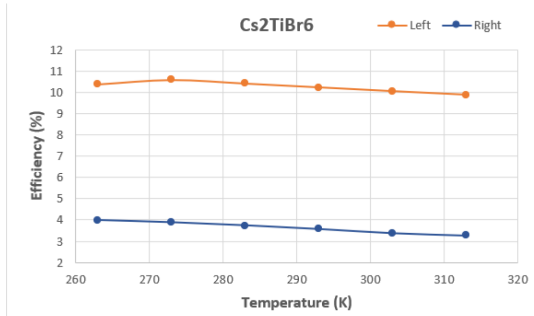
3. Effect of temperature of PVSCs on PCE (η)

For defect density= 1E+10 cm^{-3} (for all other PVSCs) and 1E+11 cm^{-3} (for $CH_3NH_3GeI_3$), at thickness HTL= 0.05 µm, optimum PVK thickness and ETL=0.3 µm, the device temperature of the PVSCs was varied and observed power conversion efficiency (η) was noted.

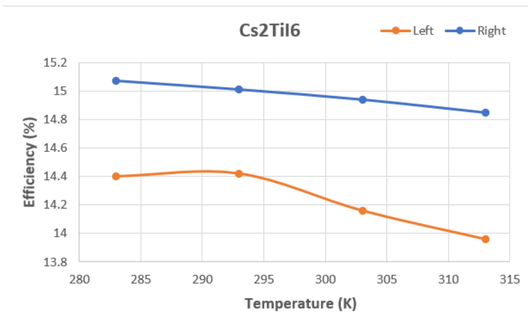
TABLE 4.4: Temperature variations on power conversion efficiency (η) in various PVSCs

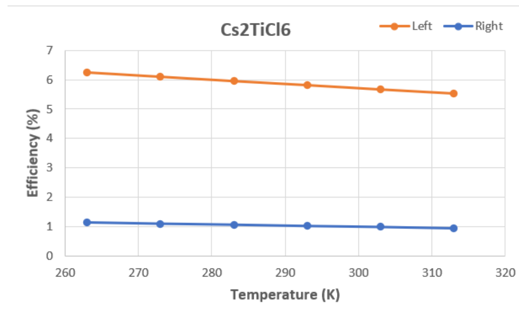
Temperature (K)	**$CH_3NH_3PbI_3$(η %)**		**Cs_2TiBr_6(η %)**		**Cs_2TiI_6 (η %)**		**Cs_2TiCl_6(η %)**		**$CH_3NH_3GeI_3$ (η %)**	
	Left	Right	Left	Right	Left	Right	Left	Right	Left	Right
263	20.47	20.47	10.37	3.98			**6.26**	1.12	**12.39**	6.34
273	20.46	20.49	**10.58**	3.88			6.11	1.08	12.34	6.32
283	20.46	20.51	10.41	3.74	14.4	**15.07**	5.96	1.05	12.27	6.31
293	20.44	20.53	10.23	3.57	14.42	15.01	5.82	1.01	12.17	6.29
303	20.43	**20.54**	10.05	3.38	14.16	14.94	5.67	0.98	12.04	6.26
313	20.41	20.18	9.88	3.27	13.96	14.85	5.53	0.94	11.85	6.22



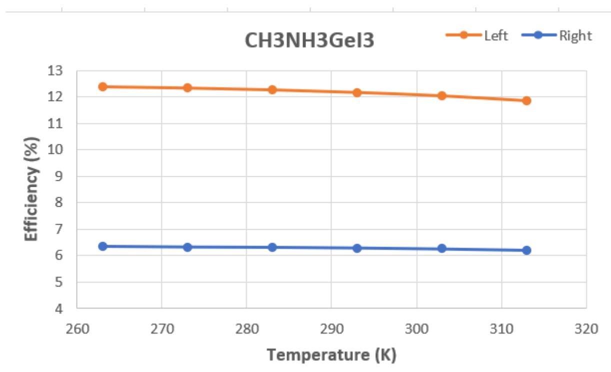


(i) (ii)



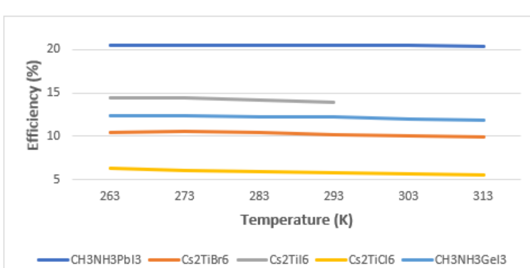


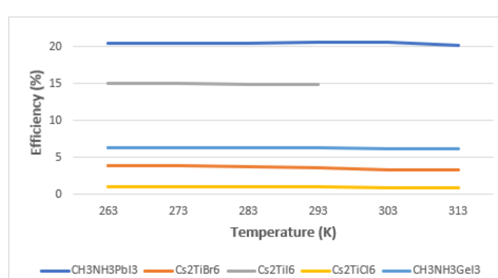
(iii) (iv)



(v)

Graph 3. Efficiency v/s Temperature curves for PVSCs when light comes from HTL and ETL side. (i)$CH_3NH_3PbI_3$, (ii) Cs_2TiBr_6, (iii) Cs_2TiI_6, (iv) Cs_2TiCl_6, (v)$CH_3NH_3GeI_3$.





(i) (ii)

Figure 4.4. Comparative Efficiency v/s Temperature curve for studied PVSCs
(i) when light comes from Left (HTL side), (ii) when light comes from right (ETL side)

It is observed that the power conversion efficiency (η) of the PVSCs increase, reaches a maximum and then decrease with increase in device temperatures. The maximum efficiency of all the PVSCs doesn't lie outside 303 K (29 ^{0}C).

Within 303 K temperature range, the solar panel efficiency is mostly affected negatively as temperature increases. The reason might be, the forbidden gap between the two bands (valence and conduction band) narrows as the temperature rises, and electrons move from the valence band to the conduction band. As a result, as the temperature of the solar cell rises, the density of charge carriers rises as well, hence increasing the efficient solar efficiency. But, after certain temperature, the efficiency starts falling. The reason being, at that certain temperature the number of charge carriers has highly increased. So, with increase in temperature now, the thermal velocity of the charge carriers increases and as a result, the number of collisions between the charge carriers increases, hence, decreasing the solar efficiency onwards.

TABLE 5: Comparison of maximum efficiencies observed for various PVSCs against various parameters(Defect density, thickness and temperature)

	Max. η (**$CH_3NH_3PbI_3$**)		**Max.** η (**$CH_3NH_3GeI_3$**)		**Max.** η (**Cs_2TiBr_6**)		**Max.** η (**Cs_2TiI_6**)		**Max.** η (**Cs_2TiCl_6**)	
	Left	**Right**	**Left**	**Right**	**Left**	**Right**	**Left**	**Right**	**Left**	**Right**
Defect density	**20.11%** (1E+10 cm-3)	19.23% (1E+10 cm-3)	9.89% (1E+10-1E+11 cm-3)	3.81% (1E+10-1E+14 cm-3)	7.42% (1E+9-1E+12 cm-3)	3.53% (1E+9-1E+12 cm-3)	14.35% (1E+10 cm-3)	14.86% (1E+10 cm-3)	5.53% (1E+10-1E+12 cm-3)	0.46% (1E+10-1E+14 cm-3)
Thickness	20.29% (0.3-0.7 µm)	**20.57%** (1 µm)	12.77% (1.4 µm)	5.58% (1.4 µm)	11.95% (2.5 µm)	3.65% (0.1 µm)	14.06% (4 µm)	15.09% (3-3.5 µm)	6.22% (4 µm)	0.47% (2-2.5 µm)
Temperature	20.47% (263 K)	**20.54%** (298 K-303 K)	12.39% (263 K)	6.34% (263 K)	10.58% (273 K)	3.98% (263 K)	14.42% (293 K)	15.07% (283 K)	6.26% (263 K)	1.12% (263 K)

CONCLUSION

In this paper, of all the PVSCs with different perovskite materials that have been studied, it is found that, $CH_3NH_3PbI_3$ shows maximum efficiency when operated under similar device temperature, layer thickness and defect density variations when compared with other PVSCs ($CH_3NH_3GeI_3$, Cs_2TiBr_6, Cs_2TiI_6 and Cs_2TiCl_6). $CH_3NH_3PbI_3$ shows maximum efficiency (> 20%) at device temperature (298 K- 303 K), layer thickness (1 µm) and defect density of 1010 cm-3. However, $CH_3NH_3PbI_3$ has a problem of toxicity, due to the presence of lead content in it. We need an environment friendly alternative for a sustainable PVSC. A comparative account of different PVSCs shown in Table 4 reveals that Cs_2TiI_6 is a secondbest choice, having device efficiencies in the range of 14-16%. Also, Cs_2TiI_6 has much lower toxicity as compared to $CH_3NH_3PbI_3$. As a result of our study, we propose Cs_2TiI_6 as a potential candidate to replace $CH_3NH_3PbI_3$.Further research needs to be undertaken in this direction to maximize the efficiencies of Cs_2TiI_6 based solar cells.

Also, it is found that, the efficiency of the solar cells depends on various factors such as defect density, layer thickness of different solar layers and device temperature of the solar cell. For obtaining a maximum solar efficiency in solar cells, a certain level of defect density, layer thickness and device temperature should be maintained, and any alternation in their magnitudes can alter the effective solar efficiency.

APPENDIX

TABLE 4.1: Parameters of ETL, different PVKs and HTL layers

	PEDOT/PSS (Hima, et al., 2019)	**$CH_3NH_3PbI_3$** (Hima, et al., 2019)	**$CH_3NH_3GeI_3$** (Singh, Agarwal, & Agarwal , 2020)	**Cs_2TiBr_6** (Chen, et al., 2018)	**Cs_2TiI_6** (Chakraborty, Choudhury, & Paul, 2019)	**Cs_2TiCl_6** (Chakraborty, Choudhury, & Paul, 2019)	**PCBM** (Hima, et al., 2019)
Thickness (µm)	0.0800	0.8	0.4	0.2	0.5	0.5	0.5
Band gap (eV)	2.2	1.55	1.9	1.8	1.8	2.23	2.100
Electron affinity (eV)	2.9	3.75	3.98	4	4.2	4	3.9
Dielectric affinity (eV)	3.000	6.500	10.00		18.00	19.00	3.900
CB effectivedensity of states (cm^{-3})	2.200E+15	2.200E+15	1.000E+16	6.000E+19	6.000E+19	6.000E+19	2.200E+19
VB effectivedensity of states(cm^{-3})	1.800E+18	2.200E+17	1.000E+16	2.140E+19	2.140E+19	2.140E+19	2.200E+19
Electronthermal velocity (cm/s)	1.00E+7	1.00E+7	1.00E+7	1.00E+19	1.00E+19	1.00E+19	1.000E+7
Hole thermalvelocity (cm/s)	1.00E+7	1.00E+7	1.00E+7	1.00E+19	1.00E+19	1.00E+19	1.000E+7
Electron mobility (cm^2/V.s.)	0.01	2.0	1.62E+5	0.236	4.4	4.4	0.001
Hole mobility(cm^2/V.s.)	0.0002	2.0	1.01E+5	0.171	2.5	2.5	0.002
Donor density Nd (cm^{-3})	1.000E+13	1.000E+13	1.000E+9	3.000E+19	1.000E+19	1.000E+19	1.000E+16
Acceptor density Na (cm^{-3})	1.000E+16	1.000E+16	1.000E+9	3.000E+18	1.000E+19	1.000E+19	1.000E+13
Defect density (cm^{-3})	1.000E+15	1.000E+15	1.000E+16	4.170E+15	4.170E+15	4.170E+15	1.000E+15

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