MINOR PROJECT -1

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JIIT'62

Team Group - 1

Optimizing Perovskite Solar Cell Performance

Team Members

- Nishant Dwivedi -22102004 (A1)
- Vibhor Yadav -22102005 (A1)
- Priyanshu Agarwal -22102236 (A8)

Supervisor

Dr. Rishibrind Kumar Upadhyay
Senior Grade Assistant Professor

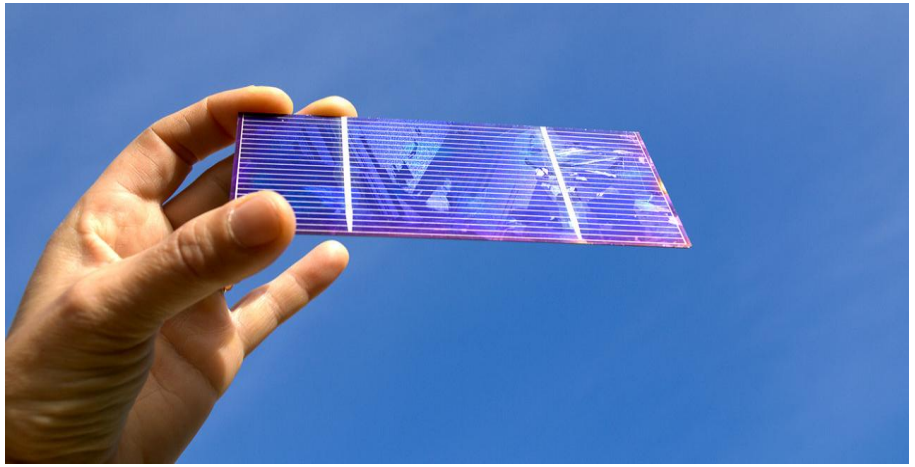
Introduction

Importance in Renewable Energy

•Solar cells are key to reducing greenhouse gas emissions and meeting global energy demands sustainably.
•Perovskites have the potential to complement or replace silicon in applications where cost and versatility are critical.

What are Silicon-Based Solar Cells?

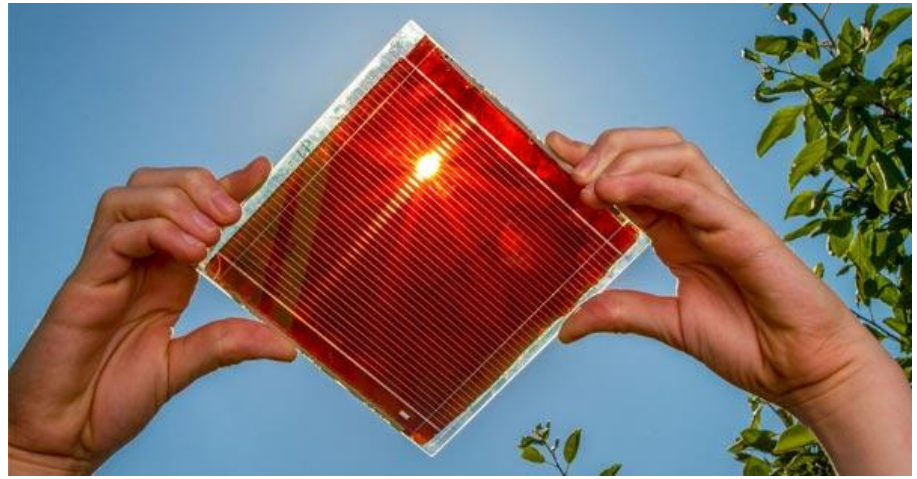
•Silicon-based solar cells are the most widely used photovoltaic technology today, dominating the market for decades.
•They rely on crystalline silicon as the primary material for converting sunlight into electricity.
•Highly reliable, they achieve efficiencies of 15–25% under standard conditions, but their performance is nearing theoretical limits (~33%).



What are Perovskite Solar Cells?

•Perovskite solar cells (PSCs) are an innovative type of photovoltaic device that use perovskite-structured materials as the light-harvesting layer.

•Known for their rapid efficiency advancements, lightweight nature, and potential for low-cost manufacturing, they represent a breakthrough in solar technology.



Perovskite vs. Silicon Solar Cells

•**Silicon Solar Cells**: Mature technology, but production is energy-intensive and costly. Their rigid structure limits applications like flexible and lightweight devices.

•**Perovskite Solar Cells**: Offer higher efficiency potential, simpler fabrication methods, and the ability to integrate with flexible or transparent substrates.

Objectives and Problem Statement

- **Objectives**:
  - To enhance the efficiency of perovskite solar cells.
  - To develop lead-free materials for perovskite solar cells to make them environmentally friendly.

- **Problem Statement**:
- Current perovskite solar cells face challenges of toxicity (e.g., lead content) and efficiency, limiting their commercial viability. Our project aims to address these issues, making them a more sustainable option for the future.

GLOBAL SCOPE

•**Justification**: The project addresses global energy challenges by improving the efficiency and environmental sustainability of solar cells, contributing to clean energy initiatives worldwide.

•**Impact**: Global adoption of perovskite solar cells could revolutionize the renewable energy sector, reducing reliance on non-renewable sources and mitigating climate change.

Methodology Overview

- **Material Research**: Focus on identifying non-toxic materials to replace lead.
- **Simulation**: Using advanced simulation tools(**SCAPS-1D**) to model the behavior and efficiency of perovskite cells.
- **Fabrication**: Developing a prototype to test material properties and performance.

Group Contributions Overview

- **Vibhor Yadav:** Methylammonium lead halide $CH_3NH_3Pb(I_{1-x}Cl_x)_3$(Perovskite) –Lead Based Simulation and optimization.

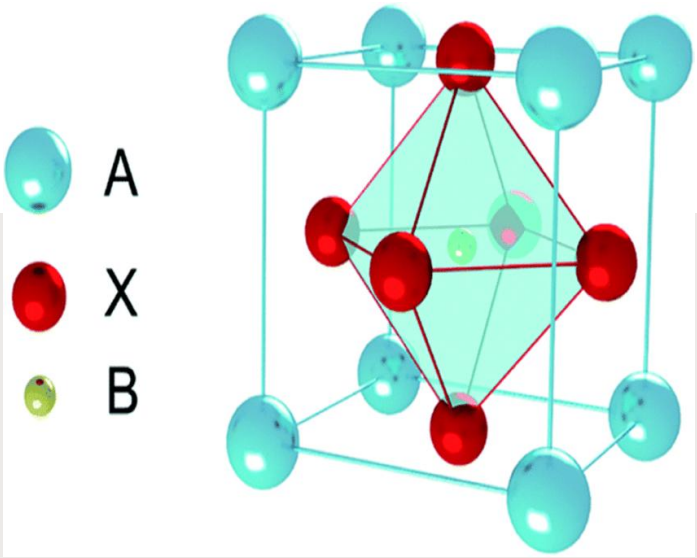
- **Nishant Dwivedi:** $CH_3NH_3SnBr_3$ (methylammonium tin bromide)– Lead Free Simulation and optimization.

- **Priyanshu Agarwal:** "Lead-Free Double Perovskite" Cs_2TiBr_6–Simulation and optimization.

Member 1's Material and Results

Material Overview

Methylammonium lead halide ($CH_3NH_3Pb(I_{1-x}Cl_x)_3$) is a hybrid organic-inorganic material used in **perovskite solar cells**. It has a unique **perovskite crystal structure**, where lead (Pb) is surrounded by halide ions (Iodine and Chlorine) and the **methylammonium (CH_3NH_3)** organic cation.



Key Points:

- **High Efficiency**: Excellent light absorption and power conversion, making it a promising alternative to silicon solar cells.
- **Tunability**: The halide composition (Iodine and Chlorine) can be adjusted to fine-tune its optical properties.
- **Low-cost**: Can be produced using simple solution-based methods at low temperatures.
- **Challenges**: Instability (degradation from moisture, heat) and **lead toxicity**, which are being addressed by researchers.

Simulation Setup and Parameter Changes

Table 1: Input parameters of the absorber layer, ETL and TCO.

Parameters	TCO[15]	TiO_2[15,16]	ZnO[17]	SnO_2[18,19]	Zn(O,S)[20]	PCBM[21]	$MAPbI(I_{1-x}Cl_x)_3$[15]
Thickness (nm)	400	70	70	70	70	70	450
Bandgap, Eg (eV)	3.5	3.2	3.3	3.5	2.83	2.0	1.55
Electron affinity χ (eV)	4	4.26	4.1	4	3.6	3.9	3.93
Relative dielectric permittivity, Єr	9	10	9	9	9	4	6.5
CB effective density of states Nc(cm^{-3})	2.2×10^{18}	2.2×10^{18}	4.0×10^{18}	2.2×10^{18}	2.2×10^{18}	2.5×10^{19}	2.2×10^{17}
VB effective density of states Nv(cm^{-3})	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.9×10^{19}	2.5×10^{19}	1.8×10^{19}
Electron mobility μn($cm^2V^{-1}S^{-1}$)	20	20	100	20	100	0.2	20
Hole mobility μh($cm^2V^{-1}S^{-1}$)	10	10	25	10	15	0.2	20
Shallow uniform donor density ND (cm^{-3})	12.0×10^{19}	6.0×10^{19}	1.0×10^{18}	1.0×10^{17}	1.0×10^{19}	5.0×10^{17}	-
Shallow uniform acceptor density NA (cm^{-3})	-	-	-	-	-	-	-
Total defect density Nt (cm^{-3})	-	-	-	-	-	-	1.0×10^{14}

Table 2 Input parameters of the HTLs.

Parameters	Spiro-MeOTAD[17]	PEDOT:PSS[15,21]	CuO[15]	Cu_2O[15,20]	CuSCN[15,19]	$CuSbS_2$[19]
Thickness (nm)	100	100	100	100	100	100
Bandgap, Eg (eV)	3.0	1.8	1.5	2.1	3.6	1.58
Electron affinity χ (eV)	2.45	3.5	4.07	3.2	1.7	4.2
Relative dielectric permittivity, Єr	3	10	18.1	7.11	10	14.6
CB effective density of states Nc(cm^{-3})	2.2×10^{18}		2.2×10^{19}	2.2×10^{18}	2.5×10^{18}	2.0×10^{18}
VB effective density of states Nv(cm^{-3})		2.2×10^{18}	5.5×10^{20}	1.9 ×1019	1.8 ×1019	1.0×10^{19}
Electron mobility μn($cm^2V^{-1}S^{-1}$)			100	200	100	49
Hole mobility μh($cm^2V^{-1}S^{-1}$)	1.9 ×1019	1.8 ×1019	0.1	8600	25	49
Shallow uniform donor density ND (cm^{-3})	50	100	-	-	-	-
Shallow uniform acceptor density NA (cm^{-3})	50	4	1.0×10^{15}	1.0×10^{18}	1.0×10^{18}	1.0×10^{18}

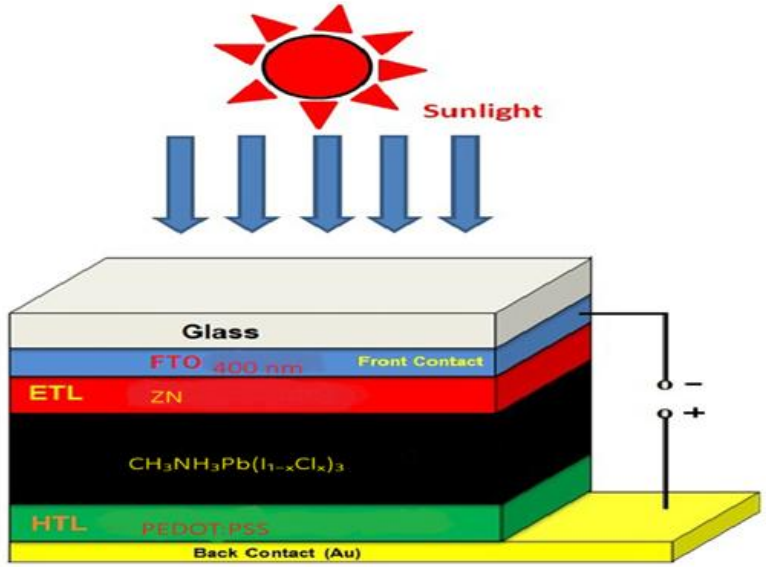


Table 3 Input parameters of interface defect and absorber defect.[15]

Parameters and units	$CH_3NH_3Pb(I_{1-x}Cl_x)_3$	ETL/$CH_3NH_3Pb(I_{1-x}Cl_x)_3$ interface	$CH_3NH_3Pb(I_{1-x}Cl_x)_3$/HTL interface
Defect type	Neutral	Acceptor	Acceptor
Capture cross section for electrons and holes (cm^2)	2.0×10^{-14},2.0×10^{-14}	1.0×10^{-17},1.0×10^{-18}	1.0×10^{-18},1.0×10^{-19}
Energetic distribution	Gaussian	Single	Single
Energy level with respect to EV (above EV, eV)	0.6	0.6	0.6
Characteristic energy (eV)	0.1	-	-
Total density (cm^{-3})	1.0×10^{13}	1.0×10^{10}-1.0×10^{12}	1.0×10^{10}-1.0×10^{12}

Results and Final Efficiency

- The maximum efficiency, FF, J_{SC}, and V_{oc} **24.98%**, 85.19%, 23.32 mA/cm^2 and 1.257 volt respectively attained by perovskite $CH_3NH_3Pb(I_{1-x}Cl_x)_3$ using PEDOT: PSS, Zn (O, S), as hole transport and electron transport layer materials respectively.

HTLs and ETLs

PSC Structure	VOC (V)	JSC (mA/cm2)	Fill factor (%)	PCE (%)
FTO/TiO2/CH3NH3Pb($_{I1-x}$Clx)$_3$/NiO/Au	1.2534	23.054548	85.7	24.77
FTO/TiO$_2$/CH3NH3Pb(I1-xClx)3/PEDOT:PSS/Au	1.2513	23.321027	85.5	24.95
FTO/ZnO/CH3NH3Pb(I1-xClx)3/NiO/Au	1.2583	23.054094	84.91	24.63
FTO/ZnO/CH3NH3Pb(I1-xClx)3/PEDOT:PSS/Au	1.2557	23.320667	84.74	24.82
FTO/SNO2/CH3NH3Pb(I1-xClx)3/PEDOT:PSS/Au	1.2569	23.322332	85.1	24.95
FTO/ZN/CH3NH3Pb(I1-xClx)3/NiO/Au	1.2601	23.057322	85.29	24.78
FTO/ZN/CH3NH3Pb(I1-xClx)3/PEDOT:PSS/Au	1.2574	23.322069	85.19	24.98
FTO/PCBM/CH3NH3Pb(I1-xClx)3/PEDOT:PSS/Au	1.2542	23.396186	85.04	24.95
FTO/PCBM/CH3NH3Pb(I1-xClx)3/NiO/Au	1.2568	23.17012	85.13	24.79

Member 2's Material and Results

Material Overview

Methylammonium tin bromide ($CH_3NH_3SnBr_3$) is a hybrid organic-inorganic perovskite material, where tin (Sn) is surrounded by bromide ions (Br), and methylammonium (CH_3NH_3) acts as the organic cation. It is used as a lead-free alternative in perovskite solar cells.

Key Points:

•**Lead-Free**: Replaces lead with tin (Sn), addressing concerns about lead toxicity in solar cells.

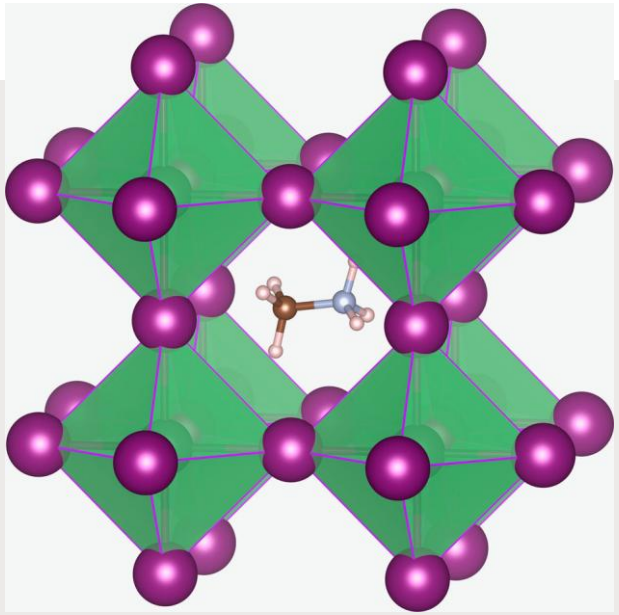
•**Good Efficiency**: Offers promising light absorption and potential for decent power conversion efficiency, although slightly lower than lead-based perovskites.

•**Tunability**: The bromide composition can be adjusted, making it possible to tailor its optical and electronic properties.

•**Low-Cost**: Similar to other perovskite materials, it can be processed using solution-based methods, reducing production costs.

•**Challenges**:

- **Lower Stability**: Tin-based perovskites generally show lower stability compared to lead-based perovskites.
- **Efficiency Gap**: While still efficient, it generally underperforms in comparison to lead-based materials, making it a subject of ongoing research.
- **Moisture Sensitivity**: Like other perovskites, it is sensitive to moisture, which can lead to degradation.



Simulation Setup and Parameter Changes

Table 1: Input parameters of the absorber layer, ETL and TCO.

Parameters	TCO[15]	TiO_2[15,16]	ZnO[17]	Zn(O,S)[16]	$CH_3NH_3SnBr_3$
Thickness (nm)	400	70	70	70	500
Bandgap, Eg (eV)	3.5	3.2	3.3	2.83	1.3
Electron affinity χ (eV)	4	4.26	4.1	3.6	4.17
Relative dielectric permittivity, Єr	9	10	9	9	10
CB effective density of states Nc(cm^{-3})	2.2×10^{18}	2.2×10^{18}	4.0×10^{18}	2.2×10^{18}	2.2×10^{18}
VB effective density of states Nv(cm^{-3})	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.9×10^{19}	1.8×10^{18}
Electron mobility μn($cm^2V^{-1}S^{-1}$)	20	20	100	100	1.6
Hole mobility μh($cm^2V^{-1}S^{-1}$)	10	10	25	15	1.6
Shallow uniform donor density ND (cm^{-3})	2.0×10^{19}	6.0×10^{19}	1.0×10^{18}	1.0×10^{19}	1×10^{13}
Shallow uniform acceptor density NA (cm^{-3})	-	-	-	-	1×10^{13}
Total defect density Nt (cm^{-3})	-	-	-	-	1.0×10^{14}

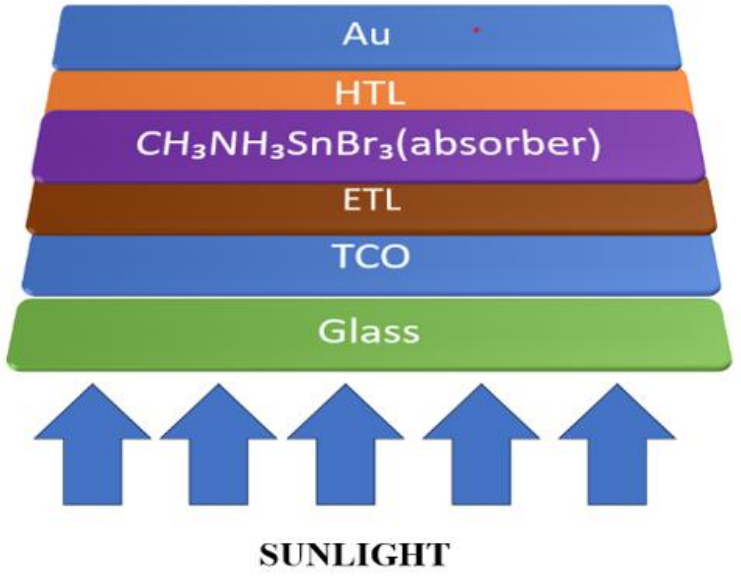


Table 2 Input parameters of the HTLs.

Parameters	Spiro-MeOTAD[17]	PEDOT:PSS[15,21]	CuO[15]	Cu_2O[15]
Thickness (nm)	100	100	100	100
Bandgap, Eg (eV)	3.0	1.8	1.5	2.1
Electron affinity χ (eV)	2.45	3.5	4.07	3.2
Relative dielectric permittivity, Єr	3	10	18.1	7.11
CB effective density of states Nc(cm^{-3})	2.2×10^{18}	2.2×10^{18}	2.2×10^{19}	2.2×10^{18}
VB effective density of states Nv(cm^{-3})	1.9×10^{19}	1.8×10^{19}	5.5×10^{20}	1.9×10^{19}
Electron mobility μn($cm^2V^{-1}S^{-1}$)	50	100	100	200
Hole mobility μh($cm^2V^{-1}S^{-1}$)	50	4	0.1	8600
Shallow uniform donor density ND (cm^{-3})	-	-	-	-
Shallow uniform acceptor density NA (cm^{-3})	1×10^{18}	2×10^{19}	1.8×10^{18}	1.0×10^{18}

Table 3 Input parameters of interface defect and absorber defect.[15]

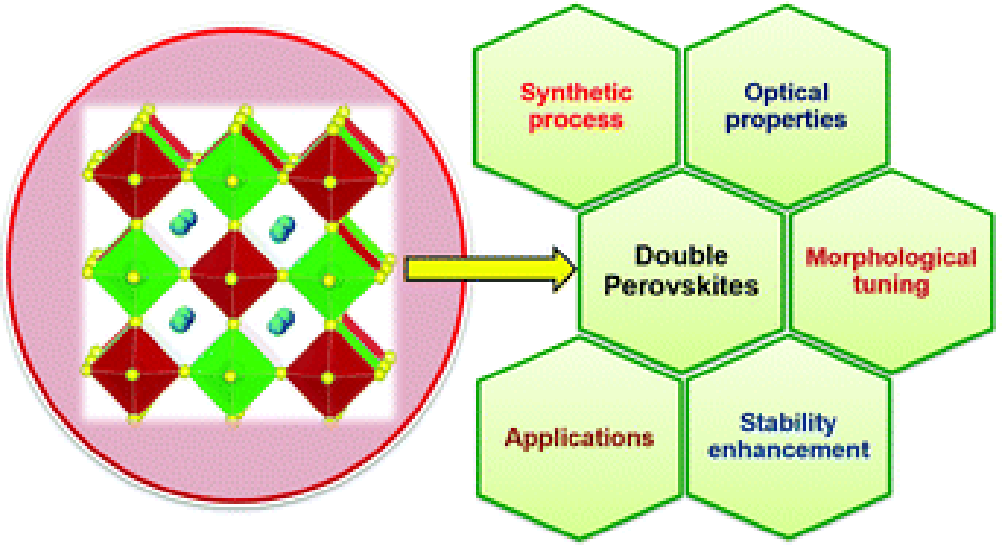
Parameters and units	$CH_3NH_3SnBr_3$	ETL/$CH_3NH_3SnBr_3$ interface	$CH_3NH_3SnBr_3$ /HTL interface
Defect type	Neutral	Acceptor	Acceptor
Capture cross section for electrons and holes (cm^2)	2.0×10^{-14},2.0×10^{-14}	1.0×10^{-17},1.0×10^{-18}	1.0×10^{-18},1.0×10^{-19}
Energetic distribution	Gaussian	Single	Single
Energy level with respect to EV (above EV, eV)	0.6	0.6	0.6
Characteristic energy (eV)	0.1	-	-
Total density (cm^{-3})	1.0×10^{13}	1.0×10^{10}-1.0×10^{12}	1.0×10^{10}-1.0×10^{12}

Results and Final Efficiency

Considering all optimization parameters, the $CH_3NH_3SnBr_3$ based perovskite solar cell achieved a maximum PCE of 27.26%, with Voc of 1.019 V, Jsc of 32.47 mA/cm², and FF of 82.37%.

Structure of PSCs	Voc(V)	JSC (mA/cm^2)	FF(%)	PCE(%)
FTO/ZnO/CH3NH3SnBr3/Spiro-MeOTAD/Au	1.019	32.473836	82.37	27.26
FTO/ZnO/CH3NH3SnBr3/PEDOT:PSS/Au	1.0135	32.552702	81.72	26.96
FTO/ZnO/CH3NH3SnBr3/NiO/Au	1.0166	32.473743	82.47	27.22
FTO/ZnO/CH3NH3SnBr3/CuO/Au	0.7812	32.771102	81.55	20.88
FTO/ZnO/CH3NH3SnBr3/Cu2O/Au	1.0151	32.499867	81.13	26.76
FTO/ZN/CH3NH3SnBr3/PEDOT:PSS/Au	1.0164	19.710055	36.33	7.28
FTO/ZN/CH3NH3SnBr3/NiO/Au	1.0195	19.787555	36.28	7.32
FTO/ZN/CH3NH3SnBr3/CuO/Au	0.7833	16.716404	39.7	5.2
FTO/ZN/CH3NH3SnBr3/Cu2O/Au	1.018	19.745987	36.31	7.3

Member 3's Material and Result



Material Overview

Cs_2TiBr_6 is a **perovskite-like compound** made up of **cesium (Cs)**, **titanium (Ti)**, and **bromine (Br)** ions. It has a similar crystal structure to traditional perovskite materials but with a different metal (titanium) instead of lead. This compound has gained attention due to its potential use in **solar cells** and other optoelectronic devices, offering a non-toxic alternative to lead-based perovskites.

- **Structure**: It adopts a **3D perovskite structure**, where titanium is coordinated by bromine anions, and cesium acts as a cation.
- **Properties**: Cs_2TiBr_6 exhibits promising **light absorption** properties and **stability**, making it a good candidate for photovoltaic applications.
- **Advantages**: The absence of lead makes it **environmentally friendly**, and its stability in moisture improves its potential for long-term applications.

Simulation Setup and Parameter Changes

TABLE 1 INPUT PARAMETERS OF ETLs

PARAMETERS	FTO	TiO2	Zno	STO	IGZO	PCBM	Znse	CdS	WO3
Thickness (nm)	500	30	30	30	30	30	30	30	30
BandGap , Eg(eV)	3.2	3.2	3.3	3.2	3.05	2	2.81	2.4	2.92
Electrno affinity X (eV)	4.4	3.9	4.1	4.0	4.16	3.9	4.09	4.18	4.590
Realtive Dielectric Permittivity	9	9	9	8.7	10	4	8.6	10	5.76
CB , Effective density of states Nc (cm-3)	$2.2X10^{18}$	$1X10^{21}$	$4X10^{18}$	$1.7X10^{19}$	$5X10^{18}$	$1X10^{21}$	$2.2X10^{18}$	$2.2X10^{18}$	$1.96X10^{19}$
VB , effective density of states Nv (cm-3)	$1.8X10^{19}$	$2X10^{20}$	$1X10^{19}$	$2X10^{20}$	$5X10^{18}$	$1.8X10^{19}$	$1.8X10^{18}$	$1.9X10^{19}$	$1.96E^{19}$
Electron mobility (cm2v-1s-1)	90	20	100	$5.3X10^{3}$	15	$1E^{-2}$	$4x10^{2}$	100	$1E^{+1}$
Hole mobility (cm2v-1s-1)	90	10	25	$6.6X10^{2}$	0.1	$1E^{-2}$	$1.1x10^{2}$	25	$1E^{+1}$
Shallow uniform donor density ND (cm-3)	$7X10^{2}$	$1X10^{19}$	$1X10^{18}$	$2X10^{16}$	$1X10^{18}$	$1E^{+20}$	$1x10^{18}$	$1X10^{18}$	$3.68E^{+19}$
Shallow acceptor density NA (cm-3)	0	0	0	0	0	0	0	0	0
Total defect density Nt (cm-3)	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$

TABLE 2 INPUT PARAMETERS OF HTLs.

PARAMETERS	Cu20	CuAlO2	CuSbS2	CuSCN	MoO3	Spiro-OMeTAD	P3HT	PEDOT:PSS	Cs2TiBr6
Thickness (nm)	30	30	30	30	30	30	30	30	900
BandGap , Eg(eV)	2.17	3.46	1.58	3.2	3	3	1.85	2.2	1.6
Electrno affinity X (eV)	3.2	2.5	4.2	1.9	2.5	2.45	3.1	2.9	4.47
Realtive Dielectric Permittivity	7.1	60	14.6	10	12.5	3	3.4	3	10
CB , Effective density of states Nc (cm-3)	$2.02x10^{17}$	$2.2X10^{18}$	$2X10^{18}$	$2.2X10^{19}$	$2.2X10^{18}$	$1X10^{19}$	$1E^{+22}$	$2.2E^{+15}$	$1E^{19}$
VB , effective density of states Nv (cm-3)	$1.1x10^{19}$	$1.8X10^{19}$	$1X10^{-4}$	$1.8X10^{19}$	$1.8X10^{19}$	$1X10^{19}$	$1E^{+22}$	$2.2E^{+17}$	$1E^{19}$
Electron mobility (cm2v-1s-1)	200	2	49	$1X10^{-4}$	100	$2X10^{-4}$	$1E^{-4}$	$2X10^{-3}$	4.4
Hole mobility (cm2v-1s-1)	80	8.6	49	$1X10^{-1}$	25	$2X10^{-4}$	$1E^{-4}$	$2X10^{-3}$	2.5
Shallow uniform donor density ND (cm-3)	0	0	0	0	0	0	0	0	$1E^{+19}$
Shallow acceptor density NA (cm-3)	$9 X 10^{21}$	$3 X 10^{18}$	$1.38X^{18}$	$1X10^{15}$	$1X10^{18}$	$2X10^{18}$	$3.17E^{13}$	$1E^{+17}$	$1E^{+19}$
Total defect density Nt (cm-3)	$1 X 10^{14}$	$1X 10^{14}$	$1 X 10^{14}$	$1 X 10^{14}$	$1 X 10^{14}$	$1 X 10^{14}$	$1 X 10^{14}$	$1 X 10^{14}$	$1 X 10^{14}$

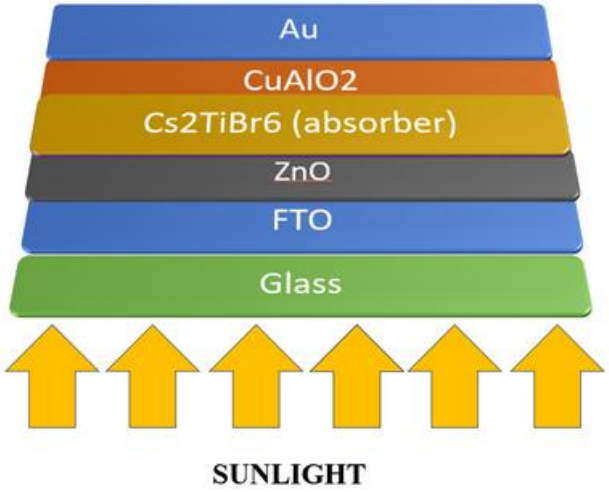


Table 3 . Input Parameters of Interface Defect and Absorber Defect.

Parameters and units	Cs2TiBr6	ETL/Cs2TiBr6 interface	Cs2TiBr6 / HTL interface
DEFECT TYPE	NEUTRAL	Acceptor	Acceptor
Capture cross section for electron and holes (cm2)	$2.0X10^{-14}$, $2X10^{-14}$	$1.0X10^{-17}$, $1X10^{-18}$	$1.0X10^{-18}$, $1X10^{-19}$
Energetic distribution	GAUSSIAN	SINGLE	SINGLE
Energy level with respect to EV (above EV , eV)	0.6	0.6	0.6
Characteristics energy (eV)	0.1	-	-
Total Density (cm-3)	$1.0 X 10^{13}$	$1.0 X 10^{10}$ - $1.0 X 10^{12}$	$1.0 X 10^{10}$ - $1.0 X 10^{12}$

Results and Final Efficiency

Considering all optimization parameters, the Cs_2TiBr_6 based device achieved a maximum efficiency of 73.88%, with Voc of 1.1231 V, Jsc of 23.54 mA/cm², and FF of 19.53%.

Structure of PSCs	Voc (V)	Jsc (mA/cm2)	FF (%)	PCE(%)
Au/ CUALO2 / Cs2TiBr6 / IGZO/FTO	1.1231	23.543828	73.88	19.53
Au/ CUALO2 / Cs2TiBr6 / ZNO/FTO	1.1231	23.543129	73.86	19.53
Au/ CUALO2 / Cs2TiBr6 / TIO2/FTO	1.1267	23.546622	72.46	19.22
Au/ CU2O / Cs2TiBr6 / ZNSE/FTO	0.6726	23.54986	69.26	10.97
Au/CU2O/ Cs2TiBr6 / PCBM/FTO	0.6732	23.551993	68.38	10.84
Au/ CU2O / Cs2TiBr6 / TIO2/FTO	0.6727	23.549836	67.41	10.68
Au/ CU2O / Cs2TiBr6 / ZNO/FTO	0.6614	24.16615	64.38	10.29
Au/ MOO3 / Cs2TiBr6 / CDS/FTO	0.6582	23.551529	60.16	9.33
Au/ MOO3 / Cs2TiBr6 / ZNO/FTO	0.6579	23.546039	60.16	9.32
Au/ MOO3 / Cs2TiBr6 / TIO2/FTO	0.6582	23.549529	58.43	9.06

Certificates of Distinction

We attended a summer school at IISC Bangalore on Advanced fabrication techniques and received a Distinction for our performance . This Achievement has further enhanced our capability to handle comples fabrication projects effectively.

Results and Discussion

- **1. $CH_3NH_3Pb(I_{1-x}Cl_x)_3$**
- **Efficiency**: 24.98%
- **Challenges**: Lead toxicity and instability under moisture and heat.
- **Discussion**: High efficiency but environmental concerns and degradation limit long-term use.
- **2. $CH_3NH_3SnBr_3$**
- **Efficiency**: 27.26%
- **Challenges**: Lower stability and efficiency.
- **Discussion**: Lead-free alternative with lower performance and stability issues.
- **3. Cs_2TiBr_6**
- **Efficiency**: 19.53%
- **Challenges**: Low efficiency, better stability.
- **Discussion**: Stable, lead-free but requires efficiency improvements.

Conclusion

- Optimizing perovskite solar cells is essential to fully realize their potential as a renewable energy source. While efficiencies over 25% have been achieved, challenges such as **stability**, **moisture sensitivity**, and **lead toxicity** need to be addressed for long-term viability.

- Efforts to improve performance focus on enhancing **material stability**, developing **lead-free alternatives**, and fine-tuning **halide compositions**. Advances in **encapsulation** and **fabrication techniques** help protect cells from degradation.

- With continued research and innovation, perovskite solar cells could become a cost-effective, high-efficiency, and environmentally friendly alternative to silicon-based cells, driving the future of **sustainable energy**.

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Thank You