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Impact of Hole Transport Layers in Inorganic Lead-Free B-γ-$CsSnI_3$ Perovskite Solar Cells: A Numerical Analysis

Adnan Hosen[1], Sabrina Rahman[1], Maroua Brella[2], Sheikh Rashel Al Ahmed[1]

[1] Department of Electrical, Electronic and Communication Engineering, Pabna University of Science and Technology, Pbana 6600, Bangladesh.
[2] Laboratoire de Rayonnement et Plasmas et Physique des Surfaces (LRPPS), Université Kasdi Merbah, Ouargla 30000, Algeria.

Outline

- Solar Energy
- Introduction
- Objectives
- Device Architecture
- Simulation
- Results
- Conclusions

Solar Energy

- ❖ Solar power is key to a clean energy future.
- ❖ Solar panels produce electricity by transforming continuous flow of energy from the sun to electricity.

- ❖ No harmful emissions are released into air.
- ❖ Photovoltaic (PV) process doesn't require any fuel and has no variable costs.

In recent years, tin-based B-γ-$CsSnI_3$ PSCs has received substantial interest as a potential material for photovoltaic applications.

- ➢ high efficiency
- ➢ significantly lower cost
- ➢ Simple processing techniques.

Introduction

- The two main types of thin film solar cells are CdTe and CIGS received much wider attention and subsequently achieved the highest cell efficiency of approximately 23%.

  - Toxic Cadmium (Cd) exists in the absorber
  - Volatility in cost of In, Te

- ❑ Black orthorhombic (B-γ) $CsSnI_3$ has several advantages
  - ✓ Reduced bio-toxicity
  - ✓ Cost-effective
  - ✓ long-term durability.
  - ✓ Suitable band gap (~1.3 eV)
  - ✓ High absorption coefficient ($\sim 10^5$ cm^{-1})

However, in the previous works, improper selection of HTL with enhanced recombination at interfaces results in low efficiency of $CsSnI_3$-based perovskite solar cell.

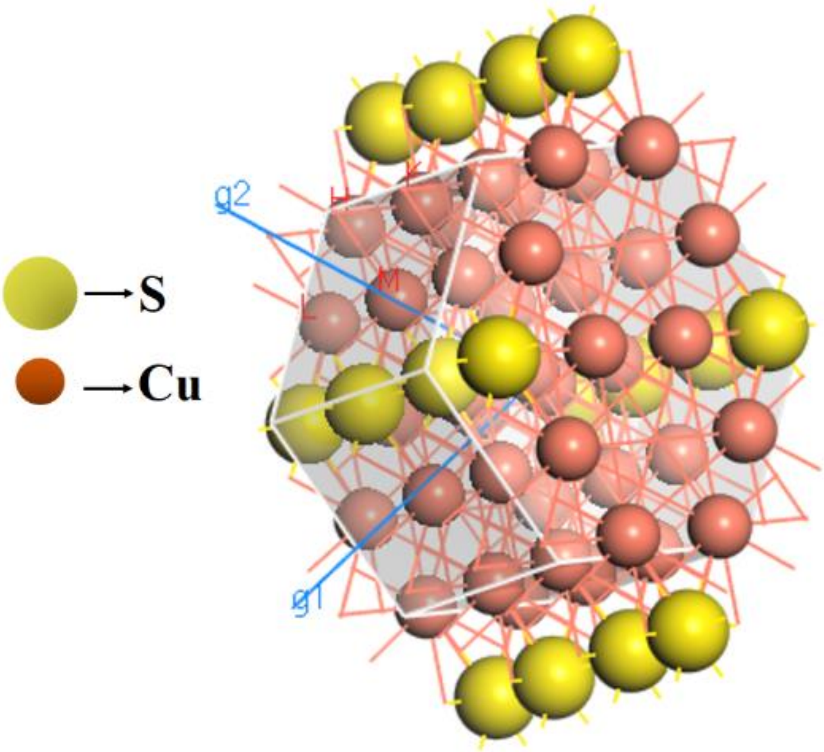
➡ Necessary to explore alternative HTL to achieve excellent PV efficiency.

Objectives

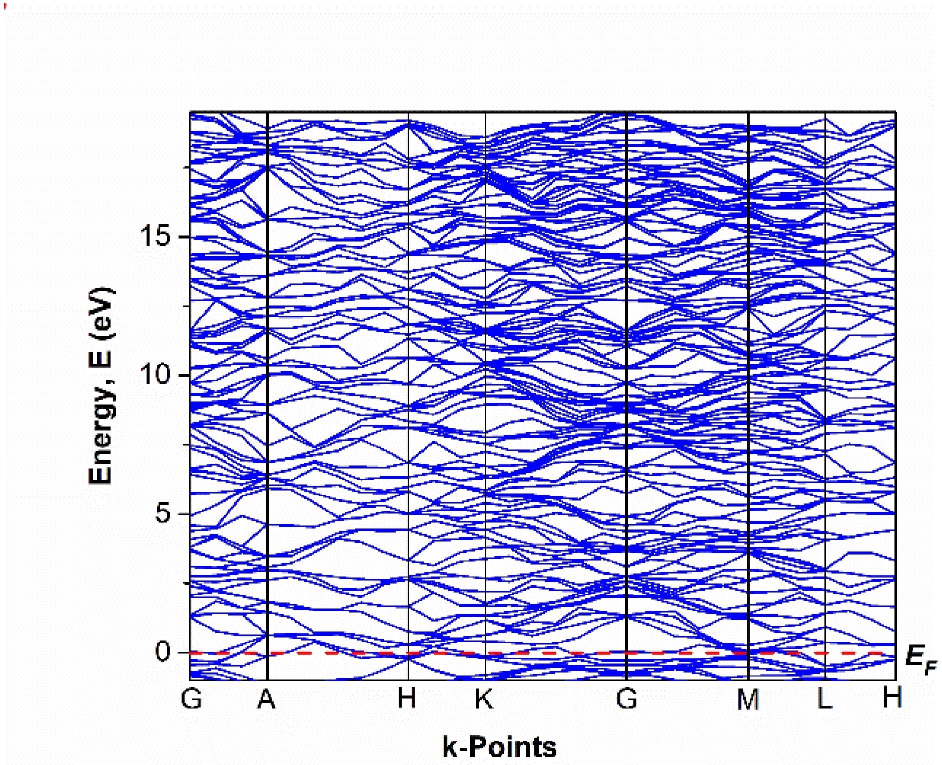
- **To enhance the PV performances of $CsSnI_3$-based PSC**

  - In this study, CuS material as a novel HTL is proposed between $CsSnI_3$ absorber and back contact.
  - Density functional theory (DFT) -extracted physical and optical parameters such as band gap and absorption spectrum of CuS are observed.
  - A comparative study is carried out among CuSCN, CuI, NiO_x, MoO_3, and CuS HTLs in Al/ITO/TiO_2/$CsSnI_3$/HTL/Ni structure using SCAPS-1D simulator.

DFT ANALYSIS OF CuS



(a) Crystal structure

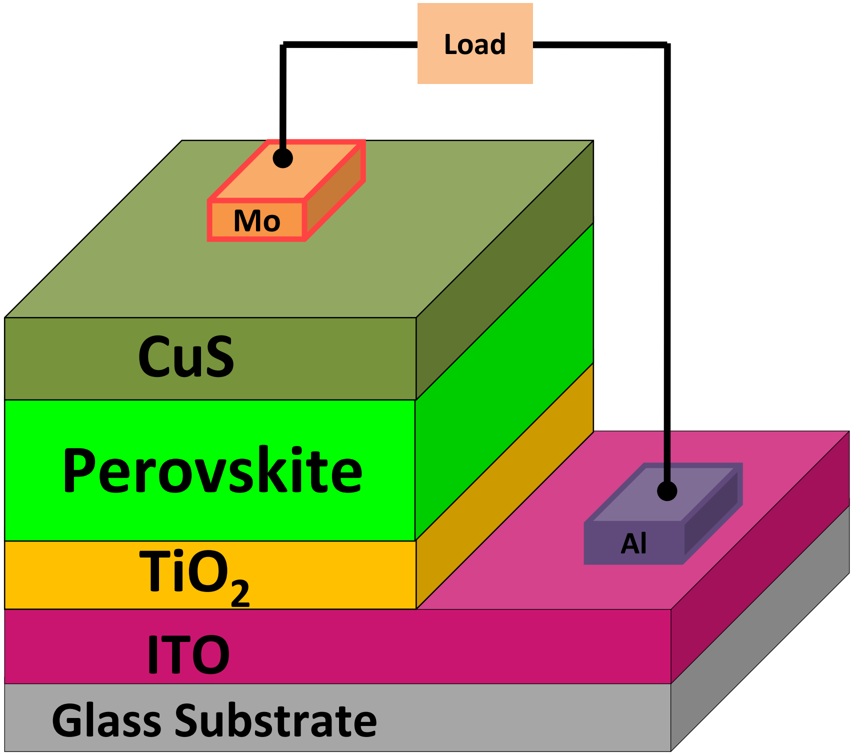


(b) band structure of CuS

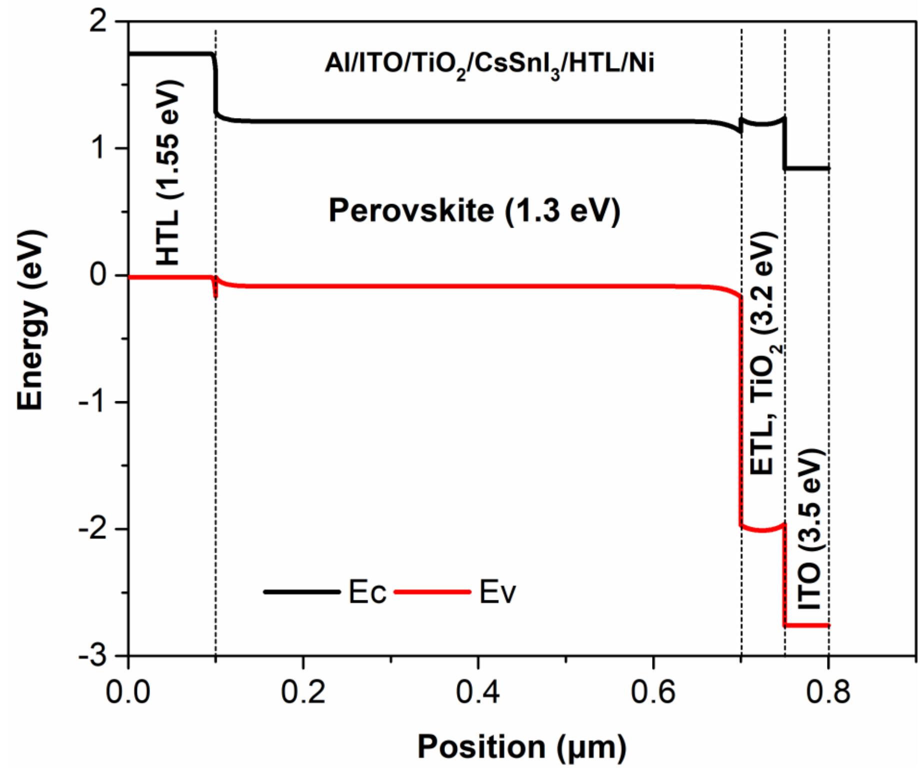
Space Group: $P6_3/mmc$ [194]

The lattice parameters of CuS are a = b = 3.797 Å, c = 16.441 Å, α = β = 90°, γ = 120°

Device Architecture



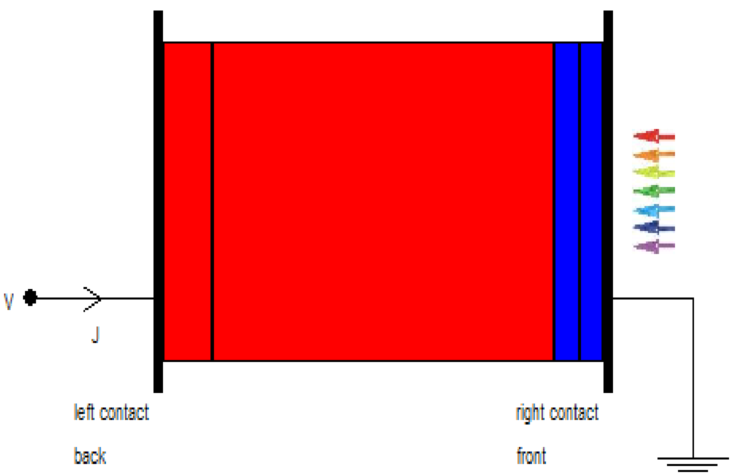
(a) Schematic diagram



(b) Energy band diagram

Simulation

- Device modeling using SCAPS1-D
- Investigation of different HTLs
- Device optimization
- Effects of thickness, acceptor density, defect, and temperature



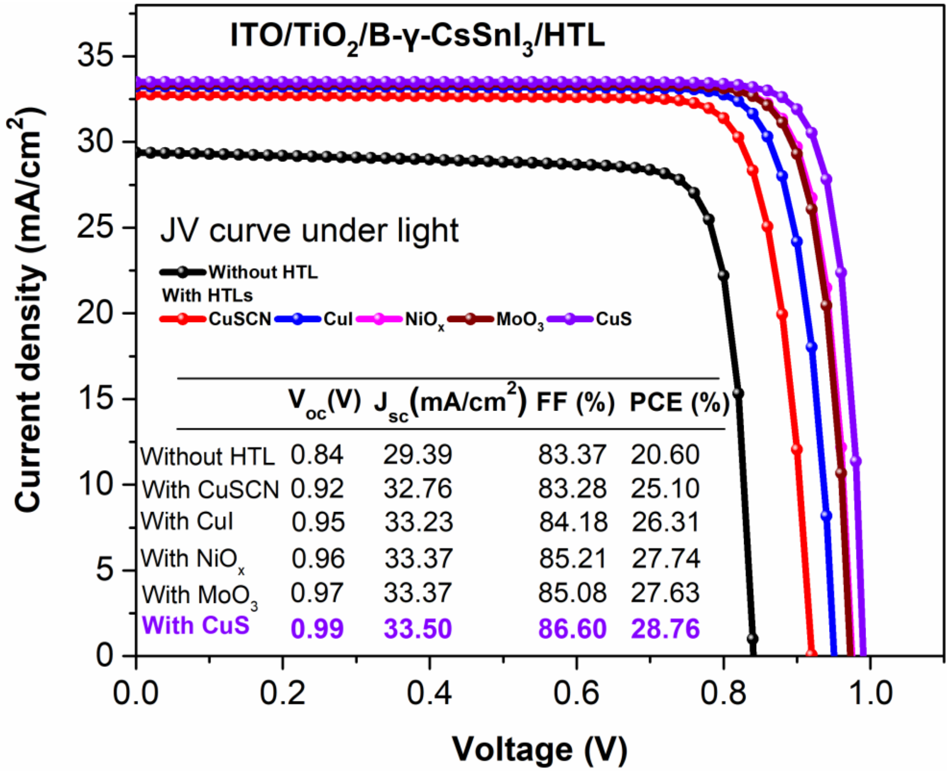
- ✓ Illumination = 100 mW/cm^2
- ✓ light spectrum = AM1.5G
- ✓ operating temperature = 300K.

Simulation parameters

Parameters	CuSCN	CuI	NiO_x	MoO_3	CuS	$CsSnI_3$	TiO_2	ITO
Bandgap, E_g (eV)	3.6	3.1	3.8	3	1.55	1.3	3.2	3.5
Electron affinity, χ (eV)	1.7	2.1	1.46	2.5	3.89	3.8	4.1	4.6
Electron/hole mobility (cm^2 V^{-1} s^{-1})	100/25	100/43.9	12/2.8	25/100	12/9	50/400	0.006	10/10
Thickness (μm)	0.1	0.1	0.1	0.1	0.1	0.6	0.05	0.05
Carrier concentration (cm^{-3})	1×10^{18}	1×10^{18}	1×10^{18}	1×10^{18}	4.7×10^{18}	5×10^{17}	1×10^{18}	1×10^{21}
Reference	[22]	[22]	[23]	[24]	[25]	[26–28]	[29,30]	[31]

Results (1)

Device Optimization



❑ The short-circuit current depends on a number of following factors

- Area of the solar cell
- Number of photons
- Spectrum of the incident light
- Optical properties
- Collection probability

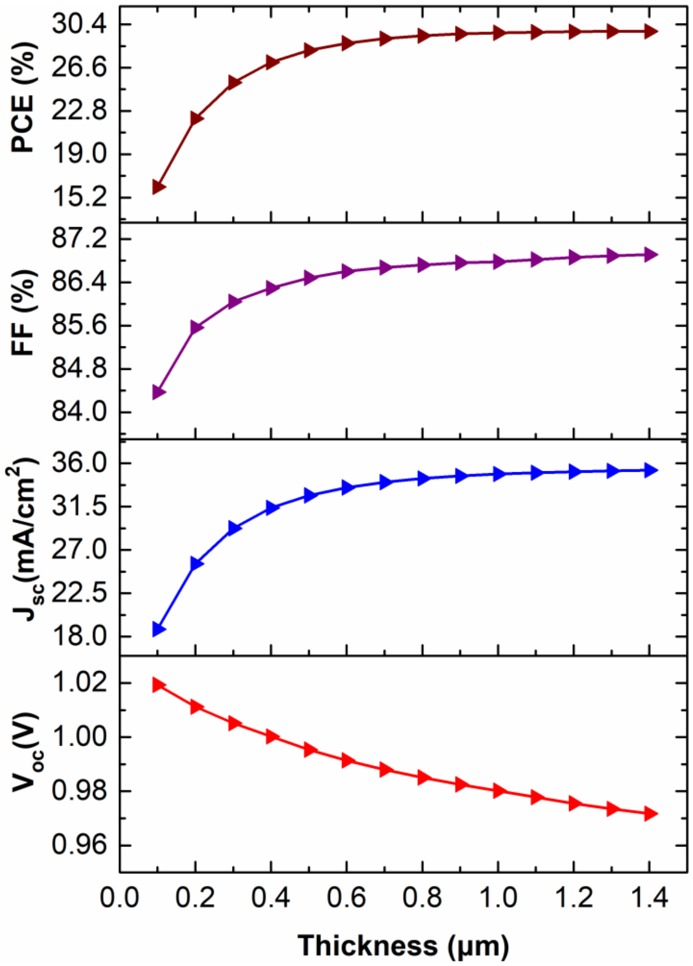
$$J_{sc} = \frac{V_{MP} I_{MP}}{V_{oc} FF}$$

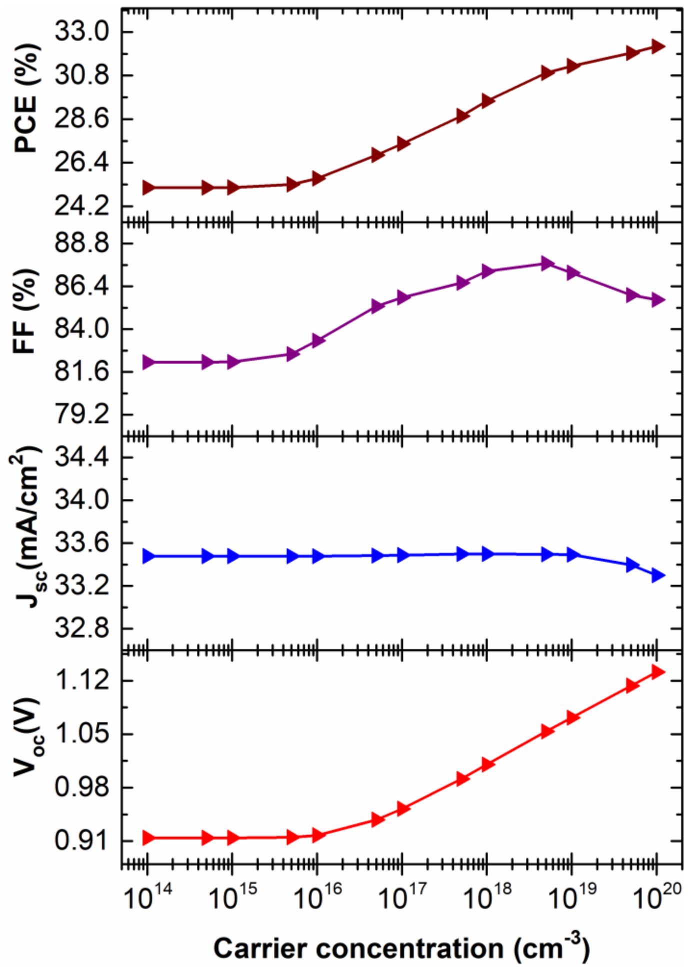
✓ CuS HTL provides better performances

✓ PCE is about 28.76%

Results (2)

Effects of Absorber Thickness and Acceptor Density





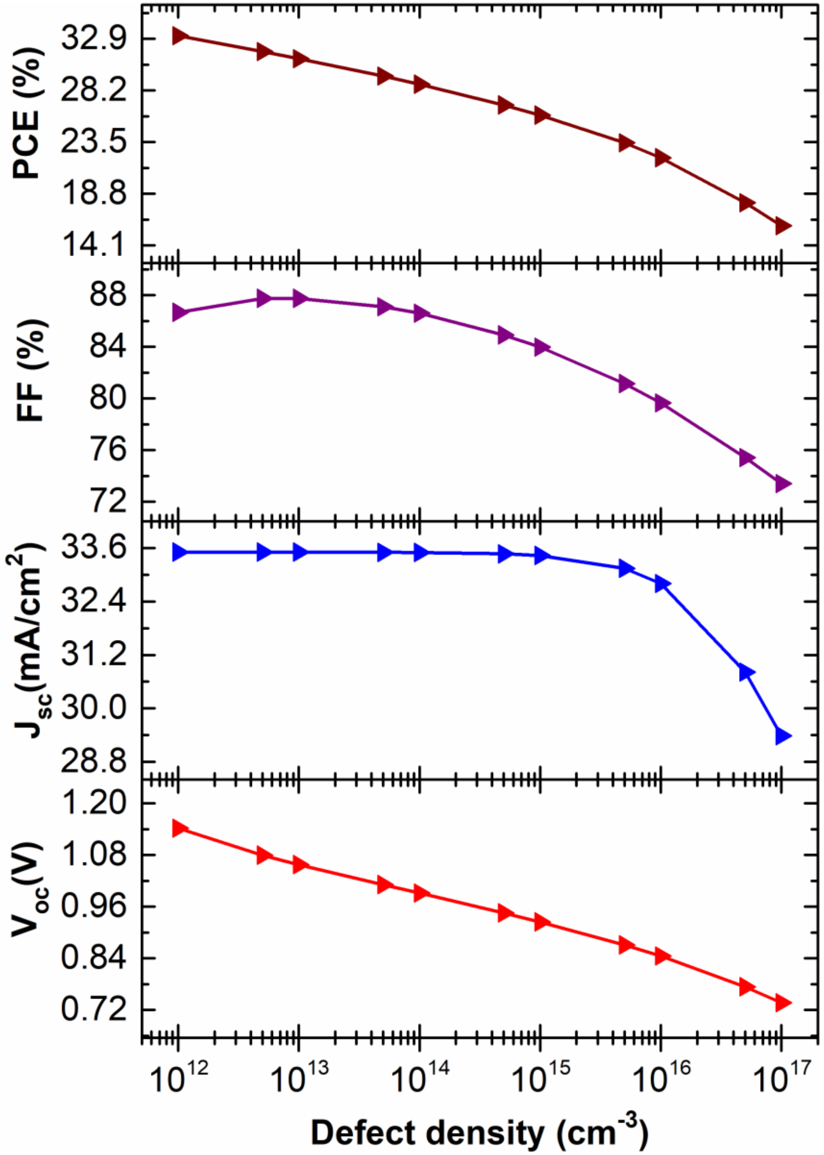
- J_{sc} rises rapidly with increasing thickness .
- Efficiency is increased.

- Efficiency is enhanced with increasing the acceptor density in absorber layer.

Thickness and acceptor density are optimized to be 0.6 μm and 5×10^{17} cm^{-3}.

Results (3)

Effect of Absorber Defect on PV Performance

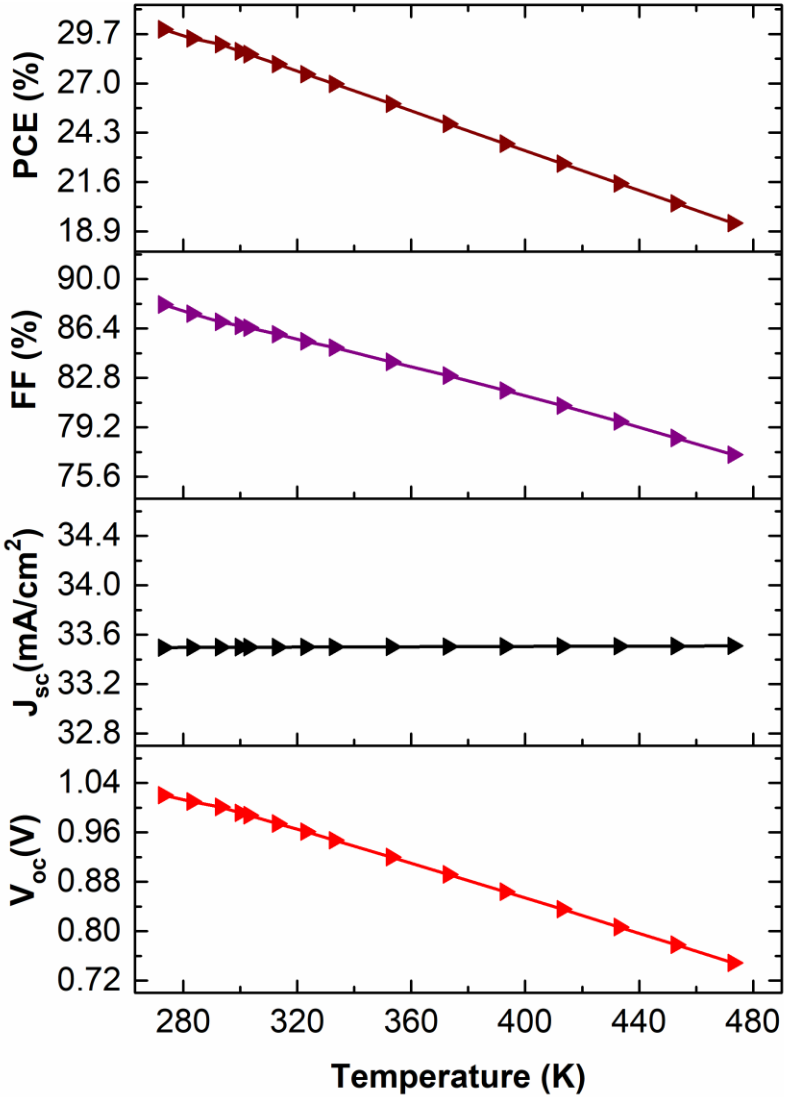


- All the performance parameters are reduced linearly with increasing the defect density.
- Increasing the defect density leads to promote the charge-carrier recombination rate.

Optimum defect density in the absorber layer is selected to be 1×10^{15} cm^{-3}.

Results (4)

Effect of Operating Temperature



- All the solar cell outputs except the J_{sc} are degraded as the increase of temperature.
- Reduction of energy band gap of the inorganic materials may results in the degradation of the overall conversion efficiency of the proposed PV device.

Conclusions

- In this work, the numerical investigation of earth abundant tin-based $CsSnI_3$ perovskite solar cell with different HTLs has been performed by SCAPS-1D program. .
  - ✓ A **new Al/ITO/TiO_2/$CsSnI_3$/CuS/Ni Perovskite solar cell** has been designed and studied.
  - ✓ The solar cell has been optimized at 0.6 µm perovskite absorber, 0.1 µm HTL, and 0.05 µm ETL, respectively.
  - ✓ It is revealed that the conversion efficiencies of 25.10%, 26.31%, 27.74% and 27.63% have been obtained for the CuSCN, CuI, NiO_x, MoO_3 HTLs, respectively. On the other hand, the enhanced power conversion efficiency of 28.74% with V_{oc} of 0.99 V, J_{sc} of 33.50 mA/cm^2 and FF of 86.60% has been achieved for the proposed structure.

Therefore, these findings may contribute insightful approach to fabricate viable, inexpensive, and highly efficient earth abundant $CsSnI_3$-based PSC with better performance.

Thank you for your attention.