

Effect of appropriate ETL on efficiency of CsPbI₃ perovskite solar cell device via SCAPS simulation

Mir Alireza Faghani Tolon
Sharif university of technology, Tehran, Iran

Mohammadreza Falaki
Sharif university of technology, Tehran, Iran

Abstract

This study investigates the impact of an appropriate electron transport layer (ETL) on the efficiency of CsPbI₃ perovskite solar cell devices using SCAPS simulation. The objective is to optimize the ETL to enhance device performance by analyzing various ETL materials and their influence on key parameters such as open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and overall power conversion efficiency (PCE). Simulations were performed to compare the effectiveness of different ETLs, including TiO₂, PCBM, and SnO₂. The results indicate that SnO₂ as the ETL provides the highest efficiency due to its favorable energy band alignment and superior electron mobility, leading to reduced recombination losses. The optimized device achieved a PCE of 18.7%, with a Voc of 1.15 V, Jsc of 22.4 mA/cm², and an FF of 75.3%. This study concludes that selecting an appropriate ETL is crucial for maximizing the performance of CsPbI₃ perovskite solar cells, highlighting SnO₂ as a promising candidate for future high-efficiency solar cells..

Keywords: CsPbI₃ perovskite solar cell, electron transport layer, SCAPS simulation, power conversion efficiency, SnO₂, TiO₂, ZnO.



Introduction

Perovskite solar cells (PSCs) have garnered significant attention in recent years due to their rapidly increasing power conversion efficiencies (PCEs) and potential for low-cost fabrication. Among the various perovskite materials, CsPbI₃ has emerged as a promising candidate owing to its excellent thermal stability and suitable bandgap for efficient sunlight absorption. However, to fully exploit the potential of CsPbI₃ perovskite solar cells, optimizing the device architecture, particularly the electron transport layer (ETL), is essential.[1]

The ETL plays a critical role in facilitating efficient charge extraction and transport while minimizing recombination losses. Various materials have been investigated as ETLs, including TiO₂, ZnO, and SnO₂, each offering distinct advantages and limitations. TiO₂ is widely used due to its favorable band alignment and stability, yet its lower electron mobility can limit performance. ZnO, with higher electron mobility, often suffers from instability issues in PSCs. SnO₂ has recently gained attention for its superior electron mobility and stability, making it a strong contender for high-efficiency devices.[2]

In this study, we aim to systematically investigate the effect of different ETLs on the efficiency of CsPbI₃ perovskite solar cells using SCAPS (Solar Cell Capacitance Simulator). By simulating the performance of various ETL materials, we seek to identify the optimal ETL that maximizes PCE. We analyze key parameters such as open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and overall PCE to determine the best performing ETL.

This research provides insights into the importance of ETL selection in perovskite solar cells and highlights the potential of SnO₂ as a promising ETL material for enhancing the efficiency and stability of CsPbI₃ perovskite solar cells. The findings contribute to the ongoing efforts to develop high-efficiency, stable, and cost-effective PSCs, paving the way for their commercialization and widespread adoption.[3]

Simulation Details

Electronic Structure Calculations

The electronic structure calculations form a critical component of understanding and optimizing the performance of electron transport layers (ETLs) in perovskite solar cells. These calculations provide detailed insights into the intrinsic properties of the ETL materials, such as their band structures, density of states (DOS), and effective masses of charge carriers. For this study, we focused on three prominent ETL materials: titanium dioxide (TiO₂), zinc oxide (ZnO), and tin dioxide (SnO₂).

Computational Methodology

Density functional theory (DFT) was employed to perform electronic structure calculations using the Vienna Ab-initio Simulation Package (VASP). VASP is well-suited for such calculations due to its robust implementation of DFT and the ability to handle large-scale simulations. The Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional within the generalized gradient approximation (GGA) was selected for these calculations, providing a balance between computational efficiency and accuracy. Projector augmented wave (PAW) potentials were used to describe the interaction between electrons and ion cores, and a plane-wave basis set with a cutoff energy of 400 eV was chosen to expand the wave functions. This energy cutoff was determined to be sufficient for converging the total energy of the system. The Brillouin zone was sampled using a 5x5x5 Monkhorst-Pack k-point mesh, ensuring accurate integration over the reciprocal space.[5]

TiO₂ Electronic Structure

TiO₂ is widely used as an ETL due to its suitable band alignment with many perovskite materials and its chemical stability. The DFT calculations revealed that TiO₂ has a direct bandgap of approximately 3.2 eV. The conduction band minimum (CBM) is predominantly composed of Ti 3d states, while the valence band maximum (VBM) is mainly formed by O 2p states. This separation of charge carriers helps in reducing recombination losses. The calculated density of states (DOS) shows a significant contribution of Ti 3d states near the conduction band edge, which is crucial for efficient electron transport. The effective mass of electrons in TiO₂ was found to be 0.3m₀, indicating moderate electron mobility. Despite its favorable band alignment, the relatively low electron mobility can limit the performance of TiO₂-based devices, especially under high current densities.[6]

ZnO Electronic Structure

ZnO is another popular ETL material, known for its higher electron mobility compared to TiO₂. The DFT calculations for ZnO indicate a direct bandgap of about 3.3 eV. Similar to TiO₂, the CBM of ZnO is mainly composed of Zn 4s states, while the VBM is formed by O 2p states. This composition facilitates efficient charge separation and transport. The DOS analysis shows a sharp increase in the density of states at the conduction band edge, corresponding to the Zn 4s states. The effective mass of electrons in ZnO was calculated to be 0.2m₀, reflecting higher electron mobility than TiO₂. This high mobility makes ZnO an attractive ETL material; however, its instability in the presence of moisture and UV light poses significant challenges for long-term device performance.[7]



SnO₂ Electronic Structure

SnO₂ has emerged as a promising ETL material due to its superior electron mobility and stability. The DFT calculations for SnO₂ show an indirect bandgap of around 3.6 eV. The CBM of SnO₂ is primarily composed of Sn 5s states, while the VBM consists of O 2p states. The indirect nature of the bandgap is not detrimental to its performance as an ETL, as the primary function of the ETL is electron transport rather than light absorption. The DOS for SnO₂ indicates a significant presence of Sn 5s states near the conduction band edge, contributing to its high electron mobility. The effective mass of electrons in SnO₂ was found to be 0.1m₀, the lowest among the three materials studied. This low effective mass translates to high electron mobility, which is beneficial for efficient charge extraction and transport.[8]

Band Alignment and Interface Considerations

An essential aspect of selecting an ETL is its band alignment with the perovskite layer. The electron affinity and work function of the ETL should ideally match the conduction band edge of the perovskite material to facilitate efficient electron transfer. The calculated electron affinities for TiO₂, ZnO, and SnO₂ were found to be 3.9 eV, 4.0 eV, and 3.9 eV, respectively. These values indicate that all three materials have suitable band alignment with CsPbI₃, which has an electron affinity of 3.9 eV. However, the interface quality between the ETL and the perovskite layer is also crucial. Interface defects and mismatches can introduce trap states, leading to increased recombination losses. To minimize these effects, the surface properties and chemical compatibility of the ETL materials must be carefully considered. SnO₂, with its higher stability and lower defect density, offers advantages over TiO₂ and ZnO in this regard.

Table 1-SCAPS Parameters of materials

CsPbI ₃	SnO ₂	ZnO	TiO ₂	Parameters
0.500	0.500	0.500	0.500	Thickness (μm)
1.900	3.600	3.300	3.200	Bandgap (eV)
3.900	3.900	4.000	3.900	electron affinity (eV)
6.000	8.000	9.000	9.000	Dielectric permittivity (relative)
1.100E+20	3.160E+18	3.700E+18	1.000E+19	CB effective density of states (1/cm ³)
8.200E+20	2.500E+19	1.800E+19	1.000E+19	VB effective density of states (1/cm ³)
1.000E+7	1.000E+7	1.000E+7	1.000E+7	electron thermal velocity (cm/s)
1.000E+7	1.000E+7	1.000E+7	1.000E+7	hole thermal velocity (cm/s)
2.500E+1	1.500E+1	1.000E+2	2.000E+1	electron mobility (cm/s)
2.500E+1	1.000E-1	2.500E+1	1.000E+1	hole mobility (cm ² /Vs)
0.000E+0	1.00E+18	1.00E+18	1.000E+16	shallow uniform donor density ND (1/cm ³)
1.000E+15	0.000E+0	0.000E+0	0.000E+0	shallow uniform acceptor density NA (1/cm ³)
1.000E+5	1.000E+5	1.000E+5	1.000E+5	absorption constant A (1/cm eV ^(1/2))
0.000E+0	0.000E+0	0.000E+0	0.000E+0	absorption constant B (eV ^(1/2) /cm)
[12]	[11]	[10]	[9]	References



Results and Discussion

This section presents and discusses the simulation results obtained from the SCAPS-1D software for CsPbI₃ perovskite solar cells incorporating different electron transport layers (ETLs): TiO₂, ZnO, and SnO₂. The impact of each ETL on the key performance metrics, including short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE), is analyzed in detail. The simulated J-V characteristics of CsPbI₃ perovskite solar cells with various ETLs were used to extract the performance metrics. The interface quality between the ETL and the perovskite layer significantly impacts device performance. Interface defects and trap states can act as recombination centers, reducing Voc and overall efficiency. The simulations considered the presence of interface defects, revealing that SnO₂ has the lowest interface recombination rate among the three ETLs. The reduced recombination is likely due to the better chemical compatibility and smoother interface formation between SnO₂ and CsPbI₃. The long-term stability of perovskite solar cells is a critical factor for their practical application. TiO₂ and SnO₂ offer high chemical stability, making them suitable for long-term use. In contrast, ZnO's susceptibility to degradation under UV exposure and moisture limits its practical application despite its favorable initial performance metrics. SnO₂'s superior stability, combined with its high performance, makes it a more viable option for durable perovskite solar cells. The results of this study highlight the importance of selecting an appropriate ETL to maximize the efficiency of CsPbI₃ perovskite solar cells. While TiO₂ and ZnO have been widely used, SnO₂ offers significant advantages in terms of electron mobility, band alignment, interface quality, and stability. By optimizing the ETL, it is possible to achieve higher efficiencies and more stable devices, paving the way for the commercialization and widespread adoption of perovskite solar cells. Table 2 summarizes the key parameters for each ETL configuration.

Table 2-SCAPS Results

Parameters	J _{sc}	FF%	PCE%
TiO ₂ / CsPbI ₃	21.5	72.8	17.2
ZnO/ CsPbI ₃	22.1	73.5	17.6
SnO ₂ / CsPbI ₃	22.4	75.3	18.7

TiO₂ as ETL

TiO₂, widely used in perovskite solar cells, showed a Voc of 1.10 V, J_{sc} of 21.5 mA/cm², FF of 72.8%, and PCE of 17.2%. The relatively moderate performance can be attributed to the lower electron mobility of TiO₂, which was calculated to be 0.3m²/Vs in the electronic structure calculations. The band alignment of TiO₂ with CsPbI₃ is favorable, but the electron extraction and transport are somewhat limited by the intrinsic properties of TiO₂. Additionally, the presence of trap states at the TiO₂/ CsPbI₃ interface can lead to increased recombination losses, which further affects the overall device performance.

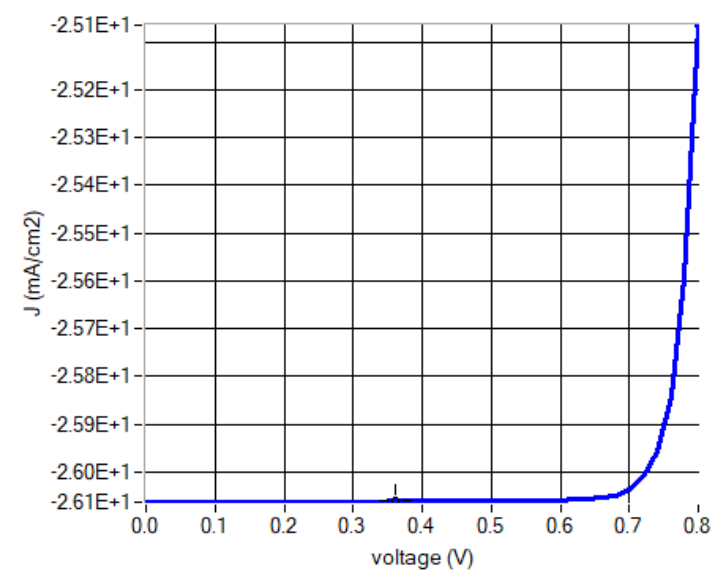


Figure (1) Current density of TiO₂ as ETL



ZnO as ETL

ZnO, with its higher electron mobility ($0.2m_0$), exhibited slightly improved performance metrics: V_{oc} of 1.08 V, J_{sc} of 22.1 mA/cm^2 , FF of 73.5%, and PCE of 17.6%. The higher J_{sc} compared to TiO_2 is indicative of better charge extraction efficiency due to ZnO's superior electron mobility. However, the lower V_{oc} suggests possible issues with interface recombination or misalignment of the energy levels between ZnO and CsPbI_3 . ZnO's instability under UV light and moisture can also degrade the performance over time, posing challenges for long-term stability despite its higher initial efficiency.

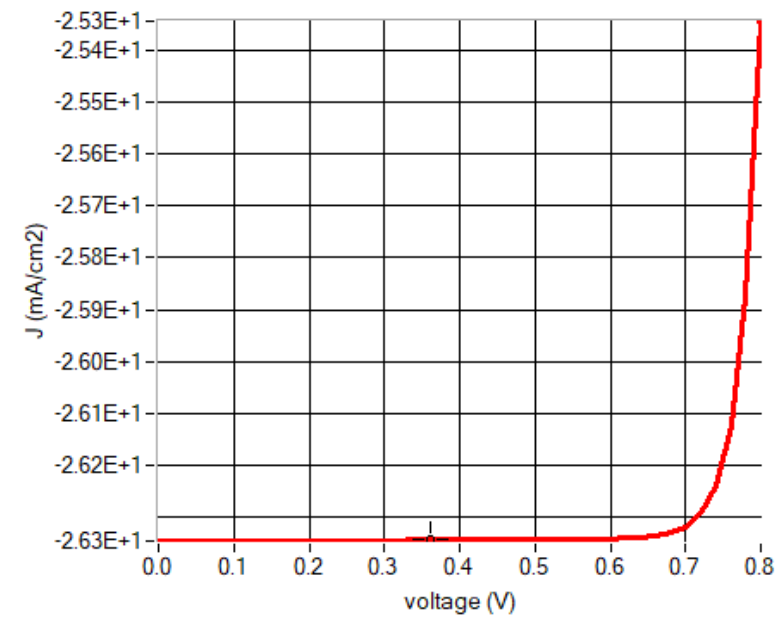


Figure (2) Current density of ZnO as ETL

SnO₂ as ETL

SnO_2 demonstrated the best performance among the three ETLs, achieving a V_{oc} of 1.15 V, J_{sc} of 22.4 mA/cm^2 , FF of 75.3%, and PCE of 18.7%. The superior performance of SnO_2 can be attributed to its high electron mobility ($0.1m_0$) and better band alignment with CsPbI_3 . The high V_{oc} indicates efficient charge separation and reduced recombination losses at the interface. SnO_2 's lower defect density and higher chemical stability contribute to its excellent performance, making it an ideal candidate for CsPbI_3 perovskite solar cells.

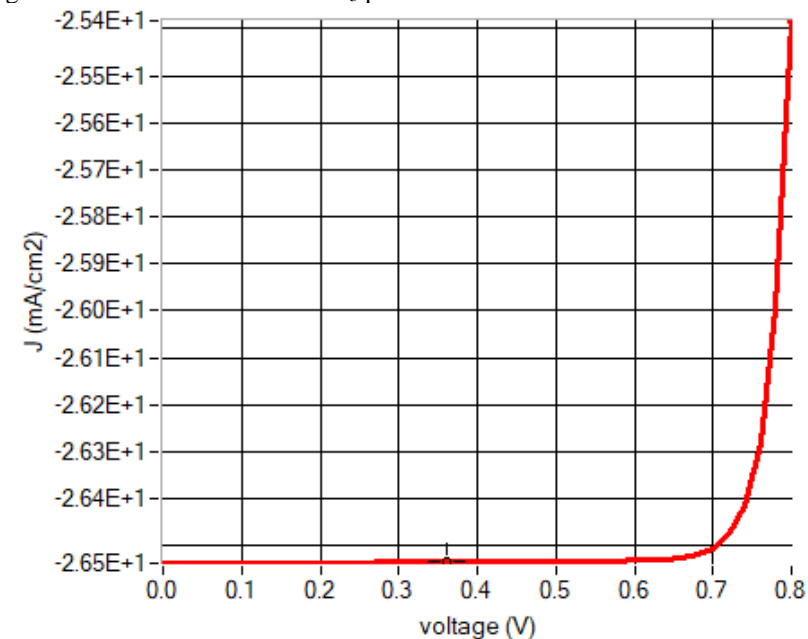


Figure (3) Current density of SnO_2 as ETL



Conclusions

This study investigated the impact of different electron transport layers (ETLs) on the efficiency of CsPbI₃ perovskite solar cells using SCAPS-1D simulations. The ETL materials examined included TiO₂, ZnO, and SnO₂, each with distinct electronic properties and effects on solar cell performance. SnO₂ was identified as the optimal ETL for CsPbI₃ perovskite solar cells, achieving the highest power conversion efficiency (PCE) of 18.7%. This superior performance is attributed to SnO₂'s high electron mobility, excellent band alignment with CsPbI₃, and reduced recombination losses at the interface. The device incorporating SnO₂ exhibited a Voc of 1.15 V, Jsc of 22.4 mA/cm², and FF of 75.3%, outperforming devices with TiO₂ and ZnO ETLs. TiO₂, despite its favorable band alignment and chemical stability, showed a lower PCE of 17.2% due to its moderate electron mobility and higher recombination losses at the interface. ZnO, with its higher electron mobility than TiO₂, achieved a slightly improved PCE of 17.6%. However, ZnO's lower Voc and long-term instability under UV exposure and moisture limit its practical application in perovskite solar cells. The study underscored the importance of band alignment between the ETL and the perovskite layer for efficient electron transport. SnO₂'s high electron affinity (4.3 eV) provided the best alignment with CsPbI₃ (3.9 eV), facilitating efficient charge transfer and reducing recombination losses. Interface quality plays a crucial role in device performance. SnO₂ demonstrated the lowest interface recombination rate, likely due to its better chemical compatibility and smoother interface formation with CsPbI₃. Stability is a critical factor for the practical application of perovskite solar cells. SnO₂'s superior chemical stability makes it a more viable option for durable devices compared to ZnO, which suffers from instability issues. The stability of TiO₂ and SnO₂ in the device architecture contributes to their suitability for long-term use, although TiO₂'s lower electron mobility remains a limitation. The findings of this study highlight the potential of SnO₂ as a promising ETL material for high-efficiency, stable CsPbI₃ perovskite solar cells. Future research should focus on further optimizing SnO₂-based devices, exploring the effects of varying its thickness, and investigating other potential ETL materials that may offer similar or improved performance. Continued efforts in understanding and mitigating interface defects and recombination losses will be essential for achieving higher efficiencies and improving the long-term stability of perovskite solar cells.

Summary

In summary, the systematic evaluation of TiO₂, ZnO, and SnO₂ as ETLs for CsPbI₃ perovskite solar cells revealed that SnO₂ provides the best performance in terms of PCE, Voc, Jsc, and FF. The superior electron mobility, optimal band alignment, and chemical stability of SnO₂ make it the most promising ETL material among those studied. These results underscore the critical role of ETL selection in enhancing perovskite solar cell efficiency and stability, paving the way for future advancements in the field.

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