IOCN 2025 Conference

The 5th International Online Conference on Nanomaterials

22–24 September 2025 | Online

MDPI

Computational study of $KSnI_3$ perovskite solar cells resulting in the power conversion efficiency of 30.44 %

BV Kheswa[1]

[1]University of Johannesburg

INTRODUCTION & AIM

- Lead-based perovskite solar cell (PSC) have highly promising performance.
- However, lead is toxic and optimization of lead-free PSCs is of global interest.
- $KSnI_3$ is a potential active absorption layer material for PSCs.
- Nevertheless, highest PCE of 22.78 % for $KSnI_3$ based PSCs is still far below the Shockley Queisser limit [1].
- The aim of this study was to optimize various configurations of $KSnI_3$ PSC.
- Specifically, we employed various ETL materials, while fixing HTL material.
- We also optimized the properties of all layers.

METHOD

- Computational modelling and optimization of four $KSnI_3$ PSC structures were achieved using SCAPS-1D software package.
- Specifically, we optimized FTO/Al-ZnO/$KSnI_3$/rGO/Se, FTO/$LiTiO_2$/$KSnI_3$/rGO/Se, FTO/SnO_2/$KSnI_3$/rGO/Se, and FTO/ZnO/$KSnI_3$/rGO/Se devices, depicted in figure 1.

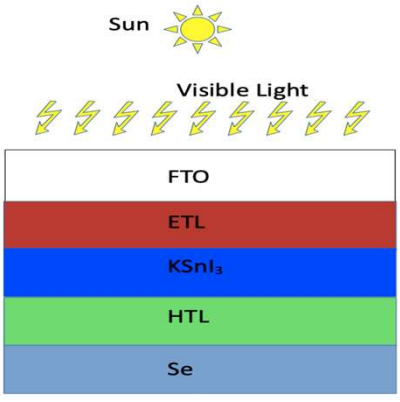

Figure 1 FTO/ETL/KSnI3/HTL/Se device.

- Al-ZnO, $LiTiO_2$, SnO_2, and ZnO, and rGO were chosen based on their band alignment with $KSnI_3$ (see figure 2), high charge mobilities, strong thermal stabilities except for the case of ZnO, and excellent conductivities.
- Simulations in SCAPS-1D are based on solving Poison's, transport, and continuity equations [2], using the finite difference method.

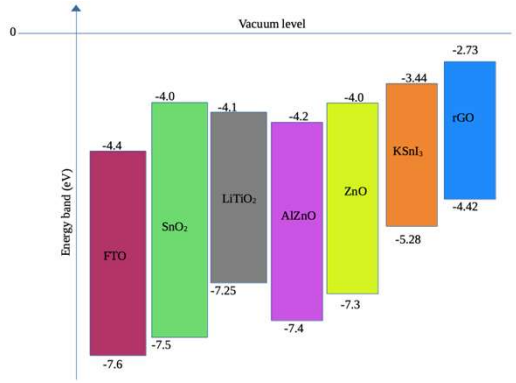

Figure 2 Band alignment of FTO, ETL, HTL and perovskite [3].

RESULTS & DISCUSSION

- We started by optimizing the FTO/Al-ZnO/$KSnI_3$/rGO/Se structure. In this optimized structure, we substituted Al-ZnO with SnO_2, $LiTiO_2$ and ZnO to get three other structures which were optimized. The results are highlighted below. In these results we assume zero series resistance, and infinite shunt resistance.

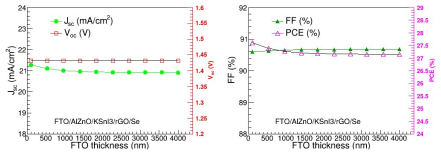

Figure 1 V_{oc}, J_{sc}, FF, and PCE as a function of FTO thickness

- Figure 1 shows final optimization stage of the FTO/Al-ZnO/$KSnI_3$/rGO/Se as function of FTO. This figure shows that V_{oc}, J_{sc}, FF, and PCE are not highly affected By FTO thickness, but we achieved the highest PCE of 27.6% on the FTO/Al-ZnO/$KSnI_3$/rGO/Se device.

- At this stage the structure has been already optimized for thicknesses and dopant densities of rGO, $KSnI_3$, and ALZnO (see table 1).

- This is the optimized structure in which ETL = SnO2, ZnO and $LiTiO_2$ were substituted.

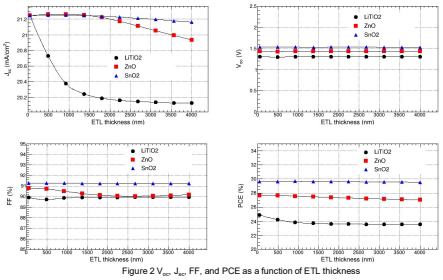

Figure 2 V_{oc}, J_{sc}, FF, and PCE as a function of ETL thickness

- Figure 2 shows performance metrics of the FTO/ETL/$KSnI_3$/rGO/Se as function Of ETL thickness. At point the $KSnI_3$, rGO, and are FTO were already optimized.

- The results Show that SnO_2 yielded the highest PCE = 29.67% and the performance didn't vary with the thickness of this ETL material, due to the high electron mobility of SnO_2.

- Thus, for further optimization, we focused on FTO/ETL/$KSnI_3$/rGO/Se. The optimal thickness of SnO_2 with deemed 489 nm.

- Varying SnO_2 donor dopant density did don't yield significant improvement on performance.

- Varying temperature (T) showed that PCE improves with rise in T up to T = 371 K, yielding PCE = 30.44%.

Table 1 The optimized properties of our four PSC structures. Optimized values are highlighted in yellow.

Parameters	FTO	Al–ZnO	$LiTiO_2$	ZnO	SnO_2	$KSnI_3$	rGO
Thickness (nm)	100	489	50	489	489	50	2670
E_g (eV)	3.5	3.1	3.15	3.28	3.5	1.84 [1]	1.69
χ (eV)	4	4	4	4	3.9	3.44 [2]	3.56
ε_r	9	9	13.6	9	9	10.4	13.3
N_c (cm^{-3})	2.02×10^{18}	2×10^{18}	3×10^{20}	2×10^{18}	2.2×10^{18}	2.2×10^{18}	10^{18}
N_v (cm^{-3})	1.8×10^{19}	1.8×10^{19}	2×10^{20}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
Vth_e (cm s^{-1})	10^7	10^7	10^7	10^7	10^7	10^7	10^7
Vth_h (cm s^{-1})	10^7	10^7	10^7	10^7	10^7	10^7	10^7
μ_e (cm^2/V/s)	2×10^1	13.84	30	43	200	21.28	2.6×10^1
μ_h (cm^2/V/s)	1×10^{-1}	25	0.01	25	80	19.46	1.23×10^1
N_A (cm^{-3})	0	0	0	0	0	8.33×10^{20}	5.45×10^{21}
N_D (cm^{-3})	2×10^{19}	10^{15}	10^{13}	10^{18}	10^{16}	1×10^{15}	0
N_t (cm^{-3})	10^{15}	10^{15}	10^{14}	10^{15}	10^{15}	10^{15}	10^{14}

Table 2 The PCE of optimized structures compared with literature

PSC structure	PCE (%)	Reference
FTO/Al–ZnO/$KSnI_3$/rGO/Se	27.16	This paper
FTO/$LiTiO_2$/$KSnI_3$/rGO/Se	24.94	This paper
FTO/ZnO/$KSnI_3$/rGO/Se	27.62	This paper
FTO/SnO_2/$KSnI_3$/rGO/Se	30.44	This paper
FTO/TiO_2/$KSnI_3$/Spiro-OMeTAD/W	9.776	[23]
FTO/F_{16}CuPc/$KSnI_3$/PTAA/C	10.83	[24]
FTO/TiO_2/$KSnBr_3$/Cu_2O/Au	8.05	[39]
FTO/F_{16}CuPc/$KSnI_3$/CuPc/C	11.91	[25]
FTO/ZnO5/$KSnI_3$/NiO/C	9.28	[26]
FTO/ZnO/$KSnI_3$/CuI/Au	20.99	[27]
FTO/SnO_2/3C–SiC/$KSnI_3$/NiO/C	22.78	[28]

CONCLUSION

- In this study we optimized In this study, we optimized FTO/ETL/$KSnI_3$/rGO/Se, where ETL = AL-ZnO, ZnO, SnO_2, and $LiTiO_2$.
- We obtained PCEs of 27.16%, 24.94%, 27.62%, and 30.44% for ETL = AL-ZnO, $LiTiO_2$, ZnO, and SnO_2, respectively.
- Our SnO_2 based PSC outperforms FTO/SnO_2/3C–SiC/$KSnI_3$/NiO/C, which is currently the most efficient $KSnI_3$ structure in the literature, by more than 7 %.

FUTURE WORK / REFERENCES

[1] Ghani, I.B.A et al. Boosting $KSnI_3$-based perovskite solar cell efficiency by 22.78% through optimized charge transport and eco-friendly buffer layer. *J. Mater. Sci.* 2024, *59*, 14547. https://doi.org/10.1007/s10853-024-10051-6
[2] Kheswa, B.V. Numerical optimization of all-inorganic CsSnBr3 perovskite solar cells: The observation of 27% power conversion efficiency. *Phys. Scr. 2025, 100, 015933.* https://doi.org/10.1088/1402-4896/ad9647
[3] Kheswa, B.V. et al. Modeling and Analysis of $KSnI_3$ Perovskite Solar Cells Yielding Power Conversion Efficiency of 30.21%. *Nanomaterials* 2025, *15*, 580. https://doi.org/10.3390/nano15080580