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Comparative Study between Lead and Lead-Free Perovskite Solar Cells: Insights from SCAPS Software Analysis

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Abstract

This paper presents a comparative study between lead-based and lead-free perovskite solar cells (PSCs) utilizing Solar Cell Capacitance Simulator (SCAPS) software. Perovskite solar cells have garnered significant attention due to their high efficiency and low-cost fabrication. However, concerns regarding the toxicity of lead in traditional PSCs have prompted the exploration of lead-free alternatives. Through simulation using SCAPS software, this study investigates the performance metrics, such as efficiency and material properties, of lead and lead-free PSCs to provide insights into their potential as sustainable alternatives for photovoltaic applications. Results show that methyl-ammonium lead iodide ($MAPbI_3$) and Formamidinium lead iodide ($FAPbI_3$) perovskite solar cells exhibit efficiencies of 16.68% and 16.65% respectively. The lead-free methyl-ammonium tin iodide ($MASnI_3$) and methyl-ammonium germanium iodide ($MAGeI_3$) achieved efficiencies of 16.59% and 12.42% respectively. The findings suggest that while lead-free perovskites offer promising alternatives, further optimization is necessary to match the efficiency of their lead-based counterparts.

Keywords: Perovskite solar cells, Lead, Lead-free, SCAPS software, Efficiency, Comparative study

1.0 Introduction

Perovskite solar cells (PSCs) have garnered significant attention in the realm of photovoltaic research due to their high efficiency and low production costs (Hougku, 2022). Among these, lead-based PSCs have been widely studied; however, concerns about toxicity have necessitated the investigation of lead-free alternatives (Niu *et al.*, 2015).

Recent advancements have leveraged Solar Cell Capacitance Simulator (SCAPS) software to model and compare the performance characteristics of lead and lead-free perovskite solar cells. Studies indicate that while lead-based PSCs continue to outperform in terms of efficiency, lead-free variants present a promising, environmentally friendly alternative (Azarhoosh *et al.*, 2016). Additionally, researches highlight the potential of tin-based perovskites as viable substitutes, though challenges such as stability and efficiency persist (Noel *et al.*, 2016; Saliba *et al.*, 2016).

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Recent studies have also explored novel lead-free materials and their integration into PSCs, furthering our understanding of their properties and performance (Park *et al.*, 2016; Kulkarni *et al.*, 2014; Byranvand *et al.*, 2022; Chen *et al.*, 2014;). Other investigations into bismuth and antimony-based perovskites have shown comparable potential, reinforcing the need for ongoing comparative analyses (Eperon *et al.*, 2014; Gratzel *et al.*, 2014; Jeon *et al.*, 2014, Hongkun, 2022; Rabia *et al.*, 2023; Roy *et al.*, 2022).

2. Materials and method

The proposed perovskite solar cells simulation is carried out with the help of SCAPS 1D software. SCAPS has been well adapted for modeling many micros, thin and polycrystalline devices, and photonic structures. Accordingly, SCAPS-1D can be used to simulate the architectures of perovskite solar cells. From the literature, the experimental results coincide with those of a SCAPS-1D simulation for the design and development of a highly efficient Tin Halide Perovskite solar cell. The SCAPS-1D has several advantages over the other simulation software, since it can grade almost all parameters of semiconductor layers.

2.1 Device Architecture

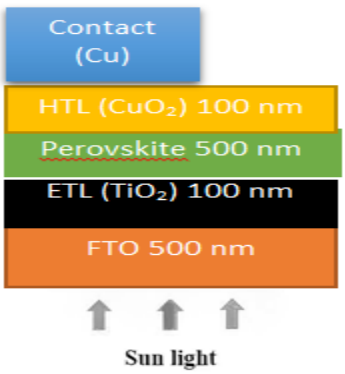

Figure 1: Perovskite solar cell architecture under investigation

Methyl-ammonium lead iodide ($MAPbI_3$), methyl-ammonium germanium iodide ($MAGeI_3$), methyl-ammonium tin iodide ($MASnI_3$), and formamidinium lead iodide ($FAPbI_3$) are the perovskites used in this study as absorber layers. Among other layers, cuprous oxides (CuO_2) and titanium dioxide (TiO_2) were used as the Hole Transport layer (HTL) and the Electron Transport layer (ETL) respectively. The solar cells' performances are displayed when the simulation parameters were successfully inputted.

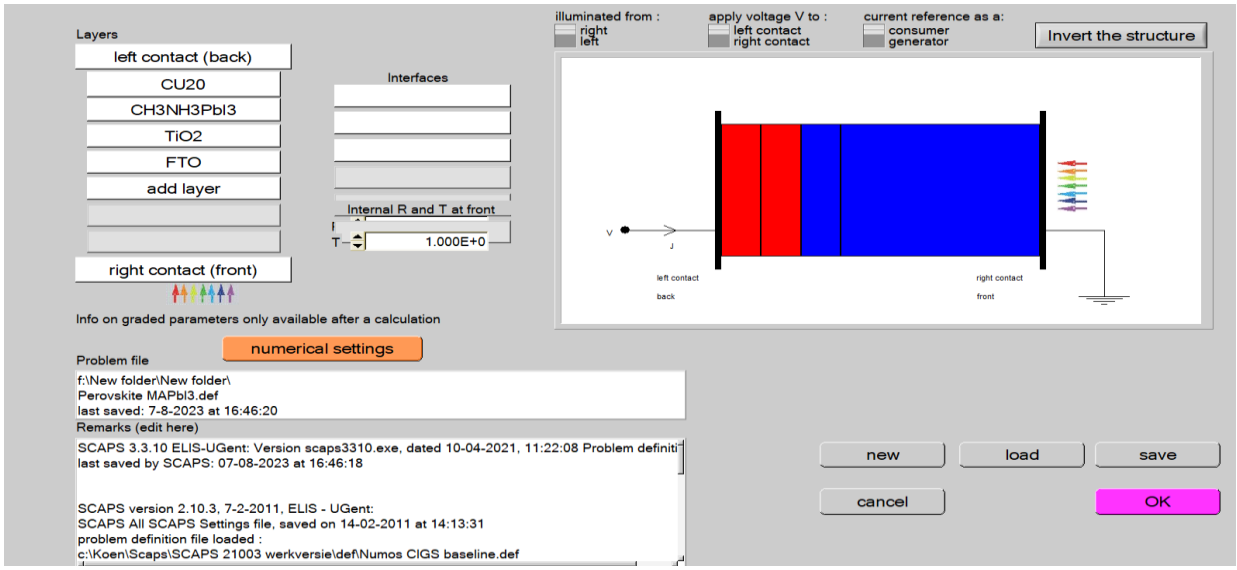

Figure 2: SCAPS-1D simulation interface showing the device architecture for $MAPbI_3$

3. Results and discussion

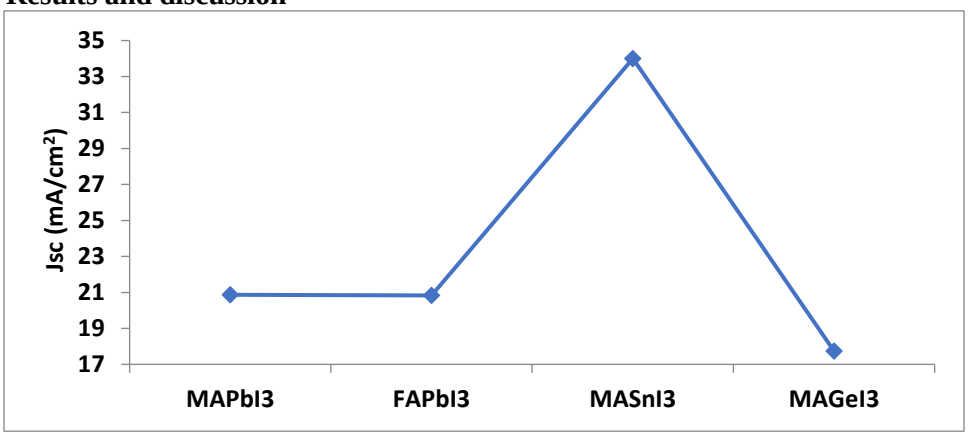

Figure 3: Short circuit current density of perovskite solar cells

One important measure of how well a solar cell converts light into electric current is the short-circuit current density (Jsc). The fact that methyl ammonium tin iodide ($MASnI_3$) has a lower band gap (~1.3 eV) than other perovskites under study means that it absorbed a wider range of the solar spectrum, including more infrared light, and resulted in a greater short-circuit current density of 34 mA/cm^2.

Near the optimal value for solar energy conversion, the band-gaps of $MAPbI_3$ and FAPbI3 are 1.55 eV and 1.48 eV, respectively. This enables effective photon absorption and electron-hole pair generation. In comparison to other perovskites, $MAGeI_3$ has a lower Jsc because of its greater bandgap (~1.6–1.7 eV), which restricts its capacity to absorb light in the near-infrared region. Perovskites based on germanium often have a higher defect count and a worse film quality, which increases recombination losses.

Lead-based perovskites ($MAPbI_3$ and $FAPbI_3$) offer a balance of good light absorption, high carrier mobility, and relatively stable performance, resulting in moderate JSC values around 21 mA/cm^2.

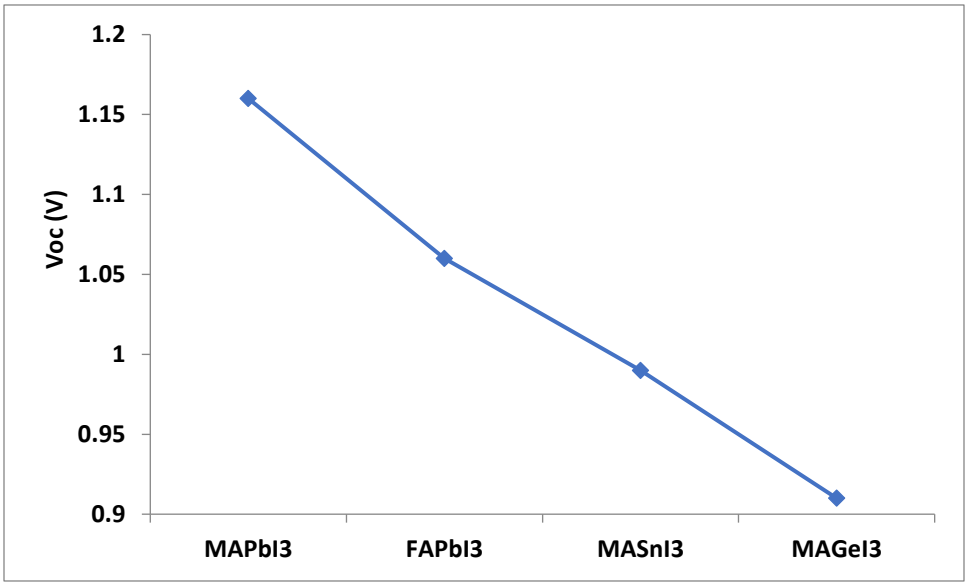

Figure 4: Open circuit voltage of the perovskite solar cells

The voltage of the cells when no current is being delivered is known as the open circuit voltage. As can be seen in this plot, the open circuit voltage of lead-based perovskite solar cells is comparatively higher than that of lead-free perovskite solar cells. Lead-based perovskite typically have favorable electronic properties for optimal solar absorption and efficient charge carrier generation. The nature of the lead-halide bonding and the structure of the perovskite lattice help in passivating defects, reducing trap states that can capture charge carriers and facilitate non-radiative recombinations, leading to higher photo-voltage.

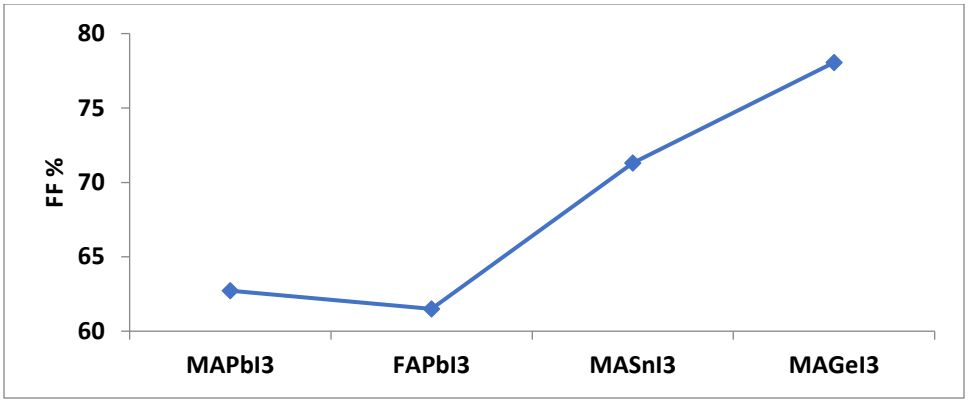

Figure 5: Fill-factor of the perovskite solar cells

The higher fill factor of lead-free perovskite solar cells can be attributed to a combination of factors, including reduced recombination losses, improved interface quality, better charge transport, and more favorable energy alignment, among others. The fill-factors of MAPbI3 and FAPbI3 are on par with approximately 63% and 62%, respectively. The lead-free perovskites have a comparatively higher fill-factor of 71% and 78% for $MASnI_3$ and $MAGeI_3$, respectively.

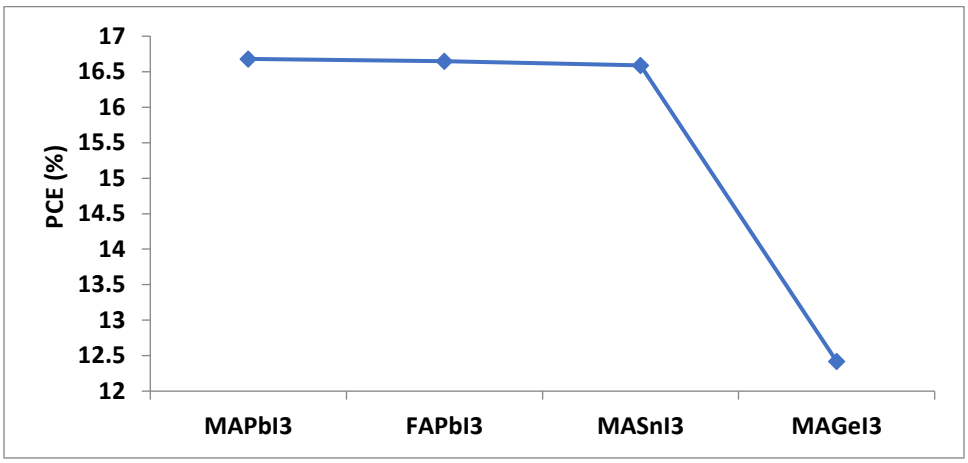

Figure 6: Efficiencies of the perovskite solar cells

The 500 nm perovskite layer thickness was used to study the perovskites solar cells' efficiency. We investigated the performances of Formamidinium Lead Iodide ($CH(NH_2)_2PbI_3$), Methyl Ammonium Tin Iodide ($CH_3NH_3SnI_3$), Methyl Ammonium Germanium Iodide ($CH_3NH_3GeI_3$), and Methyl Ammonium Lead Iodide ($CH_3NH_3PbI_3$). According to the results, the approximate efficiencies of 17 % each was obtained for $CH_3NH_3SnI_3$, $CH_3NH_3PbI_3$, and $CH(NH_2)_2PbI_3$) respectively, while $CH_3NH_3GeI_3$ had a considerably lower efficiency of 12%.

Conclusion

The electrical characteristics and individual perovskite solar cell efficiencies of both lead-containing and lead-free perovskites were examined. Methyl-ammonium lead iodide ($MAPbI_3$) and Formamidinium lead iodide ($FAPbI_3$) perovskite solar cells have efficiencies of 16.68% and 16.65% respectively. The lead-free methyl-ammonium tin iodide ($MASnI_3$) and methyl-ammonium germanium iodide ($MAGeI_3$) achieved efficiencies of 16.59% and 12.42% respectively. The findings suggests that while lead-free perovskites offer promising alternatives, further optimization is necessary to match the efficiency of their lead-based counterparts.

References

Azarhoosh, P., McKechnie, S., Frost, J. M., Walsh, A., & Van Schilfgaarde, M. (2016). Research Update: Relativistic origin of slow electron-hole recombination in hybrid halide perovskite solar cells. APL Materials, 4(9), 091501.

Byranvand MM, Zuo W, Imani R, Pazoki M, Saliba M. (2022): Tin-based halide perovskite materials: properties and applications. Chem Sci. 13(23):6766-6781. doi: 10.1039/d2sc01914k. PMID: 35774180; PMCID: PMC9200135.

Chen, Q., Zhou, H., Hong, Z., Luo, S., Duan, H. S., Wang, H. H. and Yang, Y. (2014). Planar heterojunction perovskite solar cells via vapor-assisted solution process. Journal of the American Chemical Society, 136(2), 622-625.

Eperon, G. E., Stranks, S. D., Menelaou, C., Johnston, M. B., Herz, L. M., & Snaith, H. J. (2014). Formamidinium lead trihalide: A broadly tunable perovskite for efficient planar heterojunction solar cells. Energy & Environmental Science, 7(3), 982-988.

Grätzel, M. (2014): The light and shade of perovskite solar cells. Nature Materials, 13(9), 838-842.

Hougku Li. (2022): The Recent Progress and the State-of-art Applications of Perovskite Solar Cells, Highlights in Science, Engineering and Technology, 5, 216-222.

Jeon, N. J., Noh, J. H., Kim, Y. C., Yang, W. S., Ryu, S., & Seok, S. I. (2014). Solvent engineering for high-performance inorganic–organic hybrid perovskite solar cells. Nature Materials, 13(9), 897-903.

Kulkarni, S. A., Baikie, T., Boix, P. P., Yantara, N., Mathews, N., & Mhaisalkar, S. (2014). Band-gap tuning of lead halide perovskites using a sequential deposition process. Journal of Materials Chemistry A, 2(24), 9221-9225.

Niu, G., Guo, X., & Wang, L. (2015): Review of recent progress in chemical stability of perovskite solar cells. Journal of Materials Chemistry A, 3(17), 8970-8980.

Noel, N. K., Stranks, S. D., Abate, A., Wehrenfennig, C., Guarnera, S., Haghighirad, A. A., & Snaith, H. J. (2014). Lead-free organic–inorganic tin halide perovskites for photovoltaic applications. Energy & Environmental Science, 7(9), 3061-3068.

Park, N. G., Grätzel, M., Miyasaka, T., Zhu, K., & Emery, K. (2016). Towards stable and commercially available perovskite solar cells. Nature Energy, 1(11), 16152.

Rabia S., Arshi K, Syed W. A, Abdul R, Haji G.Q, Hafiz H. A, Khalid M, Shabana A. and Faisal Saleem (2023): A comprehensive review of the current progresses and material advances in perovskite solar cells, Nanoscale Adv., 5, 3803–3833

Roy, P.; Ghosh, A.; Barclay, F.; Khare, A.; Cuce, E. (2022): Perovskite Solar Cells: A Review of the Recent Advances, Coatings, 12, 1089. https://doi.org/10.3390/coatings12081089

Saliba, M., Matsui, T., Seo, J. Y., Domanski, K., Correa-Baena, J. P., Nazeeruddin, M. K., and Grätzel, M. (2016): Cesium-containing triple cation perovskite solar cells: Improved stability, reproducibility, and high efficiency. Energy & Environmental Science, 9(6), 1989-1997.

Hongkun L. (2022): The Recent Progress and the state-of-art applications of Perovskite Solar Cells, Highlights in Science, Engineering and Technology, 5, 216-222.