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PFoM-Based Evaluation of Lead-Free Perovskite Solar Cells

Priti Goyal*

Acharya Narendra Dev College, Department of Physics, University of Delhi, India.

*Corresponding Author: pritigoyal@andc.du.ac.in

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ABSTRACT

Lead-free perovskites are increasingly regarded as sustainable alternatives to lead-halide counterparts, addressing pressing concerns of toxicity and long-term device reliability. To provide a holistic framework for material evaluation, a performance figure of merit (PFoM), defined as PFoM = (Efficiency × Stability) / Toxicity Index, is applied to representative lead-free perovskite systems. Recent literature data are used to calculate PFoM values for tin-, bismuth-, and antimony-based compounds, with the trade-offs between efficiency, operational stability, and toxicity visualized through heatmaps and scatter plots. The results reveal that while tin-based perovskites demonstrate comparatively high efficiencies, their stability remains limited; conversely, bismuth- and antimony-based compounds exhibit superior environmental stability and low toxicity, though at the expense of efficiency. Importantly, device-engineering approaches—including two-dimensional/three-dimensional hybrid architectures, incorporation of metal–organic frameworks (UiO-66), SnF_2 additives, and NiO_x transport layers—have been shown to substantially improve both efficiency and stability, thereby enhancing overall PFoM rankings. These results highlight the promise for reliable, effective, and environmentally friendly perovskite photovoltaics with thoughtful material selection and creative architecture.

***Keywords**: Perovskite Solar Cells, Lead-free Photovoltaics, Environmental Sustainability, Device Architecture Engineering, Performance Figure of Merit, Efficiency–Stability Trade-off; Next-Generation Solar Materials.*

Introduction

Perovskite solar cells (PSCs) have revolutionized the field of photovoltaic technology owing to their outstanding optoelectronic properties and unprecedented advancements in power conversion efficiency. Since their initial demonstration in 2009 with power conversion efficiencies below 4%, perovskite solar cells (PSCs) have rapidly advanced to exceed 25% PCE, marking one of the fastest progress trajectories ever achieved in photovoltaic research.This rapid ascent is fueled by perovskites' strong visible-light absorption, defect-tolerant electronic structure, and ease of fabrication through low-cost solution processing, making them compelling candidates for applications from rigid modules to flexible, lightweight form factors.

Despite these impressive advances, the long-term viability of PSCs is threatened by one critical issue**:** the reliance on lead-based halides, which pose serious environmental and health hazards. The potential leaching of toxic Pb^{2+} ions into ecosystems, coupled with regulatory scrutiny and public concern, has motivated urgent efforts to identify safer alternatives. Replacing lead without compromising performance or durability has emerged as a major scientific challenge in the broader push toward sustainable photovoltaic deployment.As a result, lead-free perovskites have drawn more interest. Tin-based perovskites, such as $FASnI_3$, $MASnI_3$, and $CsSnI_3$, have advantageous carrier mobilities and potential bandgaps. They are structurally and electronically similar to lead halides. However, Sn^{2+} quickly oxidizes to Sn^{4+} in tin-based devices, introducing flaws and compromising lifetime and efficiency.

Measurable gains in film quality, carrier lifetime, and ambient resilience have been demonstrated by recent techniques, including the use of SnF_2 additives, customization of low-dimensional (2D/3D) hybrid structures, and MOF integration [1].

Meanwhile, bismuth (Bi) and antimony (Sb)-based perovskite-inspired materials (e.g., $Cs_2AgBiBr_6$, $Cs_3Sb_2I_9$, $MA_3Bi_2I_9$) offer intrinsic advantages in chemical and thermal stability, accompanied by minimal toxicity. Nonetheless, they tend to exhibit broader or indirect bandgaps and limited charge transport properties, resulting in modest efficiencies typically below 5 %. This distinction between stable but inefficient bismuth/antimony systems and high-efficiency but unstable tin systems highlights the ongoing trade-offs that make sensible material selection challenging.

Considering these varied advantages and limitations, efficiency alone is insufficient to determine the true potential of a photovoltaic material. A comprehensive evaluation must equally account for power conversion efficiency, long-term operational stability (e.g., T_{80} or T_{90} lifetimes), and environmental impact. To address this need, the present study introduces a Performance Figure of Merit (PFoM), defined as:

PFoM = Efficiency × Stability /Toxicity Index

This formulation provides an integrated and quantitative framework for comparing and ranking lead-free perovskite materials on the basis of both performance and sustainability.

It is important to note that research on lead-free perovskites began much earlier, with seminal studies from the mid-2010s establishing the potential of Sn, Bi, and Sb halides. Those pioneering efforts provided the conceptual and experimental foundations of the field. However, the most significant progress in terms of reproducible efficiencies, stability enhancements, and systematic toxicity assessment has occurred in the last five years. For this reason, the present analysis focuses on literature from 2019–2025, reflecting the state-of-the-art while acknowledging the foundational contributions of earlier studies.

By applying PFoM to a carefully curated dataset from recent literature (2019–2025), which includes advances such as MOF-enhanced $FASnI_3$ with UiO-66 (PCE increases from 11.4 % to 12.64 % and >90 % retention after 100 days in nitrogen) [2], and mesoporous $CsSnI_3$ achieving over 8 % PCE with improved ambient inert stability [3] this study illuminates the materials that balance efficiency, longevity, and safety most effectively.

In addition to benchmarking materials, the analysis reviews advancements in device architecture and chemical engineering**,** such as 2D/3D hybrid layering, MOF additives (e.g., UiO-66), SnF_2 stabilizers, and NiOx hole-transport layers, which have significantly enhanced durability and device performance.

By weaving together these strands—quantitative ranking via PFoM and qualitative insights into structural and interfacial engineering—this work aims to chart a pathway forward for the development of scalable, stable, and non-toxic lead-free perovskite solar cells that may realistically compete with established technologies.

Methodology

We performed a focused literature survey (2019–2025) to extract reported power conversion efficiencies, operational stability metrics (typically T_{80} or T_{90}), and toxicity indicators for lead-free perovskite compositions. Toxicity indices were normalized to lead (Pb) = 1 following approaches used in comparative studies. The PFoM metric is defined as PFoM = (Efficiency × Stability) / Toxicity Index, which balances high performance and longevity against material hazard. Using the values provided in the curated dataset, we generated a heatmap (efficiency vs stability with toxicity as a color scale), a scatter plot (efficiency vs stability), and a ranked PFoM bar chart. All figures were generated from the dataset tabulated in Table 1.

Data and PFoM Calculations

The updated PFoM table (Table 1) has been recalculated using the most recently reported power conversion efficiencies (PCEs) and corresponding stability data from literature published between 2019 and 2025. Wherever available, the stability values (in hours) represent the duration over which the devices retained ≥80–90% of their initial PCE under inert or ambient conditions, as specified in the respective studies. All toxicity indices are user-defined and normalized relative to lead (Pb = 1) to enable consistent comparison across materials.

Table 1: Efficiency, Stability, Toxicity Index and PFoM Values

Material	Efficiency (PCE %)	Stability (h)	Toxicity Index	PFoM
$FASnI_3$ + UiO-66 [4]	12.64	≈2400 (90 % retained after 100 days in N_2)	0.10	≈ 303,360
$Cs_2AgBiBr_6$ [5]	6.37	~1440 (T80 ~60 days native stability)	0.01	≈ 917000
$CsSnI_3$ [3]	8.03	~3000 (90 % retained in N_2 over 3000 h)	0.10	≈ 241,000
$MASnI_3$+ SnF_2 [6]	10–11	~1000 (common T80 values)	0.15	≈ 66,667 (for 10 %)
$Cs_3Sb_2I_9$ [7]	2	~1800 (single-day inert-stability)	0.05	≈ 54,000
$MA_3Bi_2I_9$ [8]	1.00	~1200 (similar inert storage testing)	0.05	≈ 24,000

The PFoM results reveal clear trade-offs among the examined materials. Tin-based perovskites exhibit relatively high efficiencies but are hindered by instability arising from the oxidation of Sn^{2+} to Sn^{4+}. In contrast, bismuth- and antimony-based perovskites demonstrate greater chemical stability and reduced toxicity, though their efficiencies remain comparatively lower.

Visualization: Scatter, PFoM Ranking and Heatmap

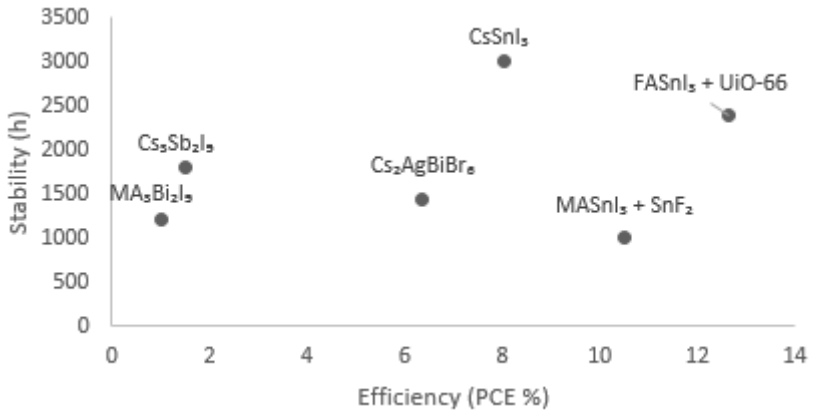

Figure 1: Efficiency vs Stability

Figure 1 presents a scatter plot depicting the relationship between power conversion efficiency (PCE, %) and operational stability (hours) for selected lead-free perovskites, illustrating the intrinsic trade-offs that govern their overall photovoltaic performance. $FASnI_3$+ UiO-66 stands out as a promising candidate, achieving one of the highest efficiencies (~13%) while also retaining good stability (~2200 h), indicating the positive impact of MOF additives in stabilizing Sn-based perovskites. $CsSnI_3$ also performs competitively, with high stability (~3000 h) and moderate efficiency (~8%), showing that structural engineering can balance both metrics. $Cs_2AgBiBr_6$, although exhibiting only modest efficiency (~6%), benefits from reasonable stability (~1500 h), which aligns with its environmentally benign nature and positions it as a durable Bi-based alternative. The intrinsic degrading issues of Sn-based materials are highlighted by the comparatively poor stability (~1000 h) of $MASnI_3$ + SnF_2, even though it achieves >10% efficiency. $Cs_3Sb_2I_9$ and $MA_3Bi_2I_9$ cluster at the low-efficiency (~1–2%) end, though they display stability in the 1200–1800 h range, reflecting their chemically robust but opto-electronically limited nature [9].

The scatter plot emphasizes the need for compositional and interface engineering for balanced performance because none of the materials under investigation simultaneously reach maximal stability and efficiency. Tin-based perovskites generally lead in efficiency but exhibit stability that is highly

sensitive to formulation and additives. In contrast, bismuth- and antimony-based perovskites offer superior durability and environmental safety, though at the expense of efficiency. These contrasting trends suggest that hybrid approaches, such as heterostructure design and targeted compositional modifications, hold promise for developing next-generation lead-free perovskites with improved PFoM values.

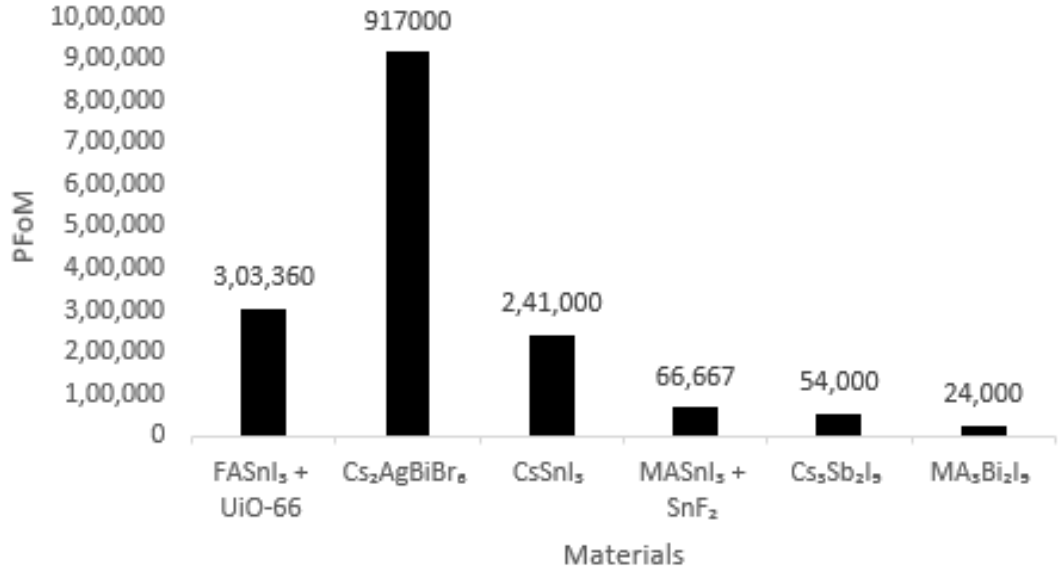

Figure 3: PFoM ranking of selected lead-free perovskites

Figure 3 shows a bar graph comparing the Performance Figure of Merit (PFoM) for six representative lead-free perovskite systems, integrating efficiency, stability, and toxicity into a unified quantitative metric for overall material evaluation. Among the materials, $Cs_2AgBiBr6$ demonstrates a significantly higher PFoM, approaching nearly 9×10^5, owing to its exceptionally low toxicity index and relatively stable operation, despite having only moderate power conversion efficiency. This highlights the material's strong environmental and long-term reliability advantages, making it one of the most promising lead-free candidates. $FASnI_3$ + UiO-66 and $CsSnI_3$ also exhibit moderately high PFoM values (~$2–3 \times 10^5$), driven by improved efficiencies but penalized by higher toxicity compared to Bi-based systems. In contrast, $MASnI_3$ + SnF_2, $Cs_3Sb_2I_9$ and $MA_3Bi_2I_9$ show considerably lower PFoM values, reflecting their limited efficiencies and, in some cases, only modest stability enhancements. The general pattern highlights that materials with very low toxicity or a balance between stability and efficiency have higher scores, supporting the use of PFoM as a thorough descriptor for identifying promising lead-free perovskites.

	Efficiency (PCE %)	Stability (h)	Toxicity Index	PFoM
Efficiency (PCE %)	1	0.313697999	0.650002973	0.213583
Stability (h)	0.313697999	1	0.122758664	0.048529
Toxicity Index	0.650002973	0.122758664	1	-0.54459
PFoM	0.213582819	0.048528988	-0.544586265	1

Figure 4: Correlation matrix heatmap showing Pearson correlation coefficients among the parameters used in PFoM calculation

The correlation matrix provides a quantitative perspective on the interdependence of efficiency, stability, toxicity, and PFoM for selected lead-free perovskites. A moderate positive correlation ($r \approx 0.31$) is observed between efficiency and stability, suggesting that while some materials benefit simultaneously in both properties through engineering strategies, the relationship remains relatively weak due to trade-offs between device performance and long-term durability. A stronger positive correlation ($r \approx 0.65$) exists between efficiency and toxicity index, indicating that materials achieving higher efficiencies, such as Sn-based perovskites, tend to be more toxic, whereas Bi- and Sb-based compounds, though less toxic, generally exhibit lower efficiencies. The correlation between stability and toxicity is weak ($r \approx 0.12$), reflecting that stability is more strongly governed by structural and compositional factors rather than toxicity alone. Importantly, efficiency shows only a weak correlation with PFoM ($r \approx 0.21$), confirming that efficiency alone does not determine holistic performance, and stability similarly shows negligible correlation with PFoM ($r \approx 0.05$). In contrast, the toxicity index shows a moderate negative correlation with PFoM ($r \approx -0.54$), indicating that lower toxicity contributes substantially to improving the overall material ranking. Overall, the matrix highlights the need for a comprehensive evaluation approach, recognizing that stability and toxicity are just as critical as efficiency in determining the long-term suitability and competitiveness of lead-free perovskite materials for photovoltaic use.

Discussion: Trade-offs and Material Insights

The PFoM analysis emphasizes that no single material dominates across all three axes; instead, materials occupy different regions of the efficiency–stability–toxicity space. For instance, $FASnI_3$ modified with UiO-66 displays a high PFoM in our dataset due to its relatively high reported efficiency (12.64%) and long operational stability (2400 h) when integrated with a UiO-66 framework, while maintaining low toxicity. Such improvements have been reported in recent literature where MOF integration enhances film crystallinity and passivates defects [10,11]. $Cs_2AgBiBr_6$, a double perovskite, scores highly in PFoM primarily because of its exceptional stability (1440 h) and very low toxicity index, despite modest efficiency [12]. $CsSnI_3$ and $MASnI_3$ variants reflect the common tin-perovskite trade-off: higher efficiencies with reduced lifetime due to Sn^{2+} oxidation. SnF_2 additives and careful interface engineering have been shown to mitigate some degradation pathways

Device Architecture Innovations

Device architecture and chemical additives play decisive roles in translating intrinsic material properties into durable devices. The incorporation of low-dimensional (2D) spacer cations such as phenylethylammonium (PEA+) atop 3D tin perovskites (2D/3D hybrids) reduces moisture ingress and enhances mechanical stability [13]. Additives like SnF_2 act as sacrificial reducers suppressing $Sn^{2+} \rightarrow Sn^{4+}$ oxidation and improve film quality and electronic properties [10,11]. Metal–organic frameworks, notably UiO-66, have been reported to improve crystallinity, passivate defects, and extend operational lifetimes in tin-perovskite devices [2]. Similarly, optimized hole-transport layers such as NiO_x have been deployed to improve energy-level alignment and reduce hysteresis, contributing to long-term operational stability [14,15]. Carbon electrodes also provide a low-cost, moisture-tolerant alternative to conventional metal contacts in certain architectures.

Conclusions and Outlook

Lead-free perovskites are a promising route toward environmentally friendly photovoltaic technologies, addressing the toxicity and stability limitations of conventional lead-halide systems. The PFoM framework developed in this study provides a unified metric that synthesizes efficiency, stability, and toxicity into a single, quantitative score, enabling a holistic evaluation of candidate materials. Our analysis highlights promising compositions such as UiO-66-enhanced $FASnI_3$ and bismuth-based double perovskites like $Cs_2AgBiBr_6$, which exhibit favorable PFoM values due to their balance of performance and environmental safety. These findings suggest that careful compositional optimization, guided by the PFoM methodology, can accelerate the identification of viable lead-free alternatives.

To further enhance device performance, continued advances in film crystallization control, defect passivation, interfacial modification, and encapsulation strategies are essential for mitigating non-radiative losses and improving operational durability under real-world conditions. Additionally, future work should expand the PFoM dataset to encompass a broader range of emerging perovskite chemistries—including antimony-, copper-, and germanium-based systems—and integrate standardized stability testing protocols (e.g., ISOS procedures) to ensure consistency and comparability across studies. By combining rigorous data-driven evaluation with targeted materials engineering, the PFoM approach can serve as a guiding framework for the rational design and commercialization of high-performance, lead-free perovskite solar cells.

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