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Probabilistic Evaluation of Lead-Free Perovskite Materials for Application Specific Photovoltaics

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Abstract: *The search for lead-free perovskite absorbers for solar cell technology has to strike a balance between performance, stability, and environmental safety, all of which have to be achieved in the presence of high material uncertainty. The traditional methods of screening materials, relying on deterministic criteria or average performance indicators, have been demonstrated to be inadequate in assessing the robustness of candidate materials in the presence of high variability. Here in this work, we propose a probabilistic material ranking scheme, which includes Monte Carlo simulation, probabilistic ranking, and the Relative Scenario Value (RSV) metric. Three scenarios for solar cell technology, including rooftop solar, long-life solar cells, and environment-friendly solar cells, have been formulated by assigning different weights to the descriptors of efficiency, stability, and toxicity. The performance distribution, uncertainty limits, and ranking stability of candidate materials have been evaluated using a typical set of lead-free perovskite solar cells. The results show a strong distinction between "generalist" and "specialist" materials, in terms of their ranking robustness. The proposed probabilistic scheme for material ranking has been able to establish a strong link between uncertainty quantification and scenario-driven decision metrics for solar cell technology.*

Introduction

Lead halide perovskite compounds have shown impressive efficiencies in solar cell applications [1]; nevertheless, issues related to toxicity and environmental sustainability have prompted extensive investigations into environmentally friendly lead free alternatives [2, 3]. Tin-based perovskite compounds, double perovskite compounds, and low-dimensional Bi and Sb-based halide compounds have been identified as potential alternatives [4-6], though none of these compounds simultaneously optimize characteristics like efficiency, durability and environment safety. Instead, material selection is now dependent on the context of applications.

Most existing material ranking and screening studies have employed a deterministic weighting method, which provides a single figure of merit for each material under consideration [7]. This method ignores material uncertainty and probability that a material could outperform others under different circumstances. Additionally, different solar cell applications require different material performance characteristics [8].

In our current work, we overcome these limitations through a probabilistic ranking scheme based on Monte Carlo simulations of application-specific figures of merit [9]. Rather than determining a single rank for a material, we compute a distribution of ranks, Top-k probabilities, and relative scenario-normalized metrics. Such a scheme allows for the identification of robust generalists, scenario specialists, and underperforming materials.

To incorporate application-driven variability, three representative photovoltaic application scenarios are considered, namely, rooftop photovoltaic systems, long-life modules for infrastructure-scale application, and environment-sensitive photovoltaic applications where material safety is a major driver. For each of the application scenarios, the relative importance of efficiency, stability, and toxicity is quantified using weighted performance metrics. Rather than using deterministic weights for each of the factors, as is typically the case, the current study incorporates uncertainty in the relative importance of the factors using Monte Carlo sampling. This results in the generation of thousands of instances of the performance figure of merit (PFoM) for each of the materials under consideration.

The resulting probabilistic framework allows for a more robust comparison of the lead-free perovskite materials. By examining the PFoM distributions, probabilistic rank stability, and cross-scenario relative performance indicators, the study offers more in-depth insights into the reliability and appropriateness of new materials. This method thus goes beyond the conventional ranking methods to provide a decision-oriented framework to select materials that are not only highly performing but also robust against uncertainties in application priorities.

Methodology

- **Application Scenarios and Descriptor Weighting**

The experimental data used in this study have been collected from the published literature between 2019 and 2025, for which the PFoM values have been computed. This range of years was chosen to ensure that the results have applicability to the latest device architectures, fabrication methods, and stability tests. Only the studies that report the complete photovoltaic metrics and the stability measurements have been considered.

Three application scenarios are considered, Rooftop photovoltaics which emphasizes high efficiency due to limited installation area [10], long-life modules, which prioritizes operational stability and reduced maintenance [11], and Environment-sensitive photovoltaics, which give emphasis on low toxicity for indoor or portable use [12]. Each scenario is represented by a set of weighting coefficients applied to efficiency, stability, and toxicity descriptors.

Material	Efficiency	Stability	Toxicity
$FASnI_3$ + UiO-66	1.0	0.96	0.56
$FASnI_3$ + PEA(2D/3D)	0.85	0.80	0.56
$MASnI_3$ + SnF_2	0.87	0.40	0.83
$CsSnI_3$ (optimized)	0.72	0.12	0.67
$Cs_2AgBiBr_6$	0.55	0.56	0.00
$MA_2AgBiBr_6$	0.35	0.44	0.00
$Cs_3Bi_2I_9$ (0D)	0.16	0.72	0.33
$MA_3Bi_2I_9$	0.09	0.44	0.33
$Cs_3Sb_2I_9$	0.13	0.72	0.33
$Rb_3Sb_2I_9$	0.18	0.60	0.33
Cs_2TiBi_6	0.28	1.00	0.11
Cs_2PdBi_6	0.21	0.80	0.22

Table 1: Application scenarios and corresponding descriptor weightings

Application Scenario	Efficiency (α)	Stability (β)	Toxicity (γ)	Rationale
Rooftop PV	0.6	0.3	0.1	Limited installation area requires high power density
Long-Life Modules	0.3	0.6	0.1	Emphasis on durability and reduced maintenance
Environment-Sensitive PV	0.3	0.3	0.4	Low toxicity prioritized for indoor or portable use

Nominal weighting factors (α, β, γ) are assigned to efficiency, stability, and toxicity for each application scenario. These values define the central tendencies around which Monte Carlo sampling is performed ($N \sim 10^4$ realizations per material per scenario). The weighting philosophy follows previously established framework previously developed by the author, reproduced here for completeness and reproducibility.

- **Monte Carlo Evaluation of Scenario-Specific Performance**

For each material, the efficiency, stability, and toxicity variables were modeled as probabilistic variables accounting for the reported variability and uncertainty associated with the material properties. Monte Carlo sampling was used to generate large sets of realizations for the descriptors [13, 14]. For each Monte Carlo iteration k, a scenario-specific performance figure of merit, denoted as PfoM, is computed as follows:

$$PfoM_k = \alpha\, \eta_k + \beta\, S_k + \gamma\,(1 - T_k)$$

Where η_k, S_k, and T_k denote the sampled efficiency, stability, and toxicity descriptors, respectively, while α, β, and γ are scenario-specific weighting factors. Extraction of the mean, standard deviation, and percentiles (P10, P90) of the computed distributions of PfoM is used to quantify the performance and associated uncertainties. Where k indexes Monte Carlo realizations. For each scenario, $N=10^4$ realizations are performed, generating distributions of the performance rather than single-point estimates.

- **Monte Carlo Sampling Strategy**

For each application scenario (Rooftop PV, Long-Life Modules, Environment-Sensitive PV), the nominal weight set (α_0, β_0, γ_0) is treated as the mean preference vector, rather than an exact prescription. Monte Carlo sampling is performed by introducing controlled stochastic variation around these nominal values:

$$\alpha^{(k)} = \alpha_0 + \delta\alpha^{(k)}$$

$$\beta^{(k)} = \beta_0 + \delta\beta^{(k)}$$

$$\gamma^{(k)} = \gamma_0 + \delta\gamma^{(k)}$$

Where the δ terms have zero mean bounded distributions, and the resulting weights are renormalized to ensure that they remain at unity. This ensures that the sampling is conducted in a manner that is realistic for decision uncertainty without breaching physical or policy constraints. Each run of the Monte Carlo method now effectively represents a realistic deployment-specific prioritization.

- **PFoM Distribution Generation**

For each material under each set of conditions for the application scenario, a set of Monte Carlo simulations, amounting to $N \sim 10^4$, is carried out to deal with the associated uncertainties in the weighting factors, each of which is scenario-specific. For each set of the above simulations, the Performance Figure of Merit (PFoM) is evaluated, giving rise to a probability distribution rather than a deterministic value. Statistical descriptors of the distribution will include the mean value of the PFoM (giving the expected value of the performance) and the standard deviations (giving the robustness of the performance to the associated uncertainties in the weighting factors). Additionally, percentile limits are also obtained, reflecting best and worst case results. Note, however, that a probabilistic approach offers a solution to three major concerns with deterministic FoMs. The first is the problem of weighting ambiguity. It is acknowledged, for example, that priorities in applications, such as relative emphasis placed on toxicity in indoor spaces, are inherently ambiguous. The second is rank instability. Although deterministic values for different materials may show similar values, their relative ranking may change with small changes in preference. Third, it offers decision robustness, acknowledging that in a real-world application, a material with a slightly lower mean PFoM value and small variance may, in fact, be a better candidate for a particular application than a material with a higher mean PFoM value and large spread of uncertainty. By incorporating the effect of uncertainty in a direct manner in a performance evaluation, the Monte Carlo-based PFoM method offers a more realistic approach to materials selection [15-17].

The Monte Carlo-based PFoM evaluation process begins with a continuous probability density function for the PFoM values for each material in each application scenario, as well as particular statistical measures such as the mean, variance, and percentile bound for each scenario. At this point in the process, no ranking is conducted; in Step 1, the process strictly isolates the intrinsic uncertainties in the performance of the materials. The values of the PFoM represent a data set that is used in the subsequent probabilistic ranking analysis. In Step 2, for each Monte Carlo simulation defined by k, the values of the PFoM are simultaneously determined for the particular materials in the scenario, with the materials then ranked according to their value of the PFoM in the particular simulation. The position of the rank is then determined for each material over the total number of realizations, N. After N simulations, the probability that material i is in the particular position in the ranking is defined by

$P_i(r)$ = Number of times material i occupies rank r / N

This two-step separation ensures conceptual clarity: performance uncertainty is first quantified independently, and only then translated into probabilistic dominance and rank stability.

- **Relative Scenario Value (RSV)**

To facilitate cross-scenario comparison, a Relative Scenario Value was defined as:

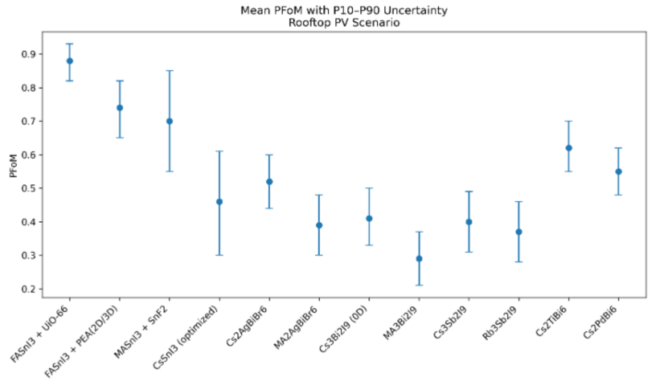
$$RSV_{m,s} = \frac{\langle PFoM_{m,s} \rangle}{\sum_m \langle PFoM_{m,s} \rangle}$$

To this aim, the Relative Scenario Value (RSV) is proposed as a normalized decision metric for quantifying the relative degree of concentration of material performance within a particular application scenario, as compared to other scenarios [18]. Although the distributions of the PFoM provide valuable information on the uncertainties associated with material ranking within individual scenarios, the RSV offers a novel approach for scenario synthesis, where probabilistic dominance is converted into a relative contribution score between scenarios. The RSV for each material is obtained by normalizing scenario-specific performance indicators, which are extracted from the mean value of the PFoM and ranking probabilities, such that their sum over all scenarios equals unity, providing a fractional distribution of material relevance for application scenarios. The RSV, which reduces the probabilistic ranking outcomes into a comparative vector, allows for clear categorization of material behavior as generalists, mostly generalists, specialists, or underperformers. This bridges the statistical uncertainty analysis with actionable materials selection.

Results and Discussion

Scenario-Specific Performance Distributions

The mean PfoM values and associated uncertainty ranges (P10–P90) for all materials under the three scenarios are shown in Figure 1.



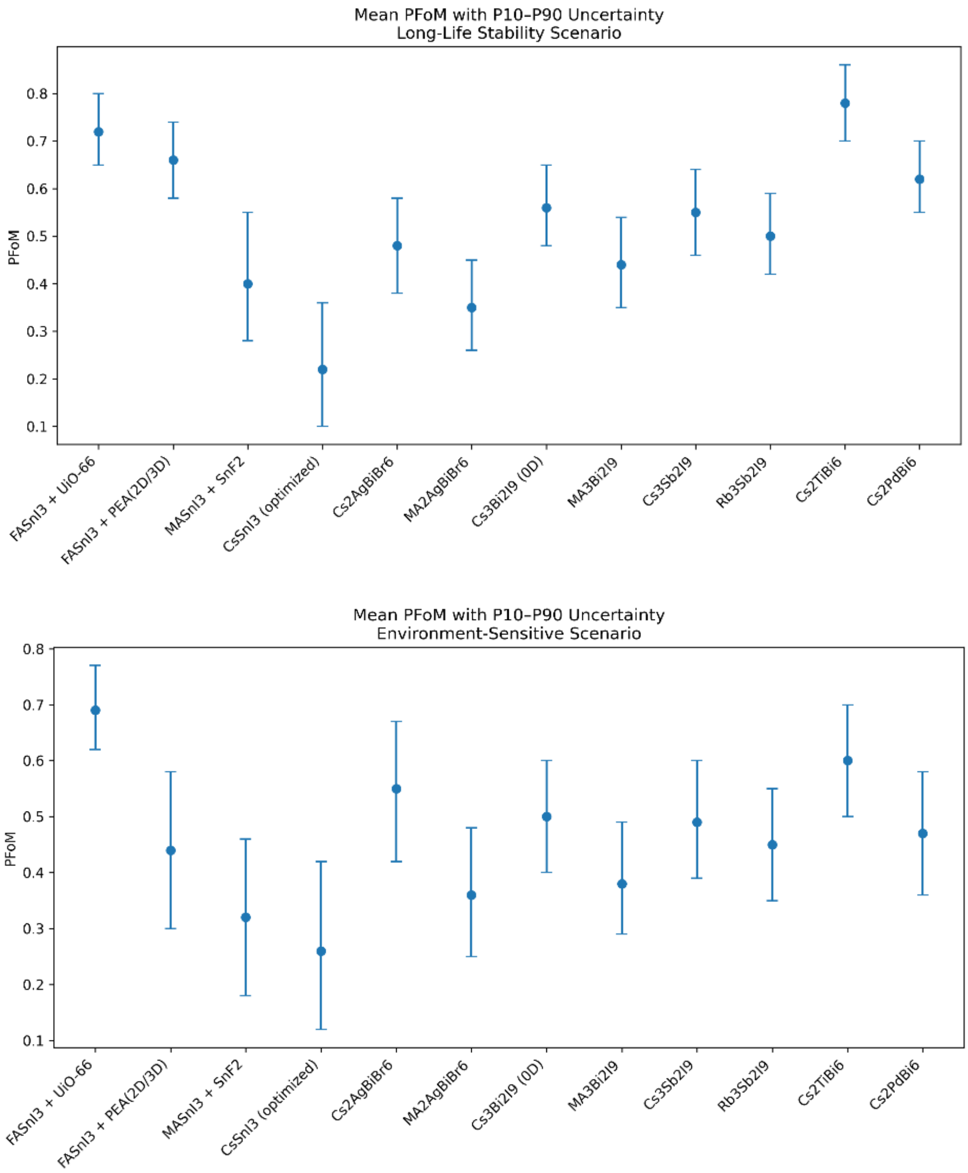


Figure 1: Mean PfoM ± P10–P90 uncertainty intervals for (a) rooftop photovoltaics, (b) long-life modules, and (c) environment-sensitive applications.

Figure 1 displays the mean figure of merit (PFoM) for each lead-free perovskite compound under the three application case scenarios, along with the corresponding uncertainty intervals given by the 10th percentile (P10) and 90th percentile (P90), obtained through the application of Monte Carlo simulations. Figures (a), (b), and (c) correspond to rooftop PV, long-life stability modules, and environment-sensitive application case scenarios, respectively.

For all three application case scenarios, $FASnI_3$ + UiO-66 maintains the highest mean PFoM value with narrow uncertainty intervals given by P10 and P90. This indicates not only its high performance but also its high robustness [19] against uncertainty, making it a top-ranked compound regardless of the application case scenario considered. Its robustness against uncertainty is confirmed in later parts by its high Top-3 probability value.

In the rooftop photovoltaic case (Fig.1a), the materials that have been optimized for charge carrier transport properties and efficiency, such as $FASnI_3$ + PEA (2D/3D) and $MASnI_3$+ SnF_2, exhibit higher mean PFoM values compared to the bismuth-based and antimony-based materials. However, the latter has a significantly wider uncertainty interval, implying that it is more sensitive to the spread of the underlying descriptors. The double perovskites and the zero-dimensional materials exhibit lower PFoM values, as well as overlapping uncertainty ranges, implying that they are less competitive in the efficiency-dominated weighting scheme.

In the case of the long-life stability scenario (Figure 1b), a rearrangement in materials is observed, where Cs_2TiBi_6 is found to be among the top-performing materials, characterized by a high mean PFoM and relatively narrower uncertainty bounds, indicating its excellent performance in stability-weighted evaluation. The hybrid tin-based perovskites are found to maintain relatively higher mean PFoM values, although with relatively wider uncertainty intervals, indicating potential degradation-related risks in the case of long-life operation. The bismuth and antimony-based materials are found to move upward from the rooftop scenario, again emphasizing the impact of stability weighting on material selection.

In the environment-sensitive scenario (Figure 1c), materials with lower toxicity are emphasized. Cs_2TiBi_6 and $Cs_3Bi_2I_9$ (0D) have high mean PFoM values compared to tin-based materials; however, their performance is penalized in terms of toxicity. Yet again, $FASnI_3$ + UiO-66 keeps its highest mean PFoM values. This implies, that its balance of efficiency, stability, and reduced toxicity remains competitive even under stringent environmental constraints [19].

As a conclusion, Figure 1 shows that mean PFoM is not sufficient for determining the material's adequacy because several materials have similar mean PFoM values but different uncertainty ranges. Therefore, the range of uncertainty between P10 and P90 is a key indicator for material performance robustness. Hence, the probabilistic ranking and Top 3 probability analysis are carried out in the subsequent section.

As such, the scenario-dependent changes evident in Fig. 1 highlight the importance of probabilistic screening, as materials optimized for one scenario may be less competitive for other weighting schemes.

Probabilistic Rank Stability and Decision Confidence

Whilst the average PFoM for each scenario gives an indication of the expected performance of the material, it does not account for the reliability of maintaining position in response to fluctuations in weighting of priorities. This has been overcome by the probabilistic rank distribution, which is constructed from the Monte Carlo simulation. The ranking of all materials according to their PFoM for each simulation, and the number of times a material achieved a certain rank, has been undertaken to obtain an empirical distribution, $P_i(r)$, accounting for performance and reliability.

In Figure 2, rank probability heat maps are provided, and from there, we can observe unique patterns in dominance and instability. Materials with a significant probability mass concentrated in Rank 1 or within the top 3 generally indicate strong decision confidence, where the dominance is maintained across a broad range of weighting configurations. Conversely, materials with a probability mass spread across multiple ranks indicate rank volatility, implying that the materials are sensitive to minor changes in application priorities, and hence, deterministic ranking is not feasible for such materials.

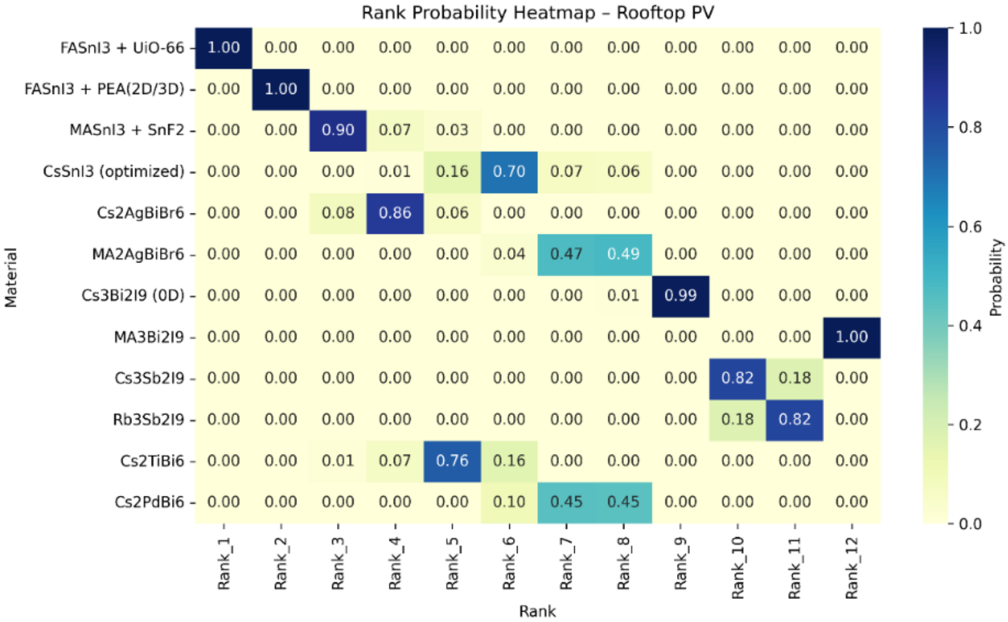
In order to hone the level of confidence in the decision even more, the cumulative Top-3 probability is also considered (Fig 3). Here, the focus is on the overall probability of the material being competitive rather than just the dominance at Rank 1. In a deployment scenario, it is arguably more important to be consistent at Top-3 rather than having the odd entry at Rank 1. Materials that have high probabilities at Rank 1 and high probabilities at Top-3 can be classified as having statistically dominant competitiveness, whereas those that have moderate mean PFoM but low probabilities at Top-3 can be classified as having fragile competitiveness.

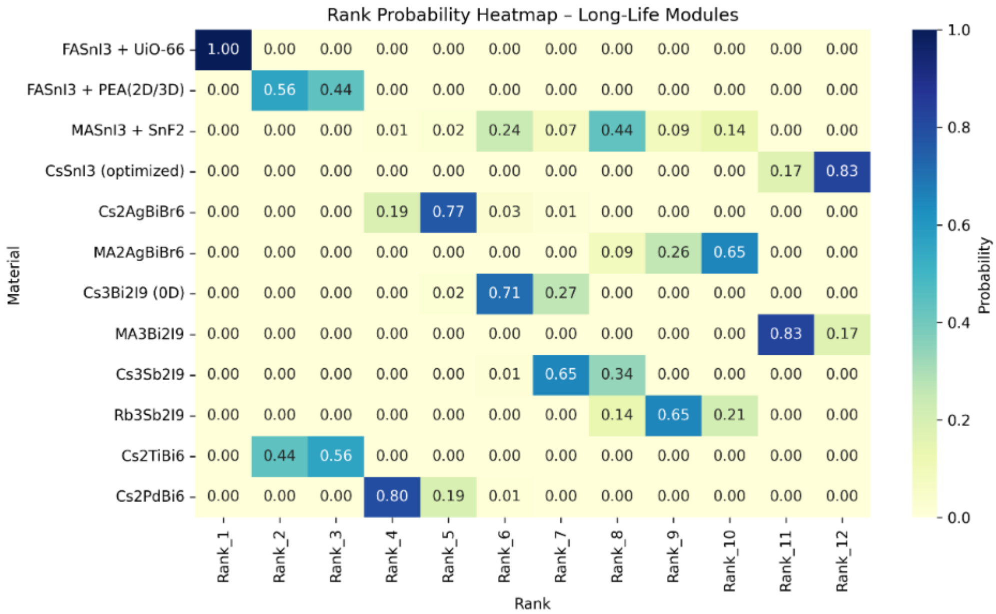
More importantly, probabilistic rank stability also offers a decision-theoretic advantage over traditional deterministic ranking approaches. Studies have shown that two materials may share similar mean PFoMs, but their rank distribution patterns may be quite dissimilar, with one consistently concentrated around Rank 1-2 and the other vacillating between Rank 1 and Rank 6. The former has higher confidence for deployment despite similar mean PFoMs. Here, uncertainty is treated as a decision variable in probabilistic ranking.

As such, this analysis has attempted to show that in the case of material selection, especially when it comes to the selection of strong materials, it is not only the performance of the material that is of interest, but also the manner in which the performance of the material can be sustained over uncertain landscapes of preference [20].

Rank Probability Heat maps under Three Application Scenarios

To quantify rank robustness, probabilistic rank distributions were constructed from Monte Carlo realizations and visualized as rank heat maps





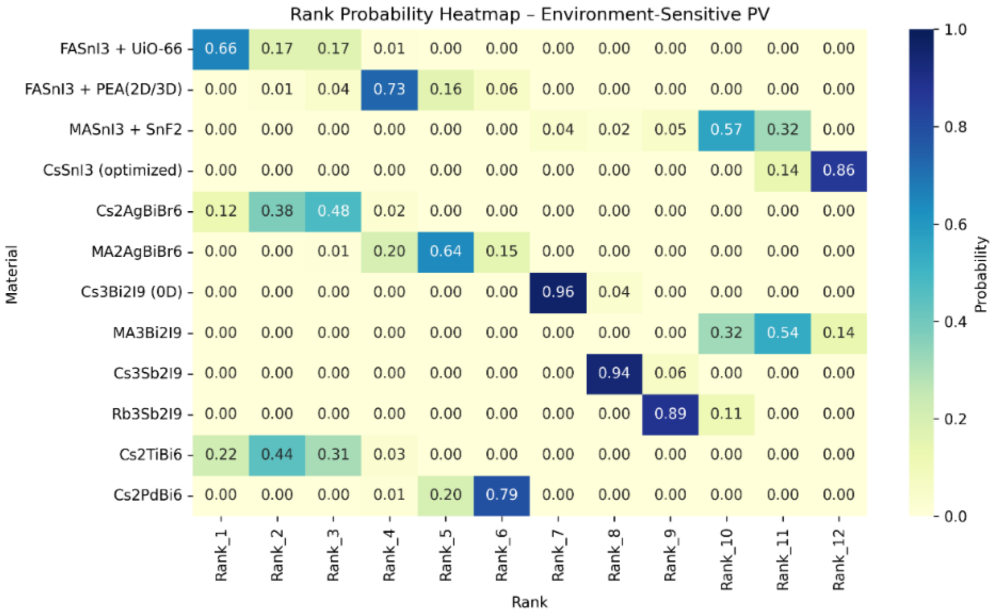


Figure :. Probabilistic rank heat map for the Rooftop PV, Long Life Stability, and Environment Sensitive PV scenarios, showing the probability of each material occupying a given rank across Monte Carlo realizations

Fig. 2 displays rank probability heat maps for all candidate materials considering the Rooftop PV, Long Life Stability, and Environment Sensitive PV scenarios. Each row in the heat map corresponds to one material, with columns representing rank position (Rank 1 being the best position). The color intensity in each heat map indicates the probability of each material at each rank position after propagating uncertainty in the PFoM computation via Monte Carlo analysis.

- **Rooftop PV Scenario**

In the case of the Rooftop PV heat map, a highly deterministic ranking is observed for the top-performing materials, where $FASnI_3$ + UiO-66 has a probability value of 1.0 at Rank 1, implying that it is always ranked as the best-performing material under the application of efficiency-dominated weight values. $FASnI_3$ + PEA (2D/3D) has a strong rank localization, implying that it is almost exclusively ranked at Rank 2, signifying its strong performance and slightly lower PFoM value in comparison to the $FASnI_3$ + UiO-66 composite material.

Materials ranked in the middle, such as $MASnI_3$ + SnF_2 and $CsSnI_3$ (optimized), indicate a probability spread between adjacent ranks, signifying a potential impact from uncertain parameters. The performance of Bi- and Sb-based vacancy-ordered materials, such as $MA_3Bi_2I_9$, $Cs_3Sb_2I_9$, and $Rb_3Sb_2I_9$, is strongly localized in lower ranks, implying that these materials are inferior performer for rooftop efficiency driven applications [21, 22].

The narrow rank distributions for top candidates indicate high confidence in material selection for Rooftop PV deployment.

- **Long-Life Stability Scenario**

As can be seen, the Long-Life Stability heat map presents a higher rank distribution than that observed in the Rooftop scenario, indicating a higher level of competition between materials when stability is given a higher weight by PFoM. While $FASnI_3$ + UiO-66 again has a high probability for Rank 1, other materials exhibit a change in rank, especially for the top five ranks.

Both Cs_2TiBi_6 and $FASnI_3$ + PEA (2D/3D) exhibit high probability values distributed across Ranks 2 to 4, indicating a higher level of competitiveness between these materials when stability is used as a weight by PFoM. Lead-free double perovskites such as $Cs_2AgBiBr_6$ and $MA_2AgBiBr_6$ exhibit an increase in rank compared to the Rooftop scenario, indicating a higher level of relevance when a higher weight is given to material longevity [23].

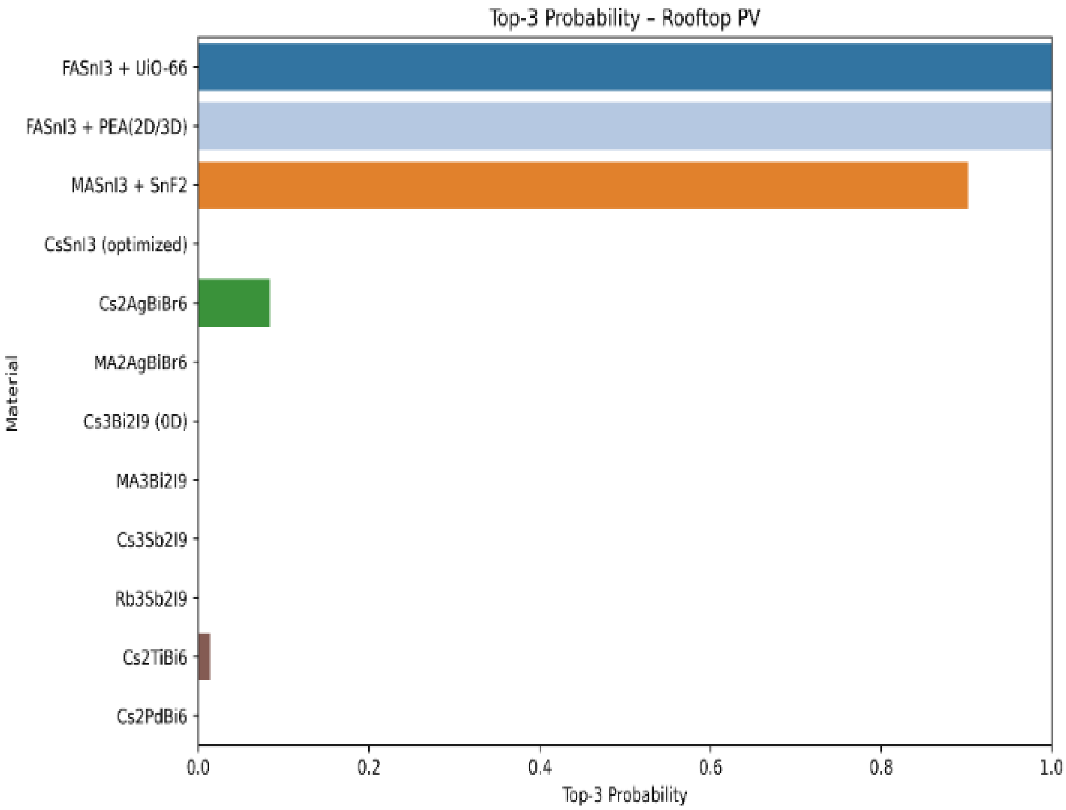
As can be seen, even though the lowest-performing materials still occupy the lower ranks, they are distributed across a higher range of values, indicating a higher impact of uncertainty related to degradation characteristics.

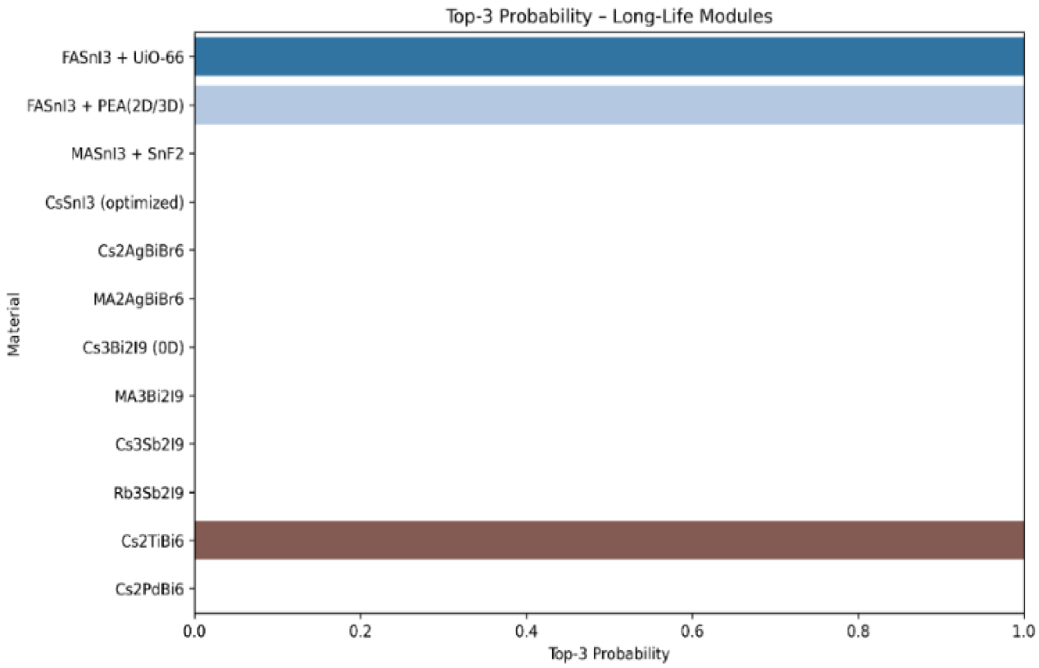
- **Environment-Sensitive PV Scenario**

The Environment-Sensitive PV heat map has the largest rank dispersion, again emphasizing the significant impact of toxicity and environmental factors on the stability of the ranking results. Unlike in the previous cases, no material is found to be a clear winner in the top rank.

$FASnI_3$+ UiO-66 is still a strong candidate, though its probability of achieving the top rank is now around ~0.66, with a significant probability mass in the second and third positions. Materials like Cs_2TiBi_6 and $Cs_2AgBiBr_6$ show broad distributions in the upper and middle ranks, again indicating that non-toxic materials are becoming competitive, even if their efficiencies are somewhat lower. Other Sn-based materials, like $MASnI_3$ + SnF_2 and $CsSnI_3$ (optimized), are shifting to lower ranks, again because of the negative impact of toxicity and stability issues. Vacancy-ordered bismuth and antimony materials are again found in lower ranks, though slightly higher than in the case of rooftop PV, because of the absence of toxicity factors. This scenario also illustrates the notion that environment-driven design results in trade-offs, where the outcomes of the ranking are less certain and dependent on the variability of the input.

For practical decision-making, these distributions were further condensed into Top-3 probabilities (Fig 3). Materials with consistently high Top-3 probabilities represent low-risk choices for deployment, even when mean performance differences are small.





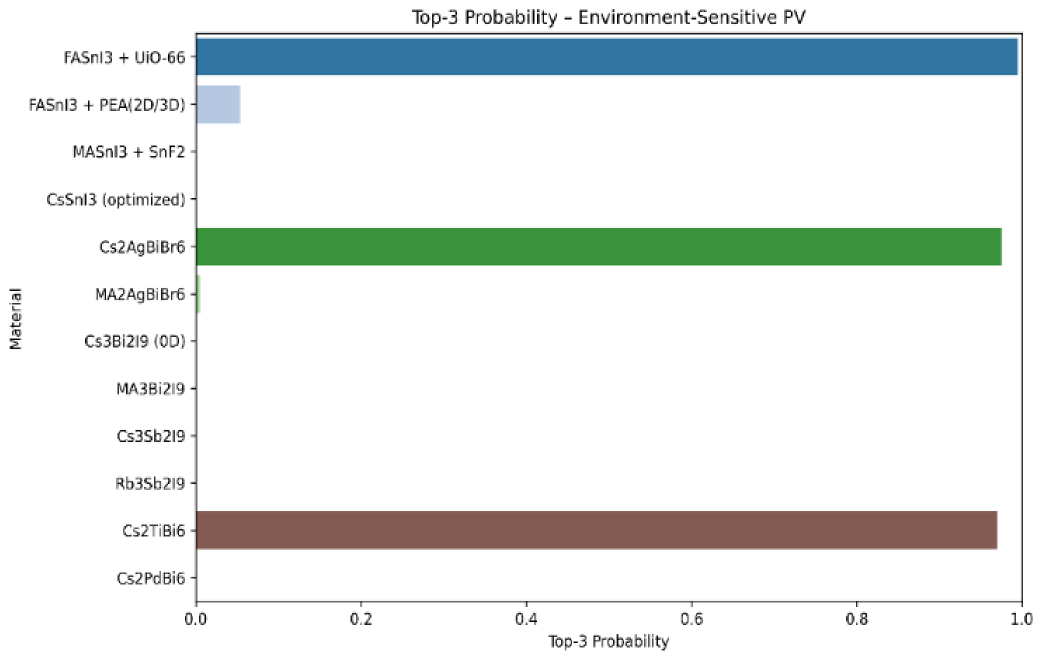


Figure 3: Top-3 probability of candidate materials under (a) rooftop photovoltaics, (b) long-life modules, and (c) environment-sensitive applications

In particular, Fig 3 shows a summary of the Top-3 probability for all candidate materials under the three application scenarios: rooftop PV, environment-sensitive PV, and long-life modules. The term "Top-3 probability" refers to the probability that a material is among the top three in a given Monte Carlo simulation, rather than relying on the average performance of a material.

In the Rooftop PV scenario (Fig. 3a), the performance of $FASnI_3$ + UiO-66 again shows an almost unity Top-3 probability, reinforcing the dominance of this compound under the conditions of efficiency weighting. $MASnI_3$ + SnF_2 also presents an extremely high Top-3 probability, suggesting the competitiveness of this compound, albeit scenario-dependent, resulting from the gains in performance at the cost of more uncertainty. Most of the lead-free double perovskites and low-dimensional compounds of bismuth/antimony have negligible Top-3 probabilities, implying that these compounds are unable to compete under the conditions of efficiency weighting, notwithstanding their occasional ranking.

For the Environment-Sensitive PV scenario (Fig. 3b), the Top-3 landscape is significantly different. $Cs_2AgBiBr_6$ and Cs_2TiBi_6 have nearly unit Top-3 probabilities, confirming the importance of both toxicity and environmental tolerance in the latter case. $FASnI_3$ + UiO-66 also maintains a high Top-3 probability, again confirming the good balance of both performance and environmental tolerance in the former case. $MASnI_3$+ SnF_2 completely loses out in the Top-3 set, again confirming the scenario dependence of the former material as opposed to the latter one.

In the case of the Long-Life Modules scenario (Fig 3c), only a handful of materials have considerable Top-3 probabilities. In particular, $FASnI_3$ + UiO-66 and $FASnI_3$ + PEA (2D/3D) have nearly unity Top-3 probabilities, signifying excellent robustness in the case of prioritizing long-term stability. In addition to these materials, Cs_2TiBi_6 also ranks high in this case, similar to its stability scores [24]. The vast majority of other materials have vanishing Top-3 probabilities, either due to low stability or high uncertainty.

Figure 3 offers a probabilistic filter that complements rank heat maps (Fig. 2), which in turn can be used to derive Relative Scenario Value (RSV) classification (Table 2). Materials with high Top-3 probabilities in all scenarios are obvious “generalists,” while materials that excel in one or more specific cases are highlighted as “specialists.” The Top-3 probabilities analysis thus connects detailed rank distributions with decision-relevant material screening in support of uncertainty-aware application-specific photovoltaic material selection.

Cross-Scenario Robustness via Relative Stability Value (RSV)

The RSV values for all materials are summarized in Table 2.

Table 2: Relative Scenario Values (RSV) and material classification across scenarios

	RSV Rooftop	RSV Long Life	RSV Env Sensitive	Category
$FASnI_3$ + UiO-66	0.333	0.333	0.332	Generalist
$CsSnI_3$ (optimized)	0.000	0.000	0.000	Low performer
$MA_2AgBiBr_6$	0.000	0.000	0.002	Low performer
Cs_3Bi2I_9 (0D)	0.000	0.000	0.000	Low performer
$MA_3Bi_2I_9$	0.000	0.000	0.000	Low performer
$Cs_3Sb_2I_9$	0.000	0.000	0.000	Low performer
$Rb_3Sb_2I_9$	0.000	0.000	0.000	Low performer
Cs_2PdBi_6	0.000	0.000	0.000	Low performer
$FASnI_3$+ PEA(2D/3D)	0.333	0.333	0.018	Mostly Generalist
Cs_2TiBi_6	0.005	0.333	0.323	Mostly Generalist
$MASnI_3$ + SnF_2	0.301	0.000	0.000	Specialist
$Cs_2AgBiBr_6$	0.028	0.000	0.325	Specialist

Fig. 2 offers the probabilistic rationale for the Rank Stability Value (RSV)-informed classification provided in Table 2. Materials with strong localization of probability mass at the top ranks in all three scenarios are found to have high and balanced Rank Stability Values and are thus classified as Generalists. For instance, $FASnI_3$+ UiO-66 has excellent localization at Rank 1 in all three heatmaps, resulting in nearly identical RSV values (~ 0.33) in all three scenarios: Rooftop, Long-Life, and Environment-Sensitive. This points to excellent robustness against shifting application priorities and uncertainty and thus meets the requirements for being classified as a Generalist.

In contrast, Specialist materials exhibit significant rank localization under specific scenarios, with near-zero probabilities in all other cases. $MASnI_3$ + SnF_2, for example, exhibits significant top-rank probability only in the Rooftop PV heat map, and $Cs_2AgBiBr_6$ is competitive under Environment-Sensitive weighting, with skewed RSV distributions that reflect scenario-dependent performance. Lastly, materials in the Low performers group exhibit localization at lower ranks with near-zero probability in the top three positions in all scenarios, as indicated by the heatmaps and confirmed by near-zero RSV values. As a result, Fig 2 and Table 2 collectively illustrate that RSV is able to effectively model probabilistic ranking behavior and map this behavior onto a useful and applicable classification scheme, beyond the simple means-based PFoM performance metrics and toward a robustness-aware decision support methodology.

Table 2 presents a summary of the Relative Stability Value (RSV) of each material over the three different application scenarios: rooftop PV, long-life modules, and environment-sensitive deployment. The RSV value essentially indicates how frequently a material is represented across the top three positions of candidate materials upon evaluation via a probabilistic Monte Carlo method, normalized such that it sums to unity across all three scenarios for consistently high-performing materials.

Among all materials considered, it is apparent that $FASnI_3$ + UiO-66 is the only material that can be considered a "generalist," with nearly equivalent RSV values across rooftop PV (0.333), long-life modules (0.333), and environment-sensitive deployment (0.332) applications. This uniformity across different scenarios clearly indicates exceptional robustness, validating that high performance is not dependent on a particular weighting criterion.

The second group of materials exhibits partial cross-scenario robustness, which is categorized as mostly generalists. In the case of the $FASnI_3$ + PEA (2D/3D), the material has high values of RSV for the rooftop and long-life scenarios (0.333 for each scenario), but the opposite is true for the environment-sensitive scenario, where the RSV is significantly lower (0.018). In the case of the Cs_2TiBi_6 material, the opposite is true, where the long-life scenario (0.333) and the environment-sensitive scenario (0.323) have high values of RSV, but the material is not present in the rooftop scenario (0.005).

Some compounds are scenario-specific specialists, recording high RSV values for a particular scenario context only. $MASnI_3$ + SnF_2 has a high RSV value only for rooftop PV systems, at 0.301, which correlates with its optimization criteria focusing on efficiency and unfavorable results for long-term stability and environmental impact. $Cs_2AgBiBr_6$ has high RSV values only for environment-sensitive deployment, at 0.325, which correlates with its advantage of having a low toxicity level, regardless of its performance in terms of efficiency and stability.

The rest of the materials, $CsSnI_3$ (optimized), $MA_2AgBiBr_6$, $Cs_3Bi_2I_9$ (0D), $MA_3Bi_2I_9$, $Cs_3Sb_2I_9$, $Rb_3Sb_2I_9$, and Cs_2PdBi_6, have negligible RSV values for all scenarios. Their absence in the Top-3 rankings signifies their continued underperformance or high uncertainty and thus places them in the low-performing materials group.

Table 2 shows that for proper material selection, one cannot solely rely on optimization in a single scenario. Rather, RSV analysis can help in identifying genuine material generalists from specialists and low-confidence materials, thus acting as a bridge between uncertainty-aware performance metrics and decision-making.

Cross-Scenario Generalist and Specialist Behavior

An important goal of this work is not only to identify the high-performing lead-free perovskites for individual deployment scenarios, but also to comprehend the progression of the ranking of the materials for fundamentally different scenarios of application. By jointly examining the probabilistic rank heatmaps (Fig 2), the Top-3 probability distributions (Fig 3), and the Relative Scenario Value (RSV) classification (Table 2), we can observe the differences among the cross-scenario generalists, scenario specialists, and underperforming materials.

An initial hint of robustness across scenarios can be gleaned from Fig 3. Materials like $FASnI_3$ + UiO-66 have their probability distribution concentrated in the upper ranks of all three scenarios: "Rooftop PV," "Long-Life Modules," and "Environment-Sensitive PV." This implies that their high performance does not depend on the weighting of certain properties in a particular scenario. This robustness in ranking can also be quantitatively supported from Table 2, where we observe almost equal contributions of RSV for all three scenarios (RSV ~ 0.33 for all three scenarios), justifying their identification as "true generalists." The limited rank dispersion in the heat maps in Fig 2 also hints at a low uncertainty in their prediction, which is an important factor in real-world applications.

In contrast, mostly generalist materials exhibit partial robustness with weakening in specific scenarios. For instance, the performance of the $FASnI_3$ + PEA (2D/3D) compound is strong with Top-3 probabilities in Rooftop PV and Long-Life Modules but experiences weakening in the Environment-Sensitive PV scenario (Fig 3). This is reflected in Table 2 with the weakening of the RSV for the environmentally weighted scenario, where the trade-off of the spacer layers is reflected. A similar trend is also observed for the compound Cs_2TiBi_6, where it performs well in the Long-Life and Environment-Sensitive scenarios but underperforms in the Rooftop PV scenario, where the compound experiences stability and toxicity-driven advantages rather than an efficiency-driven advantage [24].

Specialist behavior is clearly visible for materials where performance is significantly dependent on one particular application context. For example, $MASnI_3$ + SnF_2 exhibits high Top-3 probability almost exclusively for Rooftop PV (Fig 3), where efficiency improvements due to defect passivation play a crucial role [25], but performs much less favorably for durability- and toxicity-weighted scenarios. On the other hand, $Cs_2AgBiBr_6$ is predominantly selected for Environment-Sensitive PV, where toxicity and inherent stability of the material dominate the ranking rationale [26]. This is also reflected in their RSV vectors (Table 2), where one particular scenario significantly contributes to the final score, which confirms the specialist character of the material.

Significantly, a significant number of materials, including some bismuth and antimony-based 0D and layered materials, display a negligible Top-3 probability across all scenarios. The materials' consistently low RSV values and scattered rank distribution reflect structural limitations that make them non-competitive under any circumstance. Rather than a failing in the model, this is a testament to the overall reliability of the framework in its discriminatory capabilities.

In summary, the agreement of the probabilistic rankings in Figs 2 and 3 with the RSV-based categorization in Table 2 confirms that cross-scenario generalism is rare and non-trivial in structure, whereas specialization occurs naturally as a consequence of targeted optimization of particular physical properties. This dichotomy is of significant importance in determining the selection of materials according to the relative importance of universality vs. niche optimization in the application of choice.

Conclusion

In this work, we propose a probabilistic and application-oriented methodology for the evaluation and classification of lead-free perovskite-based PV materials under application-oriented scenarios. Unlike conventional deterministic methodologies, where a single figure of merit is assigned to each material, the proposed methodology addresses the inherent uncertainties associated with application priorities using a Monte Carlo simulation of weighted material performance metrics. This will allow for a more realistic evaluation of the suitability of materials for PV applications, as it addresses the trade-offs associated with material efficiency, stability, and safety, among other factors. Using probabilistic material rankings, Top-k probabilities, and scenario-normalized material performance, the proposed methodology will offer a systematic approach for evaluating the material ranking under varied application priorities for PV materials. It can be seen from the results that from the probabilistic rank heat maps and the Top-3 probability analysis, where the top performers in a given scenario might lose relevance if the deployment priorities are altered. This, in turn, highlights the need to take into account the uncertainties and the weighting in the materials screening methodologies. The Relative Scenario Value is a tool that brings together all this information in such a way that it is possible to see the difference between generalists, where the performance is good in all areas, and specialists, where the performance is excellent in very particular areas.

Amongst the top-ranked materials, $FASnI_3$ + UiO-66 is an efficient cross-scenario generalist, as it considers efficiency, stability, as well as sustainability issues such as the ranking uncertainty level. Conversely, materials such as $MASnI_3$ + SnF_2, $Cs_2AgBiBr_6$, etc., highlight the trade-offs that have to be made in the development of efficient versus sustainability-oriented materials, respectively. The tool also correctly identifies materials that consistently perform poorly, enabling their logical de-prioritization in the experimental design.

Aside from the aforementioned systems studied, the proposed methodology is also generally applicable to other energy systems involving competing objectives that need to be resolved, given that the proposed methodology establishes a clear connection between probabilistic ranking and data-based decision metrics. This methodology offers a clear way forward for data-based materials discovery that can help close the gap between computation and deployment.

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