

Abstract

All-inorganic metal halide (IMH) perovskites have been the subject of intensive experimental and theoretical research in the recent past for their superior thermal and chemical stability, along with high radiation tolerance relative to their organic-inorganic counterparts. IMH perovskites’ high radiation tolerance and defect-resistance make them promising candidates for photovoltaic applications in high radiation environments, such as those of outer space.

Currently, among inorganic metal halide perovskites, caesium-lead halides such as CsPbI3 and CsPbBr3 see the widest use and research attention. Their main drawback is toxicity, stemming from the lead they contain. Hence, research is now being done into lead-substituted IMH perovskites, but lead is a key component that contributes to the radiation tolerance of IMH perovskites. In this study, we have employed molecular dynamics and Monte Carlo simulations to compare the radiation damage induced by H⁺ ions in lead-based and antimony-based (lead-substituted) perovskites, aiming to elucidate the differences in radiation tolerance between the two materials.

The results show that mid-energy protons (50-100 keV) produce the greatest displacement damage and directly impact absorber-critical depths. Iodine loss is the dominant structural degradation pathway in both materials. Although Cs3Sb2I9 demonstrates slightly less B-site displacement at low energies, both compositions exhibit high halide susceptibility, since iodine loss is the dominant pathway for structural degradation, indicating that halide stabilization is essential for improving the endurance of perovskite solar cells.

Comparative Radiation Tolerance of Lead and Antimony based Perovskites under Proton Irradiation for Photovoltaic Applications

Abiha Saqib

Introduction

Why IMH Perovskites for Photovoltaics?

All-inorganic metal-halide perovskites combine high carrier mobility, long diffusion lengths, and thermal and chemical stability, making them promising candidates for photovoltaic systems operating in extreme environments.

The Lead Problem:

CsPbI₃ is a promising and widely-used perovskite for photovoltaics, but its lead content presents significant toxicity concerns. Cs₃Sb₂I₉ offers a potential lead-free alternative because of its lower toxicity, air stability, and tunable electronic structure.

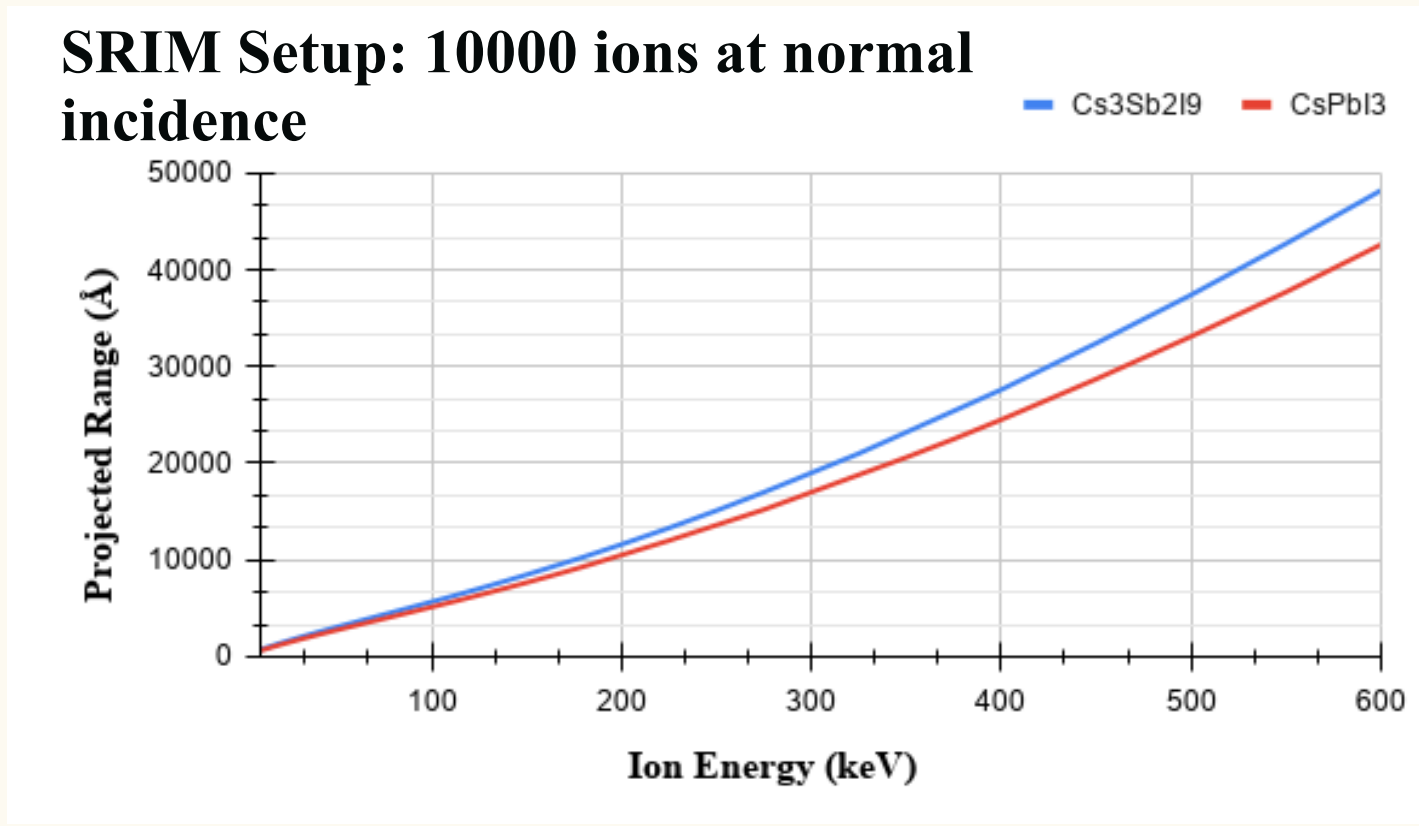
The Literature Gap and our Aim:

Lead contributes to the defect tolerance of metal-halide perovskites, so replacing lead may alter how the lattice responds to radiation. This effect of lead to antimony substitution on proton-induced displacement damage remains insufficiently understood. Therefore, the degree of substitutability of lead is being investigated in this study.

Methods

Tested Materials:

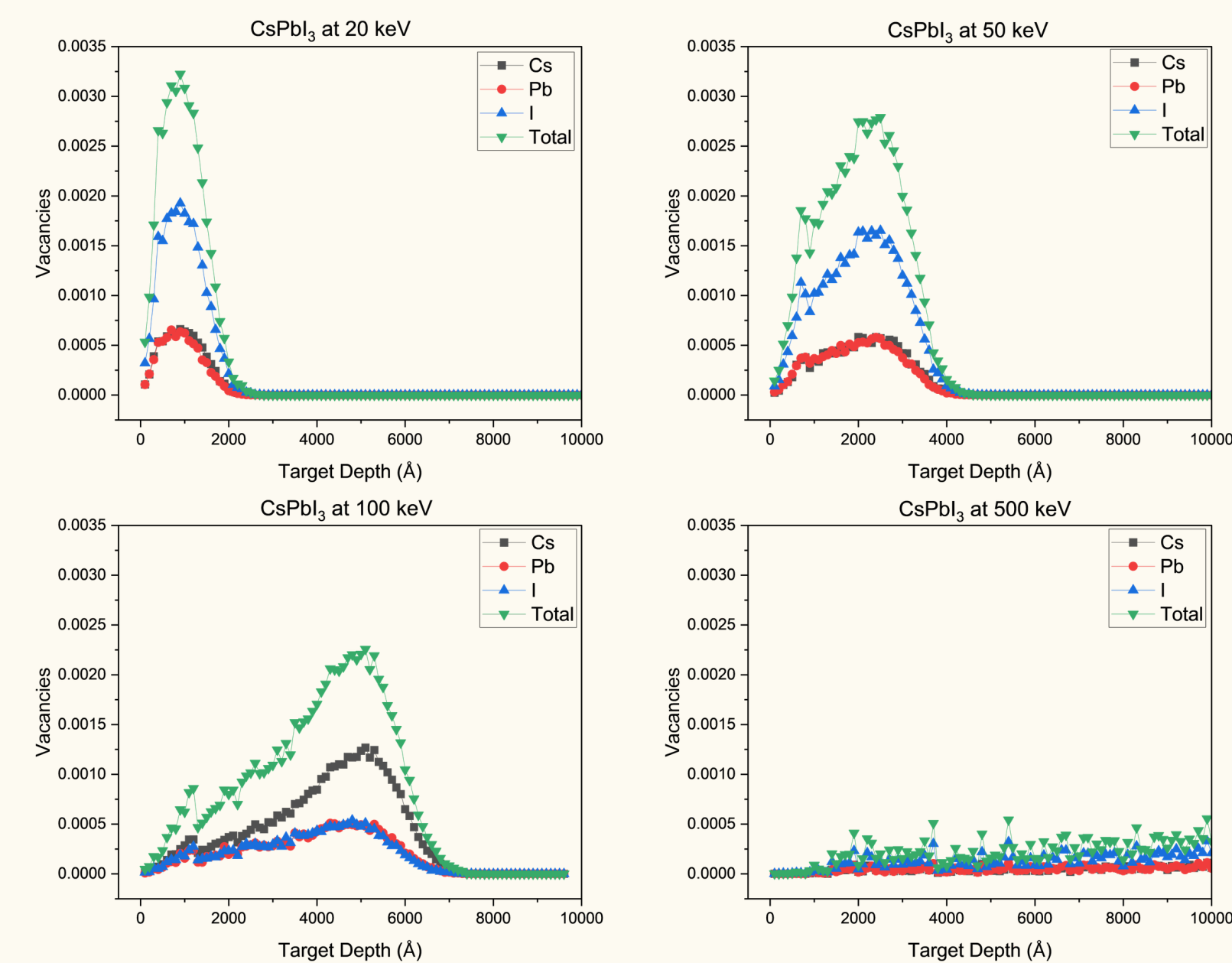
CsPbI3 (lead-based) and Cs3Sb2I9 (lead-substituted)



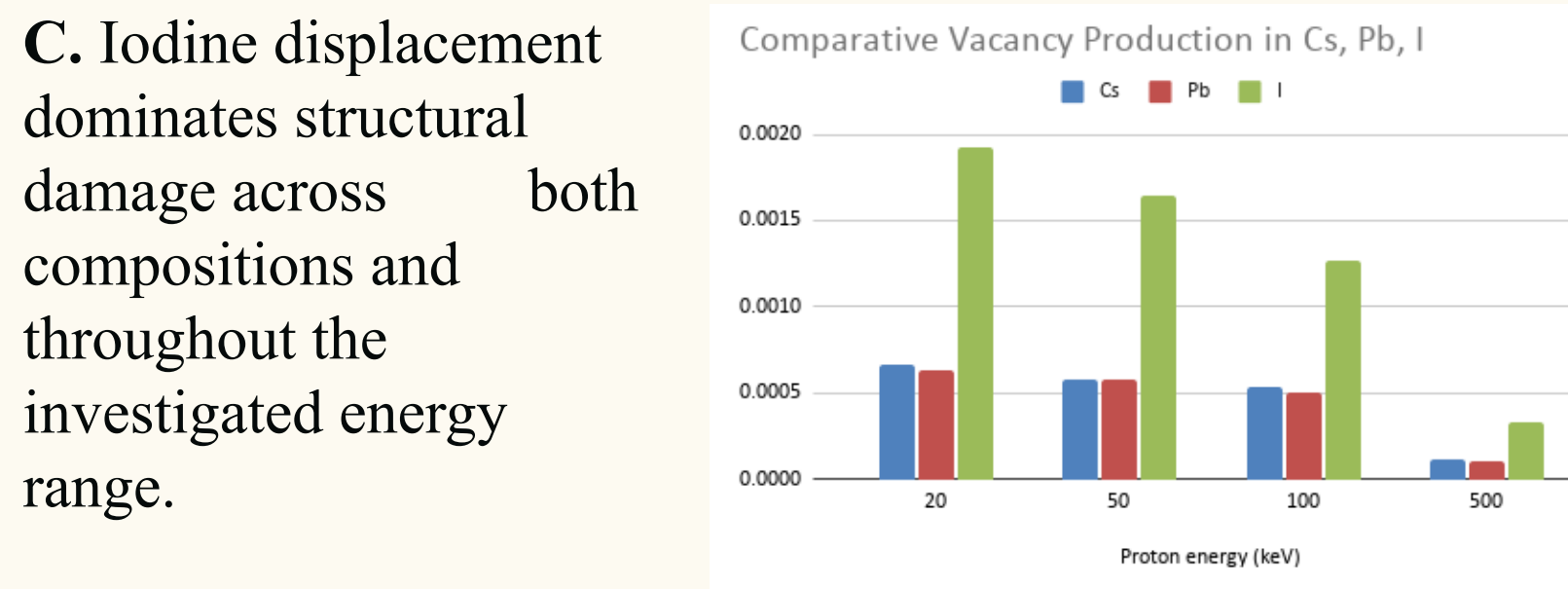
TRIM Setup	
Wafer Thickness (Å/nm)	10,000 / 1,000
No. of ions	10,000
Ion energies (keV)	20 50 100 500
Angle of Incidence (degrees)	0° (normal)
Output (Vacancies/(Å·ion))	Vacancy production rate

Results

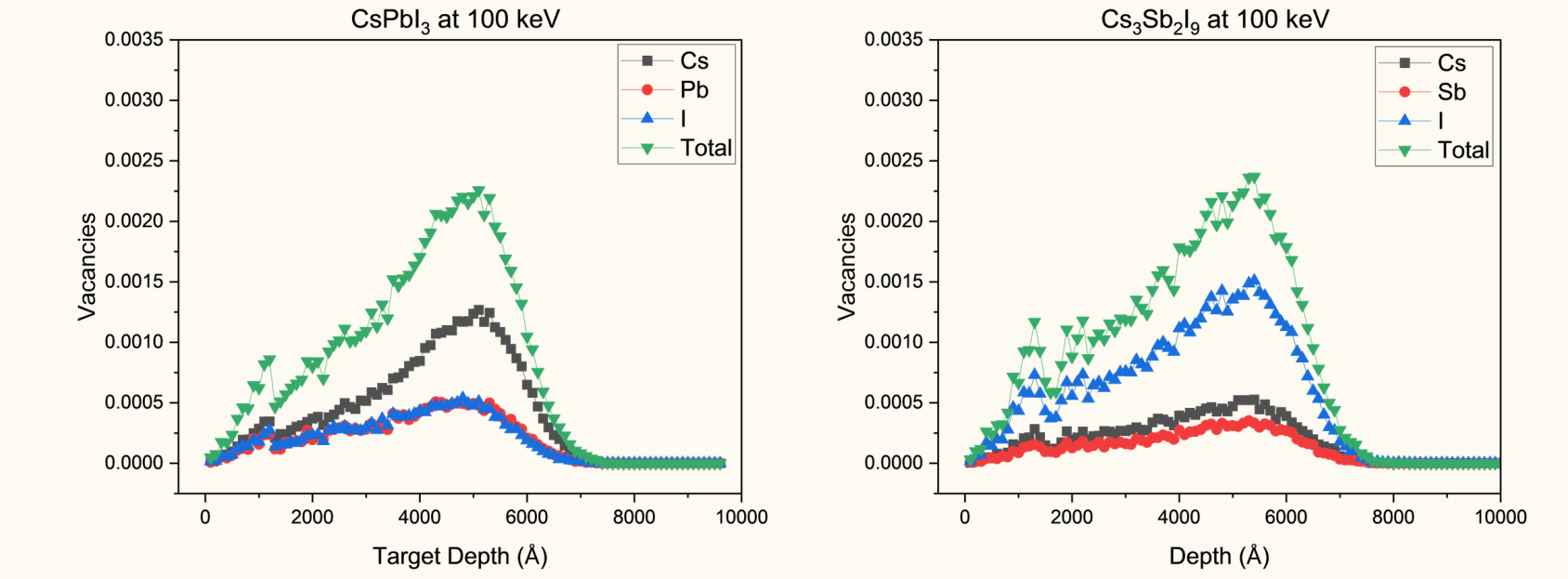
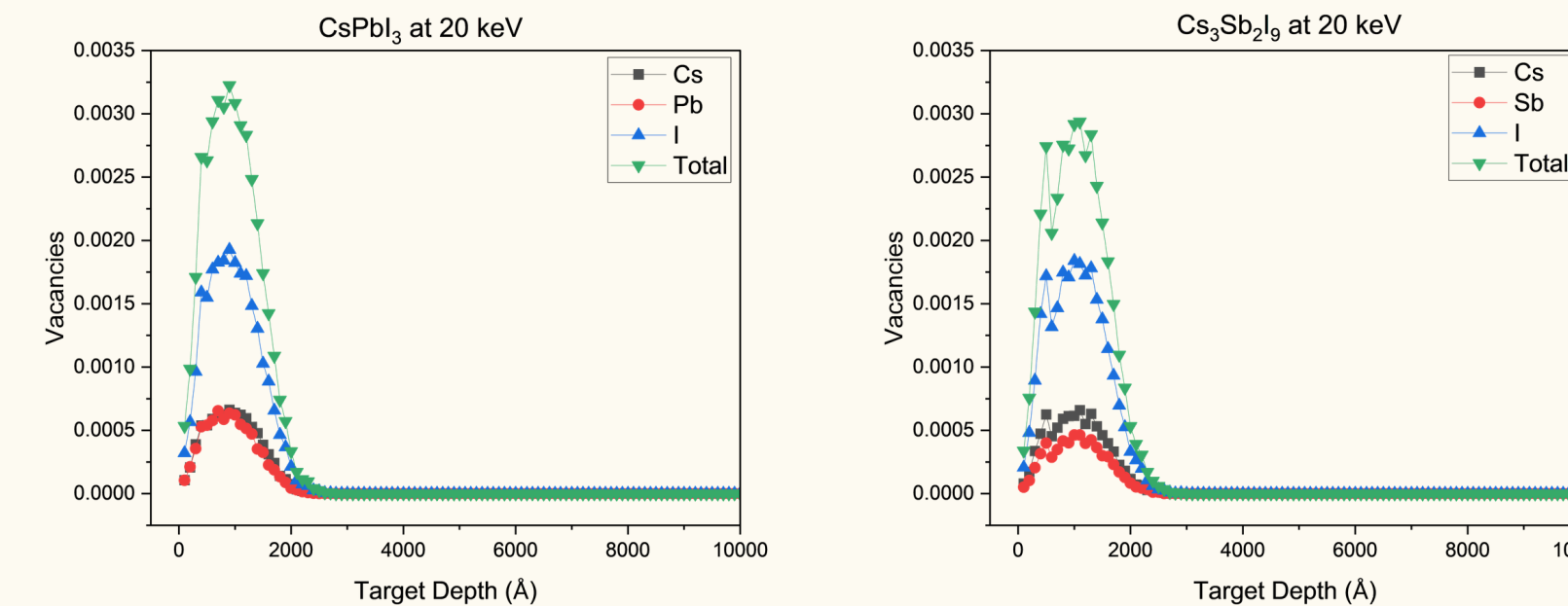
A. Maximum displacement damage occurs at intermediate proton energies, not at the highest incident energy.



B. Damage migrates into the photovoltaic absorber region
50 keV → shallower damage
100 keV → deeper absorber-region damage



D. LEAD HIGHLY SUBSTITUTABLE:
Cs₃Sb₂I₉ exhibits broadly similar vacancy-production patterns to CsPbI₃ across the tested proton energies, with the lead-based perovskite producing slightly higher vacancy rates at several energies.



Discussion & Limitations

Cs₃Sb₂I₉ demonstrates greater B-site resilience at low-to-mid proton energies, suggesting that Sb is a promising candidate for replacing toxic Pb. However, because iodine remains the dominant displacement pathway, B-site substitution alone is insufficient to produce a radiation-hardened material.

Simulated vacancies do not necessarily correspond to permanent defects; some vacancy-interstitial pairs may recombine through self-healing or thermal processes. Moreover, not all vacancies create deep electronic traps; their impact depends on defect-specific electronic structure. Hence, these atomic displacement profiles don’t directly correspond to macroscopic defect formation in photovoltaic devices.

Furthermore, this study used proton energies up to 500 keV, while extreme environments like space have considerably higher energy irradiation.

Conclusion

Monte Carlo modeling shows that both CsPbI₃ and Cs₃Sb₂I₉ remain vulnerable to halide vacancies under proton irradiation. While antimony offers modest B-site resilience and remains a promising substitute for toxic lead, halide stabilization remains essential to produce radiation hardened perovskites.

References

[1] Bouhmouche, A., Tariq, S., Jabar, A., Moubah, R., Lassri, H., & Abid, M. (2023). Electronic and thermodynamic properties of CsPbI3 halide perovskites: Ab-initio investigation. Materials Today: Proceedings. <https://doi.org/10.1016/j.matpr.2023.10.102>

[2] Hoefler, S. F., Trimmel, G., & Rath, T. (2017). Progress on lead-free metal halide perovskites for photovoltaic applications: A review. Monatshefte Für Chemie - Chemical Monthly, 148(5), 795–826. <https://doi.org/10.1007/s00706-017-1933-9>

[3] Jain, A., Ong, S. P., Hautier, G., Chen, W., Richards, W. D., Dacek, S., Cholia, S., Gunter, D., Skinner, D., Ceder, G., & Persson, K. A. (2013). Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. APL Materials, 1(1), 011002. <https://doi.org/10.1063/1.4812323>

[4] James Ziegler—SRIM & TRIM. (n.d.). <https://doi.org/10.1063/http/www.srim.org/>

[5] Kirmani, A. R., & Sellers, I. R. (2025). Are metal-halide perovskite solar cells really radiation tolerant? Joule, 9(3). <https://doi.org/10.1016/j.joule.2025.101852>

[6] Liang, J., & Qi, Y. B. (2021). Recent progress on all-inorganic metal halide perovskite solar cells. Materials Today Nano, 16, 100143. <https://doi.org/10.1016/j.mtnano.2021.100143>

[7] Martinie, S., Saad-Saoud, T., Moindjie, S., Munteanu, D., & Autran, J. L. (2014). Behavioral modeling of SRIM tables for numerical simulation. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 322, 2–6. <https://doi.org/10.1016/j.nimb.2013.12.023>

[8] Nguyen, D.-T., Walter, D., Weber, K. J., Duong, T., & White, T. P. (2023). Simulating Proton Radiation Tolerance of Perovskite Solar Cells for Space Applications. Advanced Energy and Sustainability Research, 4(12), 2370025. <https://doi.org/10.1002/aesr.202370025>

[9] Oyewande, O. E., & Akinpelu, A. (2018a). An ion-beam surface sputtering approach to the quest for lead free metal halide perovskite for solar cells. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 434, 102–108. <https://doi.org/10.1016/j.nimb.2018.08.041>

[10] Oyewande, O. E., & Akinpelu, A. (2018b). Projected Range and Sputter Yield of Ne⁺ and Ar⁺ in the Sputtering of Lead and Tin Perovskites. IOP Conference Series: Earth and Environmental Science, 173(1), 012045. <https://doi.org/10.1088/1755-1315/173/1/012045>

[11] Tu, Y., Wu, J., Xu, G., Yang, X., Cai, R., Gong, Q., Zhu, R., & Huang, W. (2021). Perovskite Solar Cells for Space Applications: Progress and Challenges. Advanced Materials, 33(21), 2006545. <https://doi.org/10.1002/adma.202006545>

[12] Yin, W.-J., Shi, T. and Yan, Y. (2014). Unique Properties of Halide Perovskites as Possible Origins of the Superior Solar Cell Performance. Adv. Mater., 26: 4653–4658. <https://doi.org/10.1002/adma.201306281>

[13] Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 19th International Conference on Ion Beam Analysis, 268(11), 1818–1823. <https://doi.org/10.1016/j.nimb.2010.02.091> Defects-Induced Voltage Losses of Perovskite Solar Cells | Encyclopedia MDPI. (n.d.). Retrieved 13September 2026, from <https://encyclopedia.pub/entry/55411>