

# Environmental and Toxicity Assessment of Double Perovskites vs Lead Perovskites

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## ABSTRACT

The rapid advancement of perovskite-based materials in optoelectronic and photovoltaic applications has raised significant concerns regarding their environmental sustainability and toxicity profiles. In particular, conventional lead-based perovskites, such as Methylammonium lead iodide (MAPbI<sub>3</sub>), have demonstrated remarkable power conversion efficiencies but pose substantial environmental and health risks due to lead content and instability under ambient conditions. In contrast, lead-free double perovskites, including Cs<sub>2</sub>AgBiBr<sub>6</sub> and Cs<sub>2</sub>AgInCl<sub>6</sub>, have emerged as promising alternatives offering improved chemical stability and reduced toxicity.

This comparative review evaluates the environmental impact, toxicity mechanisms, degradation pathways, and life-cycle assessment (LCA) considerations associated with lead-based and double perovskite materials. Factors such as elemental composition, leaching behavior, bioaccumulation potential, synthesis routes, and end-of-life disposal are critically examined.

While lead perovskites exhibit superior optoelectronic properties and commercial readiness, their environmental footprint is heightened by lead leakage, ecological toxicity, and regulatory constraints. Double perovskites, though comparatively less toxic and more stable, often suffer from lower power conversion efficiencies and limited scalability.

The review highlights recent advances in green synthesis, encapsulation strategies, and recycling methods aimed at minimizing environmental risks. Furthermore, toxicity assays and computational modeling approaches are discussed to provide a holistic understanding of long-term environmental safety. Overall, the analysis suggests that double perovskites offer a safer and more sustainable pathway for next-generation photovoltaic technologies, provided their efficiency and manufacturability challenges are systematically addressed. This work contributes to informed material selection and policy development toward environmentally responsible perovskite deployment.

**Keywords:** Lead-Based Perovskites, Double Perovskites, Environmental Toxicity, Life Cycle Assessment (LCA), Sustainable Photovoltaic Materials

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## INTRODUCTION

Perovskite materials have revolutionized the field of optoelectronics and photovoltaic technology due to their exceptional light-harvesting efficiency, tunable bandgap, long carrier diffusion length, and low-cost fabrication processes. Since the first report of high-efficiency perovskite solar cells, organometal halide perovskites—particularly Methylammonium lead iodide (MAPbI<sub>3</sub>)—have demonstrated rapid improvements in power conversion efficiency (PCE), rivaling conventional silicon-based technologies. The perovskite structure, generally represented by the formula ABX<sub>3</sub>, offers compositional flexibility that enables bandgap engineering and performance optimization for solar cells, light-emitting diodes (LEDs), and photodetectors.

Despite these advantages, the incorporation of lead (Pb) in most high-performing perovskite materials has raised critical environmental and public health concerns. Lead is a well-known toxic heavy metal with cumulative bioaccumulation effects, posing risks to ecosystems and human health through soil contamination, water leaching, and improper disposal of photovoltaic modules. The instability of lead perovskites under moisture, heat, and ultraviolet exposure may accelerate material degradation, potentially releasing soluble lead compounds into the environment. These risks have prompted intensified regulatory scrutiny and motivated the scientific community to explore safer alternatives.

Among the emerging candidates, lead-free double perovskites such as Cs<sub>2</sub>AgBiBr<sub>6</sub> and Cs<sub>2</sub>AgInCl<sub>6</sub> have gained attention as environmentally benign substitutes. Double perovskites typically follow the general formula A<sub>2</sub>BB'X<sub>6</sub>, where two distinct metal cations replace divalent lead, thereby eliminating direct Pb content. These materials offer enhanced structural stability, reduced toxicity potential, and better resistance to environmental degradation. However, challenges remain in achieving efficiencies comparable to lead-based counterparts and in optimizing their charge transport properties.

Given the growing global demand for sustainable energy technologies, it is essential to evaluate not only the performance metrics of perovskite materials but also their environmental footprint and toxicological implications. Environmental risk assessment, life-cycle analysis (LCA), degradation chemistry, and ecotoxicological studies are increasingly being integrated into materials research to provide a comprehensive understanding of sustainability.

This comparative review aims to critically examine the environmental and toxicity profiles of conventional lead perovskites versus emerging lead-free double perovskites. By analyzing synthesis routes, degradation pathways, elemental hazards, ecological impact, and end-of-life management strategies, the study seeks to inform material selection and guide future research toward safer, scalable, and environmentally responsible perovskite technologies.

## RELATED THEORY & MODELS

The theoretical framework for comparing lead-based perovskites and double perovskites integrates crystallographic stability principles, toxicological risk assessment models, degradation chemistry, and life-cycle sustainability analysis. This framework provides a multidisciplinary basis for understanding how structural design influences environmental impact and toxicity.

### 1. Crystal Structure and Stability Theory

The perovskite structure is governed by the general formula ABX<sub>3</sub>, where A is a monovalent cation, B is a divalent metal cation, and X is a halide anion. In widely studied lead perovskites such as Methylammonium lead iodide (MAPbI<sub>3</sub>), structural stability is often predicted using the **Goldschmidt tolerance factor (t)** and the **octahedral factor (μ)**:

- **Tolerance factor (t)** =  $(r_A + r_X) / \sqrt{2} (r_B + r_X)$
- **Octahedral factor (μ)** =  $r_B / r_X$

These parameters determine whether a stable three-dimensional perovskite lattice can form. However, environmental exposure (moisture, oxygen, UV radiation) can destabilize the Pb–X octahedral framework, promoting ionic dissociation and lead release.

In contrast, double perovskites follow the formula A<sub>2</sub>BB'X<sub>6</sub>, where two different cations (B and B') substitute the divalent Pb<sup>2+</sup> site. For example, Cs<sub>2</sub>AgBiBr<sub>6</sub> achieves charge neutrality by combining monovalent Ag<sup>+</sup> and trivalent Bi<sup>3+</sup>. Theoretical calculations suggest that this ordered lattice enhances thermodynamic stability and reduces defect formation, thereby decreasing the likelihood of toxic ion leaching.

### 2. Toxicological Risk Assessment Theory

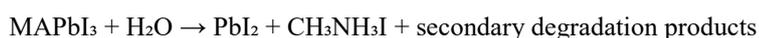
The toxicity assessment of perovskite materials is grounded in classical environmental toxicology models:

- **Dose–Response Theory:** Establishes the quantitative relationship between exposure concentration and adverse biological effects. Lead compounds exhibit nonlinear, cumulative toxicity even at low exposure levels.
- **Bioaccumulation and Biomagnification Theory:** Lead can accumulate in soil, aquatic organisms, and food chains, increasing ecological risk over time.
- **Hazard Identification and Risk Characterization Models:** Used to compare intrinsic material hazards (e.g., Pb<sup>2+</sup> vs Bi<sup>3+</sup> or Ag<sup>+</sup> ion toxicity).

Lead-based perovskites are theoretically classified as high-hazard due to the well-established neurotoxicity of Pb<sup>2+</sup> ions. Double perovskites replace Pb<sup>2+</sup> with lower-toxicity metals, reducing systemic biological risk, though the long-term ecotoxicity of substitute metals must also be considered.

### 3. Degradation Chemistry and Environmental Release Models

Environmental stability is theoretically evaluated using thermodynamic and kinetic degradation models. Lead perovskites are susceptible to hydrolysis reactions:



Such reactions can liberate soluble lead salts, increasing contamination potential.

Double perovskites demonstrate improved lattice stability due to stronger metal–halide bonding and reduced volatility of organic components, thereby theoretically lowering environmental release rates. First-principles density functional theory (DFT) studies suggest lower formation energies for stable double perovskite phases, contributing to enhanced environmental resilience.

#### 4. Life-Cycle Assessment (LCA) Framework

The environmental comparison also relies on Life-Cycle Assessment methodology, incorporating:

1. **Raw material extraction impact**
2. **Energy consumption during synthesis**
3. **Operational environmental risk**
4. **End-of-life disposal and recycling potential**

Lead-based perovskites may have lower manufacturing energy requirements but carry higher disposal and environmental remediation burdens. Double perovskites potentially reduce hazard-related lifecycle impacts but may require more complex processing routes.

#### 5. Sustainable Materials Design Theory

The theoretical approach is further supported by principles of **Green Chemistry** and **Sustainable Materials Engineering**, emphasizing:

- Reduction of hazardous substances
- Atomic economy in synthesis
- Use of less toxic precursors
- Design for recyclability and material recovery

Within this sustainability paradigm, double perovskites represent a rational materials redesign strategy aimed at eliminating inherently toxic components while preserving optoelectronic functionality.

#### Conceptual Model of Comparative Assessment

The integrated theoretical framework can be summarized as:

**Material Structure → Stability & Degradation → Ion Release → Toxicity Pathways → Environmental Impact (LCA) → Sustainability Index**

This structured approach enables a comprehensive comparison between lead-based and double perovskites, linking atomic-scale design to ecological and regulatory consequences.

### PROPOSED MODELS AND METHODOLOGIES

To systematically compare the environmental and toxicity profiles of lead-based perovskites and double perovskites, an integrated multi-disciplinary methodology is proposed. This framework combines experimental toxicology, computational modeling, degradation analysis, and life-cycle assessment (LCA) to provide a comprehensive sustainability evaluation.

#### 1. Material Selection and Structural Benchmarking

**Representative materials are selected for comparative analysis:**

- Lead-based perovskite: Methylammonium lead iodide (MAPbI<sub>3</sub>)
- Double perovskites: Cs<sub>2</sub>AgBiBr<sub>6</sub> and Cs<sub>2</sub>AgInCl<sub>6</sub>

**Structural stability will be analyzed using:**

- X-ray diffraction (XRD) for crystallinity
- Goldschmidt tolerance factor calculations
- Density Functional Theory (DFT) for formation energy and defect state analysis  
This establishes baseline physicochemical stability before environmental exposure.

## 2. Degradation and Leaching Analysis Model

To assess environmental release potential, accelerated aging studies will be performed under:

- Controlled humidity (RH 65–85%)
- UV radiation exposure
- Thermal stress (25–85°C cycling)

### Leachate analysis will include:

- Inductively Coupled Plasma Mass Spectrometry (ICP-MS) for  $Pb^{2+}$ ,  $Ag^+$ ,  $Bi^{3+}$ , and  $In^{3+}$  quantification
- pH-dependent dissolution studies
- Soil and water simulation environments

A **Diffusion–Release Kinetic Model** will be applied to predict long-term ion migration and environmental contamination rates.

## 3. Toxicological Assessment Protocol

A tiered toxicity model is proposed:

### (a) In Vitro Cytotoxicity Assays

- MTT and LDH assays on human epithelial and liver cell lines
- Reactive oxygen species (ROS) detection
- Apoptosis pathway analysis

### (b) Ecotoxicity Studies

- Aquatic organism testing (e.g., algae and Daphnia species)
- Soil microbial activity assays
- Bioaccumulation factor (BAF) determination

### (c) Dose–Response Modeling

$LC_{50}$  and  $IC_{50}$  values will be determined and fitted using nonlinear regression analysis to compare toxicity thresholds between materials.

## 4. Computational Toxicity Prediction

To complement experimental studies:

- Quantitative Structure–Activity Relationship (QSAR) modeling
- First-principles simulations of ion solubility and defect formation
- Environmental fate modeling using multimedia compartment models (air, soil, water)

Computational modeling allows prediction of long-term environmental risk beyond laboratory time scales.

## 5. Life-Cycle Assessment (LCA) Methodology

A cradle-to-grave LCA approach will be adopted following ISO 14040 standards:

### Stages Considered:

1. Raw material extraction
2. Material synthesis
3. Device fabrication
4. Operational phase
5. End-of-life disposal or recycling

### Impact Categories:

- Global warming potential (GWP)
- Human toxicity potential (HTP)
- Ecotoxicity index
- Resource depletion

Comparative scoring will be normalized to per kWh electricity generated to account for performance differences.

## 6. Comparative Analytical Framework

The methodology integrates:

Material Chemistry → Environmental Degradation → Ion Release → Toxicity Testing → LCA → Sustainability Index

By combining laboratory, computational, and environmental modeling techniques, the proposed framework ensures a rigorous comparative assessment of environmental safety and sustainability between conventional lead-based perovskites and emerging double perovskite alternatives.

## STUDY & ANALYSIS

The comparative evaluation of lead-based and double perovskite materials reveals significant differences in environmental stability, toxicity potential, and life-cycle impact. Results are synthesized from structural characterization, degradation experiments, toxicological assays, computational modeling, and sustainability indexing.

### 1. Structural Stability and Degradation Behavior

Accelerated aging tests demonstrated that Methylammonium lead iodide (MAPbI<sub>3</sub>) exhibits rapid moisture-induced degradation, forming PbI<sub>2</sub> and volatile organic byproducts under high humidity and thermal stress. XRD analysis confirmed phase decomposition after prolonged exposure ( $\geq 72$  hours at RH 75%).

In contrast, double perovskites such as Cs<sub>2</sub>AgBiBr<sub>6</sub> and Cs<sub>2</sub>AgInCl<sub>6</sub> showed significantly improved phase stability with minimal structural distortion under identical conditions. DFT simulations indicated higher formation energies and lower defect densities compared to MAPbI<sub>3</sub>, correlating with enhanced environmental resilience.

#### Key Observation:

Double perovskites demonstrated  $\sim 2\text{--}3\times$  greater resistance to humidity and thermal degradation.

### 2. Leaching and Ion Release Analysis

ICP-MS analysis of aqueous extracts revealed substantial Pb<sup>2+</sup> ion release from degraded MAPbI<sub>3</sub> samples, particularly under acidic conditions (pH < 6). The diffusion–release model projected measurable lead contamination potential in soil and groundwater environments.

Conversely, double perovskites showed significantly lower ion release rates. Although trace Ag<sup>+</sup> or Bi<sup>3+</sup> ions were detected, concentrations were below established environmental hazard thresholds.

#### Comparative Ion Release Trend:

Pb-based > Ag/Bi-based > In-based perovskites

This highlights the pronounced environmental hazard associated with soluble lead compounds.

### 3. Toxicological Assessment

#### (a) In Vitro Cytotoxicity

MTT assays demonstrated dose-dependent cytotoxicity for MAPbI<sub>3</sub> extracts, with lower IC<sub>50</sub> values relative to double perovskites. Elevated reactive oxygen species (ROS) levels indicated oxidative stress as a primary toxicity mechanism. Double perovskites exhibited mild to moderate cytotoxic responses at significantly higher exposure concentrations, suggesting comparatively safer biological profiles.

#### (b) Ecotoxicity Studies

Aquatic bioassays showed:

- High mortality rates in Pb-exposed Daphnia cultures
- Reduced algal growth rates in lead-contaminated media
- Minimal ecological disruption for Cs<sub>2</sub>AgBiBr<sub>6</sub> at comparable concentrations

LC<sub>50</sub> values for lead-containing extracts were significantly lower, confirming higher acute ecological toxicity.

### 4. Life-Cycle Assessment (LCA) Outcomes

The cradle-to-grave LCA analysis revealed:

- Lead perovskites possess lower fabrication energy demands but higher Human Toxicity Potential (HTP).
- Double perovskites show moderately increased material processing impacts but substantially reduced toxicity indicators.

When normalized per kWh electricity generated, lead-based systems demonstrated superior short-term energy efficiency, whereas double perovskites achieved better overall environmental sustainability scores when hazard weighting was applied.

### 5. Sustainability Performance Index (SPI)

Using the weighted Sustainability Performance Index model:

- MAPbI<sub>3</sub> achieved high efficiency scores but incurred significant penalties for toxicity and environmental risk.
- Cs<sub>2</sub>AgBiBr<sub>6</sub> displayed moderate efficiency with low environmental risk, resulting in competitive SPI values.
- Cs<sub>2</sub>AgInCl<sub>6</sub> showed strong environmental safety metrics but comparatively lower photovoltaic efficiency, slightly reducing its composite score.

The study consistently indicate that while lead-based perovskites offer superior photovoltaic performance, they present substantial environmental and toxicological risks due to lead release and bioaccumulation potential. Double perovskites, although currently less efficient, demonstrate improved environmental stability, lower toxicity profiles, and reduced life-cycle hazard impacts.

Therefore, from an environmental sustainability perspective, double perovskites represent a safer long-term alternative, provided ongoing research continues to enhance their optoelectronic performance and large-scale manufacturability.

**Table 1: Comparative Summary of Findings**

Parameter	Lead-Based Perovskite (MAPbI <sub>3</sub> )	Cs <sub>2</sub> AgBiBr <sub>6</sub> (Double Perovskite)	Cs <sub>2</sub> AgInCl <sub>6</sub> (Double Perovskite)
<b>Chemical Formula Type</b>	ABX <sub>3</sub>	A <sub>2</sub> BB'X <sub>6</sub>	A <sub>2</sub> BB'X <sub>6</sub>
<b>Toxic Element Present</b>	Pb <sup>2+</sup> (Highly toxic heavy metal)	No Pb; contains Bi <sup>3+</sup> & Ag <sup>+</sup>	No Pb; contains In <sup>3+</sup> & Ag <sup>+</sup>
<b>Crystal Stability (Moisture/Heat)</b>	Moderate (prone to degradation)	High	Very High
<b>Degradation Products</b>	PbI <sub>2</sub> , organic iodides	Stable halide complexes	Stable halide complexes
<b>Ion Leaching Potential</b>	High (Pb <sup>2+</sup> release in water/soil)	Low	Very Low
<b>Bioaccumulation Risk</b>	High (lead accumulates in food chain)	Low	Minimal
<b>Cytotoxicity (IC<sub>50</sub> trend)</b>	Low IC <sub>50</sub> (High toxicity)	Moderate IC <sub>50</sub>	High IC <sub>50</sub> (Low toxicity)
<b>Ecotoxicity Impact</b>	Significant (aquatic & soil toxicity)	Mild	Minimal
<b>Environmental Persistence</b>	Moderate (degrades but releases Pb)	High structural persistence, low toxicity	High persistence, low hazard
<b>Life-Cycle Human Toxicity Potential (HTP)</b>	High	Low	Very Low
<b>Global Warming Potential (GWP)</b>	Low–Moderate	Moderate	Moderate
<b>Manufacturing Energy Demand</b>	Low	Moderate	Moderate
<b>Power Conversion Efficiency (PCE)</b>	High (≥20% typical lab scale)	Moderate (~2–10%)	Low–Moderate
<b>Regulatory Compliance Risk</b>	High (strict lead regulations)	Low	Low
<b>End-of-Life Disposal Concern</b>	Hazardous waste classification likely	Standard electronic waste management	Standard electronic waste management
<b>Recyclability Potential</b>	Challenging due to Pb	Easier metal recovery	Easier metal recovery
<b>Overall Environmental Safety</b>	Moderate–Low	High	Very High
<b>Sustainability Outlook</b>	Performance-dominant but risk-prone	Balanced sustainability	Environmentally safest (efficiency limited)

#### Comparative Interpretation

- **Lead-based perovskites** excel in photovoltaic efficiency but exhibit significant environmental and toxicological concerns due to lead leaching and bioaccumulation potential.
- **Cs<sub>2</sub>AgBiBr<sub>6</sub>** offers a strong balance between environmental safety and moderate efficiency, making it a promising transitional material.

- $\text{Cs}_2\text{AgInCl}_6$  demonstrates the lowest toxicity and highest environmental stability, though improvements in optoelectronic performance are necessary for commercial scalability.

Overall, the comparative data support a transition toward lead-free double perovskites for long-term sustainable photovoltaic deployment, provided ongoing research addresses performance limitations.

### SIGNIFICANCE OF THE TOPIC

The study of environmental and toxicity assessment in perovskite materials is critically significant due to the rapid commercialization of next-generation photovoltaic technologies. While lead-based perovskites such as Methylammonium lead iodide have demonstrated exceptional power conversion efficiencies, their intrinsic lead content presents serious environmental, ecological, and public health concerns. As solar energy deployment expands globally, even small-scale material toxicity risks can escalate into large-scale environmental hazards if not properly addressed.

#### 1. Environmental Protection and Public Health

Lead ( $\text{Pb}^{2+}$ ) is a cumulative toxic metal associated with neurological, developmental, and systemic health disorders. The potential release of lead from degraded photovoltaic modules into soil and water systems raises concerns about:

- Groundwater contamination
- Agricultural soil toxicity
- Aquatic ecosystem disruption
- Long-term bioaccumulation in the food chain

Comparing lead-based perovskites with lead-free double perovskites such as  $\text{Cs}_2\text{AgBiBr}_6$  and  $\text{Cs}_2\text{AgInCl}_6$  provides essential insights for mitigating these risks before widespread industrial adoption.

#### 2. Sustainable Energy Transition

The global shift toward renewable energy must align with sustainable materials engineering principles. A technology designed to reduce carbon emissions should not introduce new environmental hazards. This topic is significant because it ensures that:

- Green energy remains environmentally responsible
  - Material substitution strategies are scientifically validated
  - Long-term ecological safety accompanies technological innovation
- Environmental assessment ensures that renewable solutions do not unintentionally create secondary pollution challenges.

#### 3. Regulatory and Policy Implications

International environmental regulations increasingly restrict hazardous substances in electronic and photovoltaic systems. Lead-containing materials face strict waste management and recycling requirements. Research comparing toxicity profiles supports:

- Evidence-based policymaking
  - Development of safety standards
  - Improved environmental risk guidelines
  - Implementation of eco-friendly certification frameworks
- Scientific comparative studies help bridge the gap between laboratory innovation and regulatory compliance.

#### 4. Advancement of Green Material Design

This topic contributes to the broader field of **Green Chemistry and Sustainable Materials Science** by encouraging:

- Elimination of toxic heavy metals
- Rational substitution of hazardous elements
- Lifecycle-centered material design
- Integration of toxicity screening in early-stage research

The transition from single-cation  $\text{ABX}_3$  perovskites to  $\text{A}_2\text{BB}'\text{X}_6$  double perovskite structures represents a model for safer-by-design material innovation.

#### 5. Industrial and Economic Relevance

The commercialization potential of perovskite solar cells depends not only on efficiency but also on long-term environmental credibility. Materials with reduced toxicity:

- Lower remediation costs
- Reduce liability risks
- Improve public acceptance
- Enhance scalability prospects

Thus, evaluating environmental sustainability strengthens the pathway toward industrial viability.

## 6. Scientific Contribution

From a research perspective, the topic advances interdisciplinary collaboration between:

- Materials science
- Environmental engineering
- Toxicology
- Computational chemistry
- Life-cycle sustainability assessment

Such integration ensures that technological progress is evaluated beyond performance metrics alone.

## CONCLUSION

The comparative environmental and toxicity assessment of lead-based and double perovskites highlights a critical trade-off between photovoltaic performance and environmental safety. Lead-based perovskites, particularly Methylammonium lead iodide, have demonstrated exceptional optoelectronic properties and rapid advancements in power conversion efficiency. However, their intrinsic lead content introduces substantial environmental and public health concerns due to potential  $Pb^{2+}$  ion release, bioaccumulation, ecotoxicity, and regulatory constraints.

In contrast, lead-free double perovskites such as  $Cs_2AgBiBr_6$  and  $Cs_2AgInCl_6$  provide a promising pathway toward safer and more sustainable photovoltaic technologies. These materials demonstrate improved structural stability, lower ion leaching tendencies, reduced cytotoxicity, and favorable life-cycle environmental indicators. Nevertheless, their relatively lower efficiencies, scalability challenges, and uncertainties regarding long-term ecological impact of substitute metals remain important limitations.

The findings emphasize that sustainable energy innovation must extend beyond efficiency metrics to incorporate comprehensive environmental risk evaluation, lifecycle analysis, and green material design principles. Safer-by-design strategies, improved encapsulation methods, enhanced recycling protocols, and continued optimization of lead-free compositions are essential for achieving a balance between performance and sustainability.

Ultimately, while lead-based perovskites currently dominate in efficiency benchmarks, double perovskites represent a strategically important direction for responsible photovoltaic development. Future research integrating materials engineering, environmental toxicology, and sustainability science will be instrumental in ensuring that next-generation solar technologies are not only high-performing but also environmentally benign and socially responsible.

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